LABORATORY DIRECTED RESEARCH AND DEVELOPMENT

Science
and Technology
Mission Technologies
Grand Challenges

A Department of Energy
National Laboratory

Cover photo (center, going clockwise): (1) testing the predictability of climate models in hindcast mode using paleoclimatic data, (2) developing an improved understanding of the physics of the gallium nitride base materials of semiconductor LEDs, (3) creating the world's smallest robots, (4) using an atomic-scale model to interpret solid-to-water interfaces on metals, and (5) designing a highly efficient catalytic purification system.

Abstract

This report summarizes progress from the Laboratory Directed Research and Development (LDRD) program during fiscal year 2002. In addition to a programmatic and financial overview, the report includes progress reports from 341 individual R&D projects in 15 categories.

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“...exceptional service in the national interest.”

Science and technology are the heart of the United States industrial competitiveness, national security, energy resources, environmental quality, and leadership in fundamental and applied science.

At Sandia, the Laboratory Directed Research and Development Program provides the knowledge that drives our future. We initiate research and development that spawn the knowledge that revolutionized technology. Areas of emphasis center on our core technical competencies and the major strategic thrusts of Sandia's Institutional Plan. Leading-edge experiments that validate our work are constructed and operated on schedule, within budget, and in a safe and environmentally responsible manner.

Our work continues to produce many scientific and technological breakthroughs that lead to new technologies, markets, and businesses for the nation.

To all those who have contributed so generously of their time and talent, thanks and congratulations for a job well done.

An Overview of Sandia's FY2002 Laboratory Directed Research and Development (LDRD) Program

K. Ortiz

September 11, 2001. Al-Qaeda terrorists hijack four transcontinental passenger flights in fully fueled Boeing 767 airplanes. Two 767s are flown into the twin towers of the World Trade Center in New York City. The structures are severely damaged, but remain standing. However, a little over an hour later, the flaming jet fuel weakens the structural frame and the towers collapse, killing over 2800 people. A third plane is flown into the Pentagon in Washington, DC, killing 184 people. A fourth plane is also headed for Washington, DC, but is prevented from reaching its target by the heroic actions of its passengers; yet, 40 more people are killed.

What if other kinds of buildings were targeted? What if the buildings contained hazardous materials? What if...?

In the days, weeks, and months following the 9/11 attacks, Sandia performed "what if" simulations of similar attacks on various important facilities. While the scenarios studied and the results cannot be made public, we can identify how some previous Laboratory Directed Research and Development projects created the capabilities that were used:

- The effect of a Boeing 767 impact on the integrity of reinforced concrete structures was simulated using Sandia finite-element codes. The constitutive model for the behavior of reinforced concrete under catastrophic loading and deformation was developed in an LDRD project.
- The intensity and duration of the ensuing jet-fuel fire was simulated. The dispersal of the jet's fuel was calculated using smooth particle hydrodynamics, a technique that was developed in an LDRD project.
- The potential dispersal of hazardous materials in the smoke plume was simulated using capabilities developed in an LDRD project.

FY 2002 Funding Levels (\$M)

FY 2002 Selected Statistics

Full-time Staff	341
Smallest Project (\$K)	6.5
Average Project (\$K)	245
Average Project (FTE)	1
Largest Project (\$M)	3.54
1st Year Projects	174
2nd Year Projects	110
3rd Year Projects	57

Sandia's prime contract states that Sandia shall anticipate national technical and scientific needs and provide practical solutions.¹ The above LDRD investments in modeling and simulation, made years ago, paid off in September 2001.

The current LDRD Program continues to invest in high-risk, high-payoff R&D projects that anticipate national needs. For example, the current LDRD Program includes several projects to improve or develop new capabilities to detect and identify chemical or biological weapon attacks that could be useful in homeland defense.

Program Strategy

The LDRD Program is authorized by DOE Order 413.2A, "Laboratory Directed Research and Development," which states that the objectives of the program are to:

- maintain scientific and technical vitality of the laboratories,
- enhance the laboratories' ability to address future DOE missions,
- foster creativity and stimulate exploration of forefront science and technology,
- serve as a proving ground for new research, and
- support high-risk, potentially high-value R&D.

LDRD projects are chosen from proposals that are reviewed for technical merit and business sense. The selected projects:

- are in the forefront areas of science and technology,
- serve a critical role in attracting and retaining top scientists and engineers,
- enhance the core capabilities and competencies required to fulfill the Laboratory's missions, and
- anticipate national needs and provide practical solutions.

In the words of Sandia's President, Ambassador C. Paul Robinson, LDRD projects are "the lifeblood of the Laboratory."

1. "The Contractor shall facilitate the Laboratory's ability to project its efforts and participate with the scientific, engineering, and technical communities on both the national and international levels with the highest degree of vision, quality, integrity and technical excellence. The Contractor shall engage in the strategic and institutional planning necessary to assure that the Laboratory maintains a posture aimed at anticipating the national technical and scientific needs and dedicated to providing practical solutions. The Contractor shall study and explore innovative concepts to minimize or mitigate possible national security threats, current and future."

—*Management and Operating Contract Between Sandia Corporation and DOE, DE-AC04-94AL85000*

The FY2002 LDRD portfolio is internally organized into four categories of investment areas: Science and Technology (S&T), Mission Technologies (MT), Grand Challenges (GC), and Other. Within these categories the individual investment areas are the following:

- **Science & Technology Investment Areas** (Advanced Manufacturing, Biotechnology, Computational and Information Sciences, Electronics and Photonics, Engineering Sciences, Materials Science and Technology, MESA Technologies, Pulsed Power Sciences)
- **Mission Technology Investment Areas** (Differentiating Technologies, Emerging Threats, Energy and Critical Infrastructures, Nonproliferation and Materials Control)
- **Grand Challenges**
- **Other** (Advanced Concepts, Corporate Objectives)

The Science and Technology Investment Areas principally support the national-security mission of the Laboratory while the Mission Technologies Investment Areas principally support other missions. However, the nature of most LDRD projects is such that multiple missions typically benefit from any given project. For example, the computer analysis capabilities described above could be equally applicable to problems in the national security, the energy and environment, or the work-for-others missions.

The Grand Challenge Investment Area is composed of large (greater than \$1M), multidisciplinary projects that address technical areas that are vital to the core purpose of the Laboratory.

Other Investment Areas include Advanced Concepts and Corporate Objectives, which in turn include University Collaborations and the Presidential Early Career Award for Scientists and Engineers (PECASE).

The individual investment areas are profiled at the beginning of each section.

FY2002 LDRD Program Measures

The LDRD Program is growing. The FY2002 program is funded at \$84.3M, which is 5.32 percent of the total operating budget, up from \$70.0M in FY2001.² Approximately 90

FY 2002 Performance

Refereed Publications	352
Other Communications	209
Patent Disclosures	133
Patent Applications	79
Patents	27
Copyrights	10

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². DOE Order 413.2A limits LDRD research funding to not more than 6 percent of the Laboratory's total operating budget for the year, including non-DOE-funded work. The Order also allows funding of capital equipment for LDRD not to exceed 6 percent of its total capital equipment budget for the year, but Sandia's LDRD Program does not assess capital equipment.

percent of the funding is defense-related, and most of that is potentially dual-use (defense and non-defense).

The process for selecting LDRD projects began early in 2001 with a call for proposals from each of the investment areas. In response, 719 brief ideas for proposals were submitted. The Investment Area Teams (IATs) reviewed these ideas and selected 471 for development as full proposals. The idea-proposal process streamlines the process, encouraging more ideas to be submitted and decreasing the time spent writing unsuccessful proposals. From these proposals, 345 projects were selected by the IATs for funding. The fiscal year ended with 341 active projects, as four projects were terminated due to job changes by the principal investigator and other reasons. Of the 341 projects, 174 are in their first year, 110 in their second, and 57 in their third.

Of note, 59 percent (63 out of 107) of Sandia's post-doctoral fellows participated in FY2002 LDRD projects.

The quality of the program remains high. For example, in 2001 Sandia LDRD journal articles across all fields represented 13 percent of all Sandia articles, and over the past five years (1997–2001), 16 percent of all Sandia articles. Also over the past five years, Sandia LDRD journal articles outranked overall-Sandia articles in terms of relative impact: 1.90 to 1.31, as measured by the Institute for Scientific Information (ISI) Science Citation Impact database. External reviews of the Science and Technology Investment Areas continue to be positive.

Conclusion

Sandia's LDRD Program continues to conduct world-class research and development that is relevant to its given missions and potentially useful to other national needs. As demonstrated in the aftermath of the September 11, 2001, attacks, the path from research to application is rarely a straight line, but the quality of this research ensures that there will eventually be payoffs, sometimes very big ones.

Additional Reading

A comprehensive discussion of DOE and Sandia's LDRD Program management and funding sources may be found in the "Sandia National Laboratories FY 2002–2007 Institutional Plan," dated December 2001.

Sandia's LDRD Program continues to conduct world-class research and development that is relevant to its given missions and potentially useful to other national needs. As demonstrated in the aftermath of the September 11, 2001, attacks, the path from research to application is rarely a straight line, but the quality of this research ensures that there will eventually be payoffs, sometimes very big ones.

National Security and Sandia National Laboratories' FY2002 Laboratory Directed Research and Development (LDRD) Program

C. Meyers and H. Westrich

Not since the founding of the national defense laboratories at the dawn of the nuclear age and the attendant Cold War has America's security been as challenged as it is today. Never have we faced such a range of unimaginable threats both at home and abroad. Any street corner, restaurant, shopping mall, office complex, or your home can, in an instant, become a war zone where Americans are in jeopardy. Our scientists are developing many of the new detection, protection, and response technologies being used by first responders and the military to ensure the safety and security of our citizens anywhere in the world.

The Laboratory Directed Research and Development (LDRD) Program at Sandia National Laboratories has been, and will continue to be, the incubator for the discoveries and enhancements to our national security technologies and devices. Now is a time when our nation's finest scientific minds must be focused on developing innovative solutions to these complex threats to our security.

Much of the technology that we have developed at Sandia sprouts from the seeds sown in the LDRD Program. Research investment decisions made ten and fifteen years ago for the LDRD Program are having a direct impact on national security programs today. For example, past LDRD advances have impacted the development of a dozen or more components currently in the weapons stockpile, including radiation-hardened microelectronics for War Reserve applications and novel ceramics for neutron generators. It was also clear decades ago that microelectronics would play a key role in how future weapon systems would evolve. As a result, Sandia made investments in various microtechnologies that laid the foundation for our current expertise in microoptics, microelectromechanical systems (MEMS), and chemical sensors.

Today we believe that all of these and similar innovations will create continued scientific and technological advancements and lead to entirely new ways of meeting the needs of the nuclear stockpile and other national security missions. Examples of current LDRD research with the potential to impact future weapons work include the ultraminiaturized radar project and the accurate timing project (an exploration to

*Ambassador C. Paul Robinson
President
Sandia National Laboratories*

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provide accurate timing in high-radiation environments without external power). Both projects utilize Sandia's MEMS and silicon substrate technologies expertise to produce imaginative solutions to national security concerns. Consistent with the past research strategies, the LDRD Program is crucial for determining current investments that the Labs will be able to capitalize on in the future. We are making LDRD Program investment decisions now in the emerging fields of biotechnology, nanotechnology, and information technology, especially at the interface where these disciplines come together.

Many of our solutions for the changing threat environment, which includes terrorism, weapons of mass destruction, major theater warfare, weapons proliferation, information security, and military operations other than war, are derived from capabilities first explored in LDRD projects and developed in weapons life-cycle applications. For example, advanced computational modeling and simulation and advanced microelectronics support capabilities have proved crucial for detecting and attacking hard targets, conducting minimally manned warfare, and developing focused logistics. Numerous LDRD innovations have supported this thrust, including robotic sensing platforms, collective sensor swarms, and direct-fire robot systems.

As part of Sandia's emerging mission to ensure homeland defense, LDRD research supports progressive solutions for some of the greatest challenges facing the nation's critical infrastructures. A single component of the nation's infrastructure, for example, the electric power grid, is complex in its own right, but when linked together with other infrastructures, notably energy production and telecommunications, complexity grows by levels of magnitude. Maintaining the physical and cybersecurity of these linkages provides an excellent opportunity to apply Sandia's extensive experience in systems engineering.

Global security is enhanced by Sandia's total nonproliferation program. Sandia's arms control, monitoring, and nonproliferation technical work forms the largest single program of its kind undertaken by any technical institution in the world. The LDRD Program, with its support for robotics, microsystems, information systems, and integrated systems that can sense, "think," act, and communicate, plays a vital role in ensuring that Sandia can meet its nonproliferation and materials control responsibilities regardless of changing regional tensions and conflicts, evolving terrorist threats, increasing or decreasing

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interest in nonproliferation, and the nation's ever-changing relationships with other world powers.

Sandia's LDRD Program provides the Labs and the nation's security complex with the blueprints and profiles of solutions for national defense for today and the future-including both foreseen and unforeseeable threats. The direct connections to national security and weapons research will continue to be the keystones of funding decisions. The LDRD Program has shown over the years that this focus pays dividends in far-reaching national security arenas.

Sandia's LDRD decision makers have never lost sight of the goal: to create world-class science, technology, and engineering by keeping our science and technology capabilities on the cutting edge. As Ambassador C. Paul Robinson, President of Sandia, said, reflecting on the thoughts of the country's scientific leadership in the days following the Manhattan Project, "They asked themselves, 'What can we do, now that we've assembled the top scientists, to make sure that the defense of this nation will always remain in the hands of scientists who are at the top of their game?' Their answer was to give creative people some freedom to have ideas, to think new thoughts, and to create the leading edge perpetually." The LDRD Program, as the direct heir of those early discretionary funding programs, is still the answer to that question.

Their answer was to give creative people some freedom to have ideas, to think new thoughts, and to create the leading edge perpetually.

Advanced Concepts

The Advanced Concepts investment area seeks solutions to future national security threats and problems that do not yet exist, but are on the horizon. Sandia has the opportunity to develop new tools that could fundamentally transform U.S. abilities to fight the “War on Terrorism.” The goals of these transformational capabilities are to create agile, networked responses utilizing the full capabilities of the nation, to deny the ability of adversaries to hide their intentions and plans, to enable exquisite situational understanding of unfolding events, to harden the homeland, to deliver discriminating effects against diffuse targets, and to alter perceptions of U.S. adversaries.

The goal of “Underground Hunter Robots: Reconnaissance, Clearing, and Securing of Underground Tunnel Complexes Using Robotic Vehicles” is to combine existing technology in advanced mobility, surveillance sensing, and both lethal and nonlethal weapons to create a robotic vehicle that can search, clear, and secure underground tunnel complexes efficiently without risking friendly forces. This project focuses on the systems issues and technology needs that must be addressed to apply mobile robotic technologies to counterterrorism and homeland

defense. Sandia will employ an intensive program of virtual design prototyping and testing such that the tools and techniques required for virtual prototyping of complex mobile systems can be validated for future use.

48212

Combating Terrorism and Homeland Security

F. T. Mendenhall, L. J. Ellis, M. B. Murphy, R. W. Stinnett, K. T. Stalker, T. D. Woodall, J. R. Yoder, L. G. Stotts, M. D. Ladd

No robust, end-to-end system to find, characterize, and track mobile targets—like mobile missiles, mobile factories, or special people—exists today. The use of mobile assets in hostile and terrorist areas is a threat against our allies and hinders our ability to operate effectively in these areas. In a diffuse war against terrorists, the ability to find specific people or mobile targets is clearly essential. During recent years, Sandia's work with robotics, unattended ground sensors (UGS), such as tactical UGS (TUGS) and STEEL EAGLE, and synthetic-aperture radar (SAR) techniques have demonstrated the ability to detect, identify, and characterize some mobile and time-critical targets such as special vehicles. However, current research focused on demonstrating a "single-point" capability; that is, a single sensor performs most, if not all, of the system's functional capability. Clearly a suite of sensors and delivery capabilities will be required to solve these problems. The solution would require small, low-cost, lightweight integrated sensors consisting of transducers—acoustic, video, electromagnetic, chemical/biological, etc.—processing, communications, command and control, and data exploitation aggregated into a large network that is capable of multisensor data exploitation and fusion. The development and demonstration of such a network is well suited to Sandia's experience in fielding end-to-end systems, including ground sensors, SAR technology, communications, and intelligent systems.

We investigated leveraging Sandia's existing and near-future technical base and systems expertise to allow Sandia to lead the country in the development of large arrays of heterogeneous sensors for use in combating terrorism. We demonstrated large arrays of sensors fielded against increasingly difficult targets in increasingly difficult environments.

In addition to fielding hardware for demonstration, we recommended development of tools to analyze the large flow of data that would result from fielding a large array of sensors and to determine the best ways of using arrays of sensors prior to their deployment into the field.

We recommended that a set of networked test-bed sensors be fielded to take stock of what is available today and to begin the task of identifying and solving the problems needed to design the ubiquitous low-cost sensor that the nation will need in the future to combat terrorism.

Sandia's work with robotics, unattended ground sensors (UGS), such as tactical UGS (TUGS) and STEEL EAGLE, and synthetic-aperture radar (SAR) techniques have demonstrated the ability to detect, identify, and characterize some mobile and time-critical targets such as special vehicles.

48213

Underground Hunter Robots: Reconnaissance, Clearing, and Securing of Underground Tunnel Complexes Using Robotic Vehicles

P. R. Klarer, J. H. Buttz, A. B. Maish, M. C. Reineke, C. G. Hobart

By combining the existing technology base in advanced mobility, surveillance sensing technology, and both lethal and nonlethal weapons technologies, a robotic vehicle can search, clear, and secure underground tunnel complexes efficiently without risking friendly forces. This project focuses on the systems issues and technology needs that must be addressed to apply mobile robotic technologies to counterterrorism and homeland defense in the context of clearing underground tunnels and/or caves. To ensure quality and functional performance of a proposed robotic-vehicle system to accomplish the tunnel-clearing task, and to accelerate the transition from design to first prototype and then to full production, Sandia will employ an intensive program of virtual design prototyping and testing such that the tools and techniques required for virtual prototyping of complex mobile systems can be validated for future use in other Sandia programs. The result of this effort shall be a virtual prototype mobile robotic system that is ready for expression in hardware and near-term deployment with operational field personnel.

We defined functional requirements for the robotic-vehicle system. We conducted a series of configuration analyses in an effort to determine what an “optimal” vehicle configuration might be. We studied a variety of vehicle design parameters using a closed-form approach to derive descriptive equations of vehicle stability and kinematic state for both wheeled and tracked designs. The fundamental issue addressed was to maximize the vehicle’s vertical step-climb ability while minimizing the vehicle’s dimensions, primarily in terms of wheel radius, track length, and wheelbase (distance between axles). We further studied the effect that the vehicle center of mass (CM) location has on step-climb height and vehicle stability on a side slope or climbing slope. The robotic-vehicle application envisioned will operate in underground tunnel complexes and operate as both reconnaissance eyes and ears for military personnel and as an armed “point man” against an armed and “dug-in” adversary. We studied potential payloads and defined a set of “standard” sensors and integrated them into the vehicle design. In addition, we considered several payload

Hunter-killer vehicle overview.

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weapons. The issue of prime concern is the forces imparted to the vehicle platform by use of the weapon and how that affects vehicle design. We conducted a parametric analysis of tracked vehicles versus wheeled vehicles that included both single-chassis designs and multichassis designs in an effort to identify a clearly advantageous configuration. Parameters included estimates of total mass, a “reliability” estimate based on mechanical complexity, estimated total power consumption, and estimated total cost. We applied a scoring system based on a decision matrix approach, with the individual criteria scores and total weighted results included in our final report. We developed a spreadsheet tool to estimate the energy requirements for the vehicle using manufacturer’s specifications for electronic components and peripherals, and using motor power data measured with existing vehicles. We outlined a mission profile for the vehicle for a typical cave/tunnel search mission that includes an on-station phase (active but immobile with the navigation sensors turned off and control, camera, and radio on). We estimated the power and energy consumption by various subsystems for this mission profile, which provides a basis for vehicle power system-configuration design. Selection of an appropriate control architecture and hardware for a small robotic-vehicle control system depends on a number of factors. This project investigated a number of these issues and identified options. We made recommendations for a hunter-killer-type vehicle, based on a set of functional requirements. We generated a concept design in a solid-modeling environment that included a range of simulated operational tests using rigid-body dynamics and finite-element stress and strain simulations. By employing the virtual prototyping tools and an analytical approach to vehicle design based on mission requirements, the resulting vehicle concept design is closer to being ready for hardware prototyping.

The issue of prime concern is the forces imparted to the vehicle platform by use of the weapon and how that affects vehicle design.

49767

Microoptical Radar: Enabling Multiple Solutions to the War on Terrorism

C. L. Smithpeter, T. D. Russ, R. D. Habbitt, Jr., J. L. Rodriguez, R. O. Nellums, A. D. Niese, T. A. Casaus, H. T. Cooley

The unique and successful development of scannerless optical radar at Sandia over the last several years has made possible the evolution of a microoptical radar (MOR) sensor system that incorporates the functions of sense, decide, act, and communicate (SDAC). Optical radar combines the principals of radar with the use of optical wavelengths such as the near infrared (NIR). MOR miniaturizes optical radar onto the micro-footprint of a chip, dramatically increasing its utility. Thus, MOR will provide a simplified and completely integrated system from which to obtain three-dimensional (3-D) or depth information of a scene. Potential antiterrorism applications include autonomous target detection and recognition, and navigation and precision strike for military applications, perimeter security, and 3-D facial recognition for reliable identification of people at border crossings and abroad.

Because of the potential benefit to border security, we proposed to first investigate the feasibility of 3-D facial recognition to autonomously and continuously screen for suspects. The demonstrated features of the Sandia laser radar, which are desirable for this application, include compact size, sub-inch range resolution, and eye safety. Current facial-recognition systems based on 2-D-intensity images have unacceptable false alarm rates (FARs) for the screening application. One MOR approach to unobtrusively identifying individuals in a crowd is comparing the 3-D geometry of a person's body and face. Another MOR approach is using the 3-D image to locate the face and estimate its orientation and scale. The scale and pose-estimate are the fundamental limitations of current 2-D algorithms. Finally, the large scale of border screening constrains the acceptable physical and performance parameters, such as cost and eye safety. Our analysis of the potential applications will derive the desired system parameters and compare them to current technology. This analysis will identify the key technology development and expected development risk.

The team utilized the existing National Aeronautics and Space Administration (NASA) scannerless laser range imager (SRI) hardware to acquire facial images of subjects. This hardware utilizes the same principles and algorithms of a MOR sensor. However, the existing hardware was not originally

Our analysis of the potential applications will derive the desired system parameters and compare them to current technology. This analysis will identify the key technology development and expected development risk.

designed for facial-recognition applications, and we expect that a new MOR sensor designed for facial recognition would have significantly improved performance. To date, MOR sensor-development work has not uncovered any insurmountable issues; in fact, the results are encouraging. Surveys of existing systems and other research have not yielded any credible alternatives.

We conducted multiple experiments utilizing the data obtained from the existing SRI sensor system. These experiments sought to answer three questions with regard to using the MOR sensor data for facial recognition.

- How does the precision of the MOR sensor affect the fidelity of the range data for facial recognition?
- How does the matching accuracy of the range data respond to scale changes in the facial data?
- How does the matching accuracy of the range data respond to rotational changes in the range data?

- *The effect of MOR range precision on facial matching.* Currently, range data obtained from the MOR sensor are subject to a large amount of noise. Range noise is currently reduced by averaging images acquired consecutively in time. For this experiment, we observed the change in matching accuracy as the number of time-consecutive images averaged increased. Results demonstrated that matching accuracy started to level off after 40 images were included in the average. Range noise variation also started to level off with 40 images at 0.2 cm, indicating a potential target-range accuracy for the MOR sensor.

- *The effect of rotation on matching accuracy.* In this experiment we compared the range data of a face acquired at approximately a frontal pose to those acquired at approximately q degrees with respect to the y -axis after rotation correction. We rotated and interpolated the off-frontal image. Thus, the experiment is really measuring the effect of the interpolation step on range accuracy and on the accuracy in registering two range images. Otherwise, the precision of the range data should be invariant to facial pose. The results demonstrated that range accuracy is only slightly compromised as the rotation angle increases. It is our hypothesis that the increase in range error can be attributed to the low fidelity of the input data, and that high-fidelity 3-D data would aid in the reconstruction of an off-axis facial image without diminishing its fidelity.

- *The effect of scale differences on matching accuracy.* In this experiment, we examined the effect of matching images of the same faces acquired at different distances from the camera. Results demonstrated no apparent trend with respect to distance

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between the two images and facial-matching accuracy. This indicates that facial matching using 3-D information may be invariant to scale.

- *Comparing different faces.* We conducted this experiment, which computes the range error associated with matching different faces, to better quantify the significance of the range errors that have been observed. We considered the faces of three individuals. Results showed that the standard deviation of the range errors for different faces is slightly higher (1.4–1.8 cm) than those observed for the same face after translation and rotation correction (0.5–1.2 cm). Typically, we would like to see larger error separation between rotated and translated versions of the same face and different faces.

Overall the experiments proved that 3-D data will greatly improve the facial-recognition process by being invariant to illumination effects and compensating for rotation and scale differences. However, the experiments also highlighted the necessity for high-fidelity 3-D data. Obtaining subcentimeter accuracy is a highly technical challenge for the MOR sensor, but one that we will have to meet.

Overall the experiments proved that 3-D data will greatly improve the facial-recognition process by being invariant to illumination effects and compensating for rotation and scale differences.

49773

Principles for Network-Security Mechanisms Utilizing Network Address Translation

J. T. Michalski, E. J. Lee, C. M. Price, E. T. Stanton

This study will provide a toolset that Sandia needs to be a leader in information network-security assessment and design. It will focus on techniques from network security through Dynamic Network Address Translation (DYNAT). It will produce a framework for operation of DYNAT-based systems, descriptions of relevant information-surety mechanisms involved, a set of operational principles, and an operational taxonomy. We will validate these components through both light-duty adversarial white boarding and more-detailed Red Team assessment to determine applicability of DYNAT functions to real systems and to outline initial vulnerabilities.

- *Completed the DYNAT framework definitions, which included the theories of DYNAT mechanisms.* Since there are a variety of ways to implement this new technology, this completed framework helps to identify the particular DYNAT implementation by providing an identified list of attributes and a classification tree to help the individual classify DYNAT types.

- *Completed the lab setup and testing of a candidate DYNAT implementation.* This “setup” included installing the software and hardware needed to build the network and devices participating in the DYNAT protocol. This lab setup allowed the research team to evaluate a DYNAT technology based on the framework definition paper. The output of this lab analysis was a report on the operations and subsequent vulnerabilities discovered in the implementation of the candidate DYNAT technology. This laboratory environment also allowed us to use valuable feedback to help refine the DYNAT framework definition document.

- *Provided a Red Team “system-analysis” review of a DYNAT implementation that uses the principals of the Information Design and Red Team (IDART).* We developed this within the Information Assurance business area to do the following: (1) identify vulnerabilities during design, (2) identify vulnerabilities in existing system architectures, and (3) provide research into better ways of securing systems.

During the laboratory research activity, we developed a software program that we can use to help in the effort of Red-teaming future DYNAT implementations. This code has the ability to track protocol parameter changes within a DYNATed

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network. It can monitor communications between end-hosts and create profiles that can identify and describe communication patterns within a DYNATed network.

51706

Feasibility Study of an Integrated-Systems Solution to the Problem of Radiological Dispersal Devices

C. A. Aas, M. W. Knazovich, J. B. Whitley, R. C. Moore, L. C. Sanchez, L. J. Dotson

Elements of emergency management and emergency response were tested on U.S. soil in the wake of the September 11, 2001, terrorist attacks. Identifiable gaps in planning, prevention, crisis management, consequence management, and recovery and restoration were noted and are becoming issues of national and international importance. Radiological dispersal device(s) (RDDs), commonly known as dirty bombs, are potential threats and pose unique challenges because of the real and perceived stigma associated with radiation and its effects. We need a total systems approach to integrate all aspects of an RDD scenario from planning to restoration to do the following:

- Improve response capabilities through planning,*
- Reduce sociological and psychological impacts through education and awareness,*
- Support policy decisions through science-based facts, and*
- Reduce potentially exorbitant recovery and remediation costs.*

Almost all of the prior U.S. work regarding terrorist acts focused on crisis management and consequence management, the technical considerations affecting initial-response organizations, and the costs and effectiveness of various decontamination operations. A total systems approach incorporating the excellent work currently under way will provide a foundation for optimizing activities and ensuring that adequate resources are applied to all aspects of an RDD program, including planning, prevention, crisis management, consequence management, and recovery and restoration.

The results of our study are as follows:

(1) Preliminary vulnerability assessment.

- What radiological materials could be used, obtained, dispersed.* An RDD is a conventional explosive or bomb containing radioactive material. A preliminary assessment indicates that the radionuclides of greatest concern include ^{60}Co , ^{137}Cs , and ^{90}Sr .

- Potential targets and impact(s).* Potential targets would likely have obvious symbolic traits and may represent governments or institutions, be the symbol of a large city, be

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politically sensitive, or represent critical infrastructures, such as electrical power, telecommunications, banking and finance, water-supply systems, transportation, emergency services, and government operations. A successful RDD attack would have health, psychological, and economic impacts.

- *Dispersal-pattern programs and current detection capability.* The Hazard Prediction and Assessment Capability (HPAC) and National Atmospheric Release Advisory Capability (NARAC) codes are both used to generate predictive plots for the atmospheric dispersion of radiological material. Detection capabilities exist for radiological and explosive materials (e.g., Sentinel II explosives-detection portal).

(2) Evaluation of need for an integrated consequence management approach.

- *Initial assessment.* Following RDD detonation, the initial assessment must:

- Determine the nature and extent,
- Identify and rank potential consequences,
- Determine the availability of needed resources for mitigation, and
- Define interfaces with crisis management and recovery and restoration components.

- *Emergency-responder actions and public response(s).*

The first responders will be the local and state police, firefighters, and emergency personnel who will require proper training and drills to handle the emergency. After that, the lead federal agency is determined as defined in the Federal Radiological Emergency Response Plan. Decisions need to be made immediately on the level of information to be released to the public and the method to convey the information.

- *Containment.* Physical and chemical containment options exist, and others are currently under development (e.g., sorbents under development at Sandia).

- *Decontamination and technology deployment.*

Decontamination and demolition technologies exist, but current technologies are labor-intensive and costly for large-scale remediation. More research is needed on decontamination of highly porous materials and building ventilation systems.

- *Forensic evidence.* Forensic evidence must be preserved to support the criminal investigation. The Nuclear Emergency Support Team (NEST) has a suite of techniques for maintaining forensic evidence.

(3) Preliminary decision maker/public information.

- *Information needs for decision makers and for public distribution.* A total system approach is needed to define programmatic needs, describe principal interactions, develop

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parametric data, and support definition of high-level requirements and lower-level derived requirements. Risk-based prioritization will provide a defensible approach to the allocation of limited expertise and resources. Information needs include:

- Interfaces, needs, and priorities between RDD components (i.e., planning, prevention, crisis response, consequence management, and recovery and restoration),
- Potential threat to be mitigated,
- Potential targets requiring protection,
- Goal quantities of material to be protected,
- Potential adversaries and capability of the adversary to pursue an attack, and
- Definition of a successful RDD event.

- *Information and training for first responders/decision makers.* First responders, including local medical, fire, and emergency personnel, need training that is sufficiently rigorous and comprehensive to adequately prepare them for their roles and responsibilities in an emergency response situation. The proficiency and level of knowledge of emergency responders need to be periodically evaluated, and strategies must be developed and implemented for those individuals who are identified as deficient. Hospitals must be prepared to handle victims of radiological contamination and/or mass casualties.

- *Panic and psychosomatic symptoms.* The psychological impact could very well drive the health and economic impacts. An RDD with a small source may cause psychological damage with limited real health or economic impact if the event is not proactively managed.

Risk-based prioritization will provide a defensible approach to the allocation of limited expertise and resources.

Other Communications

Dotson, L. J., and J. A. Jones. 2002. Feasibility study of an integrated systems solution to the potential threat of radiological dispersal devices (RDD). Paper presented at the Project Status Meeting, September, Albuquerque, New Mexico.

52175

Feasibility Study: Development of a Computational Sociopsychological Model for Understanding Terrorist Behavior

N. M. Berry, N. G. Brannon, J. G. Turnley, S. Y. Goldsmith, T. D. Moy, S. V. Spires

Sociophysics is a rapidly emerging interdisciplinary field that combines computational and social sciences in the form of complex adaptive agents that can then be used in simulation models of society. Sociologists have long recognized the critical interdependence of individuals on society and vice versa, but up to now no tool has existed for analyzing such nonlinear behavior in a complex system.

Leading social scientists, most notably psychologists, have made significant progress in understanding the minds of terrorists, primarily their state, but they under-emphasize the important social processes that created the terrorists in the first place. The primary challenge is that often only synchronic data (snapshots) are available. The nascent field of sociophysics is poised to help fill in this gap in psychological understanding.

If developed, the objectives of a computational societal model would be to (1) understand the dynamic social processes that lead to terrorist behavior; (2) test the effectiveness of different actions on terrorism—gaming—that cannot be tested any other way, and finally, (3) develop effective strategies for combating terrorism.

Sandia will develop and explore credible approaches to building a computational model with sufficient fidelity to provide meaningful and insightful results. From these approaches, we will then identify the critical subelements (technologies) that will be required, e.g., algorithms, cognitive models, behavioral frameworks, etc.

We explored the feasibility of developing a complex simulation system depicting social dynamic aspects of terrorist and terroristlike organizations and their impact on the greater society. The team concluded that while the concepts behind this idea are sound, the magnitude of the work required to deliver a complete social simulation system, as defined by numerous use cases, in a reasonable timeframe is daunting. Instead, we pursued a tractable proof-of-concept demonstration. The accomplishments from this project support these views and our suggestions.

- Explored several universal modeling language (UML)-like techniques for assisting team domain experts, a clinical

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psychologist, a historian, and a cultural anthropologist, in capturing and representing their knowledge.

- Generated use-case scenarios and analyses to describe desired system functionality, end-user perspective, system requirements, conceptual representation, and associated relationship diagrams.

- Generated detailed analysis characterizing use-case variables with respect to terrorist group activities and government assessment of known violent activities.

- Constructed a structural organization model depicting top-level view of associations between use-case variables and knowledge organization.

- Constructed use-case system behavioral model depicting how the user views the relationships for the given use-case within the organization of the overall system.

(We) generated detailed analysis characterizing use-case variables with respect to terrorist group activities and government assessment of known violent activities.

52176

Feasibility of Microsensors for the War on Terror

P. J. Eicker, R. L. Burchard, R. W. Stinnett

The Advanced Concepts Group (ACG) study on the War on Terror (WoT) identified the potential of Sense, Decide, Act, and Communicate (SDAC) modules to be a key technical element of the WoT. An SDAC is a microsystem composed of microcomponents, each of which is capable of carrying out one of the modalities of sensing, deciding, acting, or communicating with a controlling authority or another SDAC. The study postulated that SDACs would be valuable to the WoT.

This project will make a preliminary assessment of the value of SDAC microsystems in several applications of importance to the WoT.

Steel Ratler is a high-capability ground sensor that has been developed and deployed. Steel Ratlers today cost on the order of \$20,000 per unit. Given the potential of microsystems, we estimate that within 5 years, Steel Ratler-type capability could be produced for approximately \$200 per unit, i.e., a two-orders-of-magnitude reduction in cost. There are two factors involved: first, advances in microtechnologies will permit fundamental changes in the design of Steel Ratlers, and second, when produced in quantity, additional savings will be realized. Thus, Steel Ratlers, which today are precious, will no longer be so dear and will be considered essentially expendable. These inexpensive Steel Ratlers will allow the U.S. to accomplish extensive monitoring of trails and caves.

As another example in the 5-year window, we will be able to produce very capable sensor systems that contain a camera, image analysis, motion detection, sound analysis, and transmission for approximately \$100 per unit in the size of a sugar cube. While it is not surprising that systems this capable can be produced in the size of a sugar cube, it should be at least modestly surprising that we could produce them for \$100 in the near term.

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52397

Feasibility Study for Improved Nonlethal Weapon Based on Disruption of Postural Reflexes

R. P. Toth

Sandia will explore a new type of nonlethal weapon (NLW) based on disruption of postural reflexes. The principle of operation is the use of repetitive, high sound-pressure-level (SPL) pulse packets that induce disinformation in the vestibular system. Access to the vestibular system is achieved via that portion of the inner ear common to balance and hearing, the fenestra ovalis. The predicted consequences of such disinformation in the vestibular system are nystagmus, nausea, loss of postural control, disorientation, and fear. The applications where this could have utility are building denial and tunnel clearing.

The prototype electroacoustic generator is based on a repetitively triggered Marx bank and a transducer based on a plasma discharge in a heavy-walled cylinder terminated at one end by shorting plate and radiating from the opposite end via an acoustic impedance transformer into free space. Pilot-level results from the prototype electroacoustic generator suggest that SPL of 200 dB can be produced at a distance of 3 m from only 176 J of energy.

This is a project to further develop and test a new concept for an acoustic NLW based on induction of sensory disinformation in the vestibular system by a high SPL pulse train. The intended area of application is facility protection where the NLW operates in reverberant or semireverberant (tunnel) environments to obviate the need for high SPL at long ranges.

Progress included operation of the electroacoustic generator at variable energy delivery (to control dose), and at a maximum rep rate of 20 pulses/min. The electroacoustic generator is a variable-rep-rate, high-voltage discharge in a 6 in.-diameter, 12 in.-long cylinder with a shorting plate at one end, and a variety of projectors that act as impedance converters to free space at the other end. The discharge takes place across a pair of titanium spherical electrodes supported by adjustable insulators through the ½ in. wall thickness of the cylinder. High voltage is supplied by a two-stage Marx generator designed and built for this purpose. The Marx generator charges in parallel a bank of 50 kV energy-storage capacitors of low equivalent series resistance and series inductance. The Marx is erected by a trigger pulse that connects the two stages in series by

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pressurized air and gas switches to produce twice the charge voltage. The electrodes are spaced to hold off the charge voltage, but break down under the voltage produced by erection of the Marx. Under these conditions, we measured pulse power parameters for ~ 200 J pulses at 4 kA, 20 kV charge, and 40 kV discharge over 200 ns. The peak SPL produced by this discharge is very high, perhaps as much as 200 dB at 3 m. SPL measurements are complicated by overload and electromagnetic interference (EMI) not defeated by a Faraday cage. This implies that a low-impedance magnetic wave is produced by either the trigger or the Marx or the discharge.

Specific goals were rep-rate operation, measurement of pipe pressure, and evaluation of projector designs that may be expected to alter the possible formation of a MACH plate at the exit aperture of the generator. We were able to rep the system only at the comparatively low rate of 20 pulses/min. We acquired a constant-current high-voltage power supply (HVPS), but the trigger switches could not operate fast enough to take advantage of the improvement. Pipe pressure measurement was a major problem due to EMI and propagation of a plasma over the face of the pressure transducer. We ameliorated the last of these with a special piezoelectric (quartz) element recessed from the ground-isolated mount and covered with a heat-ablative layer. This yielded peak pressures of about 2000 psi. We also lifted the ground electrode from the pipe with a second standoff to reduce ground bounce. This changed the time history from a dampened sinusoid to an exponential decay with two time-constants, but the peak pressure was about the same. We evaluated three projectors: a simple conical horn with a 15-degree half-angle, an obturated conical horn of the same angle and length, and a deLaval nozzle also with 15-degree expansion after the throat over a 15 in. distance. We tested the performance with both high SPL (175 dB overload) microphones and blast probes. On direct comparison, the deLaval nozzle seemed to produce higher SPLs, but EMI added variability, and the high pressures may have damaged the transducers. Sound maps in the transverse plane seemed to indicate vortex propagation, hence MACH plate formation; but again, EMI and transducer damage prevented unequivocal interpretation.

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53373

Detection, Classification, and Multitarget Tracking in a Sensor-Rich Environment

M. L. Yee, M. D. Ladd, H. G. Nguyen, D. I. Toledo, D. C. Craft, D. J. Gallegos

In the next decade there will be a paradigm shift in unattended sensors. Driven by inexpensive commercial-off-the-shelf (COTS) hardware, next-generation sensing concepts and low-power communications and large networks of sensors will be fielded. Research needs to be done on how to perform detection, classification, and tracking of multiple targets in this type of sensor-rich environment. Development of algorithms that perform these functions utilizing large networks of sensors is a critical next step. A key concept is the fact that detection and classification of targets is an integral part of tracking multiple targets, in that classification is beneficial to solving the track-to-target data-association problem. Conversely, track-history information is beneficial to classification of targets as it facilitates the use of sequential classification techniques. Therefore, it is crucial to understand how the information available within a network of sensors can best be used to contribute to this synergy.

We identified key concepts and algorithm architectures. We also collected field-test acoustic data for multiple targets from multiple sensors for the purpose of testing tracking and classification algorithms.

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Advanced Manufacturing

The objective of the Advanced Manufacturing investment area is to support manufacturing technology advances with an emphasis on process-based quality. Process-based quality is a systematic approach to generate superior manufactured goods (i.e., nuclear weapon components and sub-systems) with little or no product inspection or testing. Advanced Manufacturing promotes understanding the interactions between the design, fabrication processes, and environmental constraints, making it possible to ensure product that meets functional requirements the first time, every time. Research priorities in this investment area support the miniaturization and cost- and time-reduction requirements for future nuclear weapon manufacturing needs. Manufactured products, particularly microdevices, have the potential to reduce defects and costs.

Integrated microelectro-mechanical systems (MEMS) offer the opportunity to miniaturize key components in military and commercial applications at low cost. Many advantages of this miniaturization are subsequently sacrificed in packaging MEMS structures. "IMEMS Packaging and Interconnection Technology" will resolve multiple micropackaging issues to efficiently and reliably take advanced MEMS structures from

functionality in a laboratory setting to fielded applications. Ultimately, wafer-scale packaging techniques that make the device into its own package will be developed. As a measure of this success, this project is directly associated with 23 technical advances, and three patents have been granted.

10721

Volumetric Displacement Control (VDC) of Manufacturing Tools

L. F. Bieg, M. T. Ensz, B. Jokiel, Jr., C. J. Atwood

Performance analysis of equipment utilized in production, and mainly production equipment requiring motion, has been historically neglected or is performed while allowing the equipment to become static (gain a stable steady state). Furthermore, machinery used for final inspection and quality assurance acquires data off of a previously manufactured piece part by taking one data point at the time, mostly using a touch-trigger probe. These types of data-gathering devices render the inspection machine static prior to moving on to the next probing point. Conversely, to fabricate piece parts in a metal-removal process, for instance, equipment is used that requires continuous motion of various speeds. This project addresses these issues and demonstrates a solution from conceptual design, evaluation, calibration, and prototype implementation. Sandia developed a portable three-axis coordinate-measuring machine (CMM) allowing for the gathering of data while in motion. We can ally this novel mechanism to inspect piece parts dynamically prior to the manufacturing process, intermittently during the manufacturing process, and after fabrication has been completed. Furthermore, the mechanism finds applications in the performance evaluation of machine tools, inspection equipment, or any machinery employing motion.

- *Developed software for independent metrology applications.*

(1) We designed and implemented data-acquisition software providing the ability to perform pertinent studies and corrections.

(2) We evaluated the Sandia-designed joint-feedback system and calibrated it to provide accurate angular resolution in the count domain of three counts per arc second for joints one and two, and five counts per arc second for joint three.

(3) We performed a long-term drift study. This study included different altitudes within a 2 cu ft working volume and resulted in a one-count drift stability within a 24-hour period. Joint three, being the farthest away from the base-plate kinematic mount, was analyzed to be most sensitive to drift.

(4) We purchased Spatial Analyzer, a commercially available metrology software. This software module allowed the volumetric displacement control (VDC) team to evaluate

MPEG video of VDC in motion.

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the performance of a Zeiss CMM with a Laser Tracker and compare both these devices with the VDC system.

- *Applied VDC system to in-process workpiece inspection.*

(1) Commercial metrology software is driving the inspection performance of the VDC system, allowing for the evaluation of every known geometrical element.

(2) A real-time graphical representation of the VDC system is provided in software, providing for a state-of-the-art graphical user interface (GUI).

(3) The VDC system is applied for in-process inspection by the operator/machinist as needed to define datum features, part orientation, maximum material condition, out-of-tolerance conditions, or for final feature inspection after part manufacturing.

- *Evaluated process performance with and without the VDC system.*

(1) We designed and fabricated an artifact that will serve the function of on-machine certification and calibration of the VDC system.

(2) Conversely, we can evaluate displacement performance of the manufacturing tool against the artifact. Multiple ANSI B5.54 circle-diamond-square test parts have been fabricated by our machining test-bed and have been inspected on the machine by the VDC system. Subsequent post-manufacturing inspection on a CMM will determine and document process-improvement levels.

- *Implemented VDC system on the shop floor as process-based quality for application modes 1 and 2.* As application mode 1 is defined as in-process inspection, application mode 2 addresses the use of the VDC system as a three-dimensional ball bar. This mode allows for “dynamic” evaluation of motion in the entire workspace of production equipment. We demonstrated this mode of operation on a real production machine tool on the shop floor.

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Other Communications

Bieg, L. F. 2002. Development of a portable, three-axis, 3-dimensional Ball Bar™. Paper presented at Spring 2002 Tri-Joint IMOG–JOWOG Meeting, 14–17 May, at NIST, Washington, DC.

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10722

Process-Based Quality Tools to Verify Cleaning and Surface Preparation

J. A. Emerson, P. A. Lemke, E. D. Reedy, Jr., D. P. Adams, N. R. Moody

Specifying material choices and the method for processing does not always ensure the long-term reliability of an adhesive bond. Manufacturing quality and control are crucial, and one must be able to fully characterize and certify the entire fabrication process. From a recent cleaning study, Sandia learned of the need to develop and move to the factory floor a tool to identify surface-preparation requirements and guarantee their effectiveness. This tool utilizes a method for measuring adhesion of small areas in conjunction with combinatoric testing. The development of a small plate containing many masked-off regions follows combinatoric techniques. Processing this plate through a production line exposes a new region during each step of the fabrication process. Now the plate contains the combined effects of all the processing steps, as well as any contamination added during storage and transit. This combinatoric process characterization plate (PCP) is interrogated to determine if the desired adhesion level exists when the fabrication process is complete. We developed a method based on nanoindentation and contact mechanics testing to interrogate the PCP. For example, a thin layer of the adhesive is cast over the plate, followed by a stressed overlayer. The radius of the blister generated during indentation is directly related to interfacial fracture toughness. To correlate the data from nanoindentation-generated interfacial fracture energy, we used a tensile Brazil nut (TBN) sandwich specimen to measure the interfacial fracture toughness of a millimeter-scale epoxy bond constrained by metal adherends. The ultimate goal of this work is to develop the concept for a tool that could be used on the factory floor and would be viable for small-lot and rarely used processes.

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The unique aspect of this project is to develop and move to the factory floor a combinatorial PCP to identify surface-preparation requirements and guarantee their effectiveness. No other tests or inspection would be necessary to guarantee acceptance of the final product. Although this is a new concept for certifying War Reserve parts, the core idea of maintaining process control is critical to modern manufacturing. This tool would represent the combined effects of all the processing steps, as well as any contamination added during storage and

transit; it also carries the history of sequential surface preparation and subsequent processes.

The Honeywell/Federal Manufacturing and Technologies (FM&T) Kansas City Plant initiated studies on characterization of cleaning and surface-preparation processes for adhesive bonding. In principle, the concept could work; however, more work is needed to develop the reliability of the concept. Because of the lack of a good tool, we did no design of experiments. We did further work on developing adhesion tests for small areas that are accurate, convenient, and scalable from conventional adhesion tests. Stressed layers placed on a polymer film can induce delamination. We completed studies for developing known and adjustable stress overlayers with tungsten (W) and Ta₂N-superlayer stressed thin films under various vacuum-deposition pressures. These stressed superlayers trigger delamination in weakly bonded films but not in strong adhering films. Deposition of the overlayers can result in stresses ranging from 1 GPa tension to 4 GPa compression. When combined with controlled thickness, the total stored energy can be tailored to induce fracture in each film. We showed with the nanoindentation of thin epoxy films on aluminized glass that delamination occurs readily along the film-metal interface. To measure the interfacial toughness for 0.2–1 μm -thick epoxy films, we found that a critical indenter displacement is required to create stresses that drive interfacial crack growth. We started an initial investigation in collaboration with Cornell University and the University of New Mexico into a theory defining the fracture mechanics of thin bond lines. We began the effect of contaminants on interfacial fracture toughness using indentation techniques and stress overlayer techniques. However, analysis of the data has proven difficult because of the lack of a suitable theory.

We completed the use of JKR (Johnson, Kendall, Roberts theory) contact mechanics for detecting trace amounts of surface contamination. The approach capitalizes on the difference in surface energy between the epoxy probe and organic contaminant. We were unable to determine the lower limits in contamination because of difficulty in accurately determining the level of contamination by a secondary technique. Future work should include correlation with contact-angle data.

We used the TBN sandwich specimen to measure the interfacial fracture toughness of a millimeter-scale epoxy bond constrained by metal adherends. We varied the applied mode mixity by using a different set of loading holes, and an 80-degree variation in applied crack-tip mode mixity is possible.

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These stressed superlayers trigger delamination in weakly bonded films but not in strong adhering films.

The ability to easily adjust the applied mode mixity over a wide range of potential values is a substantial advantage over other common types of interfacial fracture specimens. We used a calibration function, which depends on failure load, initial crack length, and the position of the loading points, to determine interfacial toughness and the associated crack-tip mode mixity. We use self-assembled monolayers (SAMs) to simulate a contamination. The interfacial adhesion is susceptible to fracture of epoxy on aluminum (Al) because of the change in the practical work of adhesion. We apply the monolayers to the polished Al surfaces at high density such that the terminal groups determine the interfacial interactions with the epoxy adhesive. Without SAMs, the epoxy on Al samples failed adhesively at an energy of nearly 20 J/m^2 . The increase in fracture energy can be attributed to the need for higher stresses and more extensive deformation prior to film failure.

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Other Communications

Emerson, J. A., N. R. Moody, R. K. Giunta, M. S. Kent, and E. D. Reedy, Jr. 2002. The effect of sample preparation on interfacial fracture for thin epoxy films. *Proc. 25th Annual Meeting of the Adhesion Society, Inc., and The Second World Congress on Adhesion and Related Phenomena (WCARP-II)* 25 (February, Orlando, Florida): 110.

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Moody, N. R., M. S. Kent, E. D. Reedy, Jr., J. A. Emerson, and D. F. Bahr. 2002. Effects of self-assembled monolayers on interfacial fracture of thin epoxy films. *Proc. 25th Annual Meeting of the Adhesion Society, Inc., and The Second World Congress on Adhesion and Related Phenomena (WCARP-II)* 25 (February, Orlando, Florida): 458.

10723

Fabrication of Three-Dimensional Microstructures Using Soft Lithography

R. L. Myers, D. P. Adams, A. D. Oliver, J. A. Emerson

Microstructures are becoming increasingly important in technological advances in many fields, including the upgrade and maintenance of the nuclear weapons stockpile. Microstructures are fabricated primarily by photolithography, a process that produces two-dimensional (2-D) parts. However, photolithography has intrinsic limitations in making 3-D structures. The LIGA (acronym for the German term Lithographie, Galvanoformung, und Abformung, for lithography, electroforming, and molding) process requires x-ray radiation, making it costly and not readily accessible. The ability to fabricate 3-D microstructures of a wide range of materials using a soft lithography technique (e.g., microcontact printing) makes it possible to achieve unprecedented levels of system functionality for microelectromechanical systems (MEMS), microsensors, and microoptical devices at a much lower cost. Soft lithography techniques use a patterned elastomeric stamp or mask.

Sandia is investigating the fabrication of 3-D microstructures using microcontact printing. This process could be used to create MEMS devices. Microcontact printing is a soft lithography technique in which a self-assembled monolayer (SAM) is patterned by transfer printing. A macroscopic analogy is linoleum block printing, which offers low-cost, high-precision replication. The thin patterned layer can be an etch resist or a foundation upon which to build new types of microstructures. Since an elastomeric stamp is flexible, it can be used to transfer a pattern to 2-D or 3-D substrates. For example, metallized glass capillaries can be patterned by microcontact printing and then selectively etched in an aqueous etchant to form microstructures such as microcoils.

Current university research demonstrates that microcontact printing can achieve nanometer-level resolution on planar substrates. Our particular application requires a much larger feature size that should be easier to pattern with this technique. We propose the fabrication of 3-D microstructures with feature sizes in the tens of microns.

While electroplating a substrate patterned in gold (Au), we discovered that our original microchain design needed modifications to accommodate the electroplating process. We made a new master and then a new stamp that incorporated the modifications needed for electroplating. By transferring the

Printing microcoil pattern on 3-D part.

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microchain pattern to two metallized glass capillaries and then adjoining them, we can form interlocking links through electroplating. This electrochemically welds the two halves of each link together and builds up the thickness of the links to make them more robust. We successfully produced the new microchain pattern in Au on 3-D metallized glass capillaries using microcontact printing followed by selective wet etching in an aqueous cyanide bath. The new pattern gives the electrical continuity needed for electroplating. We aligned and joined several pairs of patterned capillaries using silver epoxy and submitted several samples for electroplating.

The geometry of the long, thin capillaries raised many complications for the electroplating process. Even after several hours of electroplating in a Au cyanide bath, there is no increase in thickness. Troubleshooting efforts are under way but have not revealed the problem. No contaminants have been identified. Electroplating long, thin capillaries in our traditional setup may not be possible. We purchased new equipment that will allow us to more evenly electroplate small cylindrical parts such as capillaries by using a rotating-disc electrode. The uniformity of the coating around a capillary can be greatly improved by spinning it. Efforts are currently under way to install the new equipment and to acquire the needed fixtures for the rotating-disc electrode to hold the capillaries.

We transferred the microcoil pattern to Au-coated glass capillaries. Several factors are critical in effectively transferring the microcoil pattern to a 3-D substrate. For example, if the capillary is not placed on the stamp at the desired angle, the lines of hexadecanethiol “ink” will not match up to form a helix. After numerous attempts to transfer the microcoil pattern by hand, we employed a micromanipulator to get proper alignment of the capillary on the stamp. The micromanipulator works very well in microcontact printing as long as the thickness of the stamp is uniform from one end to the other. If the stamp is too thick at one end, this will cause the capillary to push down too hard on the stamp at that end, thereby distorting the pattern. If the stamp is too thin at one end, the capillary will skip over the recessed section of the stamp, causing discontinuities in the pattern.

Due to the difficulties encountered in the electroplating process, we do not yet have any final parts for functional testing. However, we wound numerous small coils that replicated the expected size of our parts. We conducted preliminary testing on the wound coils, which allowed us to check the limits of test equipment to ensure the reading of very

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small quantities. In addition, we can use these data as baseline data when we test our final parts.

Microcontact printing is a promising method of making microcoils from both 3-D (cylindrical) and 2-D (planar) substrates. One advantage of planar microcoils is the ability to stack numerous coils in a tight space. We are currently in negotiations to fabricate stackable planar microcoils using the techniques established in this project.

We are currently in negotiations to fabricate stackable planar microcoils using the techniques established in this project.

Other Communications

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10751

Automatic Design of Practical Fixtures

J. C. Trinkle, R. J. Gross, P. G. Xavier, E. Gottlieb

The cost of designing and manufacturing fixtures has driven significant research in the automatic design of fixtures at Sandia (e.g., Holdfast™), in academia, and in industry. Nonetheless, automated fixture design systems are not widely used. The two primary problems are (1) lack of generality (i.e., arbitrary 3-D parts and fixturing element geometries cannot be handled), and (2) inability to accurately predict important performance criteria (i.e., tolerance stack-up, loading difficulty, and thermal expansion mismatches). These problems lead to failures. For example, in the Neutron Generator (NG) Facility, fixture failures cause significant costs and delays.

Fixture design systems have fallen short because there have been no underlying theory or analysis tools to efficiently predict loading difficulty and problems associated with dimensional errors and changes in parts and fixtures. Sandia seeks to develop new fixture design techniques and a new idea for mitigating the effects of dimensional errors. The new results allow more general analysis of stability, realistic simulation of fixture loading, including sliding and rolling, and sticking contacts. Our work will yield a principled way to include unstructured and systematic dimensional variations in the design process.

The proposed approach can be broadly classified as simulation-based design and, as such, will require the simulation of multiple scenarios, each corresponding to possible unknown loading conditions and manufacturing errors. To maximize the effectiveness of this approach, we will apply variants of bundle methods to minimize the number of scenarios to be analyzed while still guaranteeing the achievement of fixture design specifications and on experiments to validate our simulations. Also, since the approach is simulation-based, any phenomenon that can be simulated can be included without changing our approach.

- *Design and implement kinetic data structures for toleranced parts.* The kinetic data structures were intended to improve the performance of the multibody dynamics code that underlies much of the work performed in this project, and that will be increasingly important in future fixturing work in the same vein as this project. We designed and implemented kinetic data structures and tested them in some special simple cases. We determined that this enhancement was not effective, so we refocused our efforts in directions not planned in the original

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proposal. Specifically, we collaborated with Argonne National Laboratory and the University of Wisconsin, the developers of the software that underlies our multibody dynamics work. They are studying our typical datasets and will design preprocessing algorithms to improve the performance of our multibody simulator. Our simulator is arguably the best in the world for systems where bodies are nominally rigid and experience intermittent contacts. A brief description and some animations can be found on www.cs.sandia.gov/~jcitrink.

- *Test tolerance stack-up method on NG parts.* This work was folded into the next task.

- *Make final algorithm enhancements and deliver software to designers.* We prototyped our software, which is now undergoing development in SolidWorks for use by actual designers. Current capabilities include interactive fixturing of multiple parts with complex geometry and real-time tolerance stack-up analysis for arbitrarily chosen key points.

Refereed

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Our simulator is arguably the best in the world for systems where bodies are nominally rigid and experience intermittent contacts.

10770

IMEMS Packaging and Interconnection Technology

K. A. Peterson, C. A. Reber

Microelectromechanical systems (MEMS) and integrated MEMS (IMEMS) offer the opportunity to miniaturize key components in nuclear weapons at low cost. Many advantages of this miniaturization are subsequently sacrificed, however, by packaging MEMS structures with the present understanding of conventional microelectronic packaging processes. The resulting low yields of MEMS packaging are a “showstopper” for the eventual success of MEMS. This project will resolve multiple micropackaging issues to efficiently and reliably take advanced MEMS structures from functionality in a laboratory setting to fielded applications. Sandia will practice concurrent engineering to develop the interconnection, micropackaging, post-processing, and, ultimately, wafer-scale packaging concepts that will make consistent, process-based quality a reality.

We will study and improve packaging materials and processes so they don’t “kill” released, functional MEMS. We will investigate a new processing sequence utilizing high-capacity commercial polymer encapsulation to afford complete protection to conventional wirebonds and die-attach prior to the release of the MEMS devices. We will investigate a new approach for ruggedizing released and treated functional MEMS wafers through the use of encapsulation in a vacuum-deposited, carbon-based material. This approach protects MEMS devices through some potentially damaging micropackaging processes, such as backside preparation, die separation, handling, die-attach, interconnection, and possibly even transfer molding. Packaging innovations that reduce the number and complexity of processing steps will be instituted in a package design with an integral, optical-quality window. Ultimately, we will investigate wafer-scale packaging techniques that make the device into its own package.

This project will complete these evaluations with the goal of ensuring advanced manufacturing at higher yield. The success of this project will be a major step in the advanced manufacturing of reliable MEMS structures in industry and will make them more available to Sandia weapon applications.

Certain areas not foreseen in the original proposal demonstrated applications that are extremely useful. Some of the unforeseen applications involve the direct interconnection of gold packaging materials to polysilicon MEMS bondpads,

This image depicts successful implementation of windowed package structures.

The success of this project will be a major step in the advanced manufacturing of reliable MEMS structures in industry and will make them more available to Sandia weapon applications.

which resulted in an allowed patent and will result in another patent application. Another is the post-processing of commercial packages for applicability to MEMS and other microelectronics, which resulted in disclosure of a technical advance (TA) and generated no fewer than five distinct program applications, with more arriving each month.

The method for the temporary encapsulation of MEMS devices for packaging resulted in a patent and sparked even higher interest in alternative ways to accomplish the same goal in a more straightforward manner. This alternative approach will become straightforward only if additional effort is invested. The method for plastic encapsulation of devices prior to release was prototyped and resulted in a patent. This additional work would take the form of additional characterization of the release process. This technique sparked interest in an additional modification that could revolutionize certain aspects of MEMS packaging and will result in a patent application. The work on the windowed structures succeeded beyond our expectations, resulting in a patent, an allowed patent, a number of applications, and a TA. These structures survived temperature cycling and proved to be hermetic. The project goal was to show preliminary feasibility of the approach, but the results have gone beyond that goal, potentially resulting in a product that is valuable to the microelectronics community. Finally, we realized the need for a parallel approach to wafer-scale processing of MEMS, an approach that we call “wafer-scale-like packaging.” This method overcomes a foundry’s reluctance to incorporate additional area to the perimeter of a device to increase packaging yield.

This project has facilitated interactions with a number of projects that have overlapping interests, including Defense Programs with packaging needs, separate project efforts with packaging needs, and several other projects on the horizon. The knowledge base created by this project led to interactions with companies as large as Lockheed Martin and as small as Intellite. One of the key TAs in this project, “sacrificial volumes,” is applicable to microoptoelectromechanical systems (MOEMS) packaging, microfluidics, microgyro packaging, and an ion-mobility spectrometer, in addition to its applications in MEMS packaging.

When we started this project, MEMS packaging was a complicated venture, responsible for much of the cost and some of the growing pains of MEMS. After three years of effort, that is still the case in the industry. Even so, we made significant strides in facilitating the packaging of MEMS by better characterizing existing and new methods for interconnection,

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die-attach, release etching, process order, and the visibility of packaging as a necessary entity for the success of MEMS. As a measure of this success, this project is directly associated with 23 TAs and partly associated with several more. Three patents have been granted, a few others allowed, and a number of others will likely result in the future.

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10793

Computer Numerically Controlled Micromachines

B. Jokiel, Jr., E. E. Wyckoff, L. F. Bieg, J. J. Allen, D. P. Adams

Historically, microelectromechanical systems (MEMS)—type micromachines are fabricated to function in two-dimensional (2-D) workspace. Sandia will design, manufacture, package, and apply computer numerically controlled (CNC) silicon (Si) micromachines. These multiple-degree-of-freedom (DOF) machines (including 3-D) would serve as the basic building block for a variety of applications. Its use in micromilling, microcoordinate measuring, microalignment, optical switching, laser pointing, rastering, and a device that performs surgery on living cells is contemplated. A micromilling machine, capable of machining nanosized features, can be built by employing a high-speed motor holding a cutting tool all on one chip. Some of the innovative technologies that are needed to enable CNC micromachines include the following:

(1) A parallel mechanism is the only method of fabricating a multi-DOF microstage on a chip, since serial mechanisms require the stacking of actuators.

(2) Sputtering or chemical vapor deposition (CVD) can apply non-Si material to a poly-Si part.

(3) A focused ion beam (FIB) can fabricate micro-sized cutting tools.

(4) A micromachine stepper motor can provide open-loop positional control.

(5) Non-Si-based microfabrication can provide packaging of Si micromachines.

CNC micromachines will have weapon reserve (WR) and commercial applications. CNC micromachines can be used to machine or inspect nonplanar parts to dimensions previously unheard of. A mirrored platform can couple optical energy to multiple sensors or detonators. Safety-critical parts can be micromilled immediately before detonation. Medical applications include micromanipulation of biological specimens using a dexterous CNC manipulator.

(1) A design methodology and parts toolbox for creating planar-fabricated, spatially deployable, computer-controlled MEMS mechanisms. We leveraged criteria for the design of parallel kinematic mechanisms (PKM) from the field of robotics and machine tools to develop a design methodology for Si MEMS PKMs. From this work, we can determine the configuration and type of control linkages for a spatial motion-

MEMS double-sided linear stepping-track drive.

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control platform, including the number and type of unconstrained DOFs in each control linkage.

Certain types of joints are necessary to design spatially deployable mechanisms: different types of 2DOF rotary joints, spatial four-bar linkages, and 3DOF joints. We created a toolbox of joints and assorted other parts to enable the quick design of different device configurations. It is possible to create motion-control stages in MEMS with up to six independently controlled DOFs.

(2) *Perfection of stepping-track drive actuators capable of 0.4 mN of force and controlled motion at 100 mm/s.* We created a family of linear drives and parts, and we developed a generalized theory and design methodology for stepping-track drives complete with parts toolbox. By inputting the desired actuator resolution and force range, we can easily determine all of the design parameters for a feasible stepping-linear-track drive. Unlimited-stroke, bidirectional track drives with resolutions down to > 250 nm are possible. We designed and successfully tested seven successful permutations of these drives ($2.0\ \mu\text{m}$ resolution) around Sandia's high-performance comb drive. They demonstrated position repeatability perfectly at 100 mm/s track speeds with upwards of 0.4 mN force.

(3) *A packaged and bonded set of devices.* We fabricated two versions of XYZ translation only, and four versions of piston-tip-tilt MEMS microstages on a single concatenated SUMMiT-V™ (Sandia Ultraplanar Multilevel MEMS Technology) module. The largest device was $3\ \text{mm}^2$. These devices were successfully released and coated with a vapor-deposited self-assembled monolayer (SAM) antifriction coating. The die were wire-bonded to a ceramic 68-pin leadless chip carrier (LCC), which we mounted in a package on a printed circuit board for testing. Since this occurred very late in the project, the die have not undergone rigorous testing. Preliminary tests indicate that they work as designed.

(4) *Control software complete with a graphical user interface (GUI) for the stages and the linear drives built around MATLAB.* We developed software for the stepping-track drives to facilitate rapid testing of the linear track devices. The user inputs total actuation distance and maximum velocity, acceleration, and drive voltage. The software then computes the voltage-time profiles for each actuator using constant jerk acceleration-deceleration curve. A "record notes" function allows the user to record observations with a log of the drive parameters.

We developed a more complex package for the XYZ translation stages. The microstage control software reads a user-

XYZ microstage popped up from fabrication plane.

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created, high-level path plan file (M/G-code machine tool language). It computes the trajectories for each of the drives and computes the voltage-time records for each of the actuators.

A package for the piston-tip-tilt device is currently in development. The equations for the XYZ stage are simple and relatively quick to solve on the fly. The piston-tip-tilt equations require an iterative solution and are solved *a priori* and stored in the form of a lookup table. The software interpolates between solutions using the table.

(5) *An infrastructure to design, engineer, and test spatial MEMS mechanisms.* Software design tools include AutoCAD2002 (and related MEMS software tools created by Sandia), SolidWorks, COSMOS/DesignStar, and COSMOS/Motion. These are used for solid-model visualization, rapid-prototyping model generation, finite-element analysis (FEA), and dynamic analyses. We built a probe station and MEMS test stand that reside in a clean room. The station has 10 signal channels, 12 amplification channels, 10 probe positioners, a digital 1.3 megapixel still camera, and a digital live-video-collection system. The cameras and MATLAB software are driven by an 800 MHz Pentium III computer system.

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Refereed

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26508

Mesoscale Wide-Bandwidth Linear Magnetic Actuators

L. A. Jones, R. Chanchani, T. K. Mayer

The purpose of this project is to develop and integrate the technologies to efficiently manufacture mesoscale wide-bandwidth linear magnetic actuators. Mesoscale actuators are defined here as actuators that have linear travel beyond that which can be achieved using electrostatic, piezoelectric, or magnetostrictive technologies, but that are small enough in overall size that mesoscale and micromachining methods are required to fabricate them. This work leverages the results of recently completed and ongoing projects at Sandia concerning the fabrication of mesoscale magnets and coils. It seeks to supply mesoscale magnetic actuator technology to a host of applications at Sandia.

We are developing a mesoscale moving-magnet planar x-y actuator using planar batch-fabrication technologies. The planar stator coils in the actuator are extremely compact and could not be implemented using traditional wire-wound coils. Instead, we are using the benzocyclobutene/copper high-density interconnect (BCB/Cu HDI) process to make the stator coils. We successfully fabricated the moving magnets in the actuator using microelectrodischarge machining (micro-EDM) and special tooling.

Applications of this technology include pointing actuation as required by optical switches, lithography, telescopes, radars, control and propulsion surfaces, wide-bandwidth valve modulation, active vibration damping, and micromaterials testers.

In earlier work, Sandia investigated a novel four-sided linear magnetic actuator concept. The concept was a moving-magnet design with the magnets suspended via magnetic bearing forces generated by the stator. The four planar sides of the stator were specifically designed for batch fabrication using a particular planar-fabrication technology under development at Sandia. Detailed analysis of this novel concept indicated that the actuator would develop sufficient bearing forces and motoring forces for wide-bandwidth movement.

Subsequent investigation of the favored planar process for fabricating the stator coils determined that the process is not mature enough to fabricate the required stator coils. We sought and identified an alternative process and developed the alternative process for HDI. Standard lithography techniques are used to define layers of Cu conductors with intervening

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layers of BCB, in a process known as BCB/Cu HDI. We investigated BCB/Cu HDI and used it to fabricate five layers of conductors with four intervening layers of BCB. The disadvantage of this alternative process is that it is currently optimized for high-frequency, low-current circuits, which means that the (sputtered) conductors are very thin, whereas the actuator stator coils operate at low frequency and high current, ideally requiring thick conductors. With additional development, we could fabricate thicker conductors with the BCB/Cu HDI process, but due to resource limitations, the actuator will be fabricated with the current BCB/Cu HDI process.

The BCB/Cu HDI process is fundamentally planar and unable to fabricate structures many hundreds of micrometers high, thereby precluding the implementation of a four-sided actuator. Therefore, we decided to pursue a single-sided planar actuator, i.e., only one side of the four-sided actuator. A macroscale version of just such an actuator capable of two-dimensional motion (x - y) was presented in a thesis at the Massachusetts Institute of Technology. We designed a similar actuator for this project, but in the mesoscale—millimeter-sized, with the stator coils designed for batch fabrication using the planar BCB/Cu HDI process.

Because of the conductor thickness limitations imposed by the current state of the BCB/Cu HDI process, the performance of the prototype planar actuator will be reduced. The resistance of the stator coils will be high, resulting in relatively high power consumption and heating in the stator. Nevertheless, the prototype actuator will be useful for control-system development, overall proof-of-concept, and applications that require lower-bandwidth actuation.

To date, we have not successfully fabricated a complete set of stator coils because of wafer contamination problems. Therefore, we redesigned the stator coils to be smaller and will assemble them from four separately fabricated pieces, as opposed to fabricating them simultaneously in place, as in the previous design. This new design with smaller stator coils should improve the odds of successfully fabricating a full stator, with the tradeoff being that the actuator will have a reduced x - y throw. We currently are fabricating masks for this new stator design.

We fully fabricated Halbach arrays for the moving-magnet structures in the actuator using micro-EDM to cut bulk high-energy magnet material and by assembling the magnetized magnets with specially designed tooling.

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We selected and acquired a digital-signal processor (DSP) system for motor control. We designed and implemented circuitry that interfaces six laser-displacement sensors in a test stand to the DSP system. We implemented transimpedance amplifiers to drive stator-winding currents as commanded by the DSP system. We are continuing DSP software development work in anticipation of the successful fabrication of stators.

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26509

Levitated Three-Axis Microaccelerometer*F. J. Peter, R. D. Kinney, J. C. Gilkey, S. H. Kravitz*

Sandia's objective is a significant advancement in the state of the art of accelerometer design for tactical-grade (or better) applications. The design goals are < 100 micro-G bias stability across environments and a \$200 cost. This quantum leap in performance improvement and cost reduction can be achieved only by a drastic new approach, not incremental improvements to existing concepts. This novel, three-axis, closed-loop accelerometer is implemented as a hybrid micromachine. The hybrid approach frees the designer from the limitations of any given monolithic process and drastically expands the available design space. The design can be tailored to the dynamic range, resolution, bandwidth, and environmental requirements of the application while still preserving all of the benefits of monolithic microelectromechanical systems (MEMS) fabrication—extreme precision, small size, low cost, and low power.

- *Design concept.* Liquid fill is no longer considered a viable design option because (1) it results in a grossly overdamped system for accelerometer applications, and (2) the electrical properties of fill liquids are too unstable to yield stable, predictable performance.

- *Detailed design.* Based on a balance of ease of fabrication and control-system stability, we found a 10 mm air gap to be optimal. We completed the detailed stator/rotor design and submitted technical advances for several novel electrode concepts.

- *Fabrication.* We addressed three process-development challenges: inconsistent gold via plating, resulting in undesirable voids; insufficient via and wafer flatness, resulting in poor patterning of stator electrodes; and short circuits through the conductive vias during the anodic wafer-bonding process. We resolved the plating problem by process refinements enabled by acquisition of the appropriate plating equipment. We resolved the flatness problem by recent acquisition of a world-class lapping capability. We resolved the anodic bonding problem using a novel wafer-stacking approach, which the experts said “couldn’t be done.” We reduced total process flow time by 50%.

- *Control-system modeling.* A revised control-system model revealed two key findings. (1) Stability is very sensitive to the rotor/stator air gap. The choice of air gap is a tradeoff among stability, the maximum available control voltage, and

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controller bandwidth. (2) Decoupling each degree of freedom simplifies the control algorithm immensely and improves stability.

- *Revised performance prediction.* We updated the calculation of performance based on actual closed-loop operation of a test structure developed for the rotating microgyro: 2 milli-G at 100 Hz bandwidth. We made two improvements: more-optimal electrode geometry and a three-times reduction in charge-amplifier noise, which yields a predicted bias stability of 80 micro-G.

- *Control electronics and test equipment.* We made significant hardware and software upgrades that increase functionality and performance while reducing size dramatically.

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26510

Microfabrication Processes Combining Focused Ion-Beam Machining and Thin-Film Vapor-Deposition Techniques

D. P. Adams, T. M. Mayer, M. J. Vasile

This project seeks new techniques for fabricating complex-shaped microscale devices, components, and instruments. Currently, there is a need for numerous devices with nonplanar features and substrate geometries. This includes components critical to nuclear weapons (NW) and to emerging threats such as microactuators, microsolenoids, micropumps, and microsensors. Devices built on nonplanar substrates are also desired for biomedical (e.g., endoscopes) and pharmaceutical applications.

Sandia's goal is to develop innovative techniques for fabricating curvilinear, micrometer-size features of various materials onto planar and nonplanar substrates (e.g., cylinders). Development of novel microfabrication techniques is required since current processes are limited in either dimensionality, material complexity, or microstructure control. Also, we are investigating methods that shape geometrically complex instruments, such as cutting tools that enable microfabrication.

In this work, we used focused ion-beam (FIB) sputtering for defining features. This may involve direct ion sputtering, direct-write FIB chemical vapor deposition (CVD), or sputter-shaping of microcutting tools and subsequent ultraprecision machining. Direct-write FIB sputtering allows feature definition on nonplanar substrates with nanometer precision. Our research includes an ion-beam lathe process for fabricating coils.

In a second process, we researched FIB sputtering as an enabling technology for microfabrication. FIB sputtering is useful for shaping complex-shaped cutting tools with dimensions $\sim 10\ \mu\text{m}$. We then used these microcutting tools to define features on nonplanar components by ultraprecision machining. For some applications, we researched techniques that combine precision machining with thin-film deposition to make miniature coils. In general, our techniques fabricated coils covering a range of feature sizes from 500 nm to 100 μm . This overcame limitations of conventional techniques such as wire-wrapping. In addition, we targeted film materials other than those used in silicon (Si) microelectromechanical systems (MEMS). This work started with single-conductor coils, such as gold, but included multilayers. For example, zero-magnetic-susceptibility multilayer coils for micronuclear magnetic resonance (micro-NMR) spectrometers are feasible.

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- We researched electromagnetic/electric properties of single-layer coils. We produced continuously conducting coils with diameters as small as 1 mm on insulating substrates by an adaptation of the Damascene process, which is a combination of precision-machining and thin-film processes. We also fabricated and measured cylindrical coils with 3 mm diameters and 25 μm conductors for continuity.

- We demonstrated the ability to tailor thin-film wire cross-section in micromachined coil substrates. We cut double-triangle grooves 15 μm deep on a pitch of 150 μm with excellent replication of the cutting tool.

- We demonstrated deposition of multilayer thin-film microcoils, with chromium and titanium adhesion promotion layers.

- We incorporated ion-beam-induced CVD gasjet assembly.

- We developed techniques for making very small coils onto cylinders using direct-focused ion-beam sputtering.

- Research included shaping of diamond and tungsten carbide microcutting tools by ion-beam sputtering. We researched chemical-enhanced techniques to increase the rate of shaping and to improve microtool cutting-edge roughness. We thoroughly studied the surface morphology of ion-bombarded diamond. We established the sputter rate for diamond as a function of ion incidence angle, with and without chemical assist from water vapor.

We made two specialized prototype diamond tools of interest to Lawrence Livermore National Laboratory using the ion-beam process.

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Refereed

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26511

Resolving Fundamental Limits of Adhesive Bonding in Microfabrication

R. K. Giunta, J. A. Emerson, M. S. Kent, D. R. Adkins

Sandia is developing microsystems for the Nuclear Weapons Strategic Business Unit (SBU), including a Sandia Ultraplanar Multilevel MEMS Technology (SUMMiT™)—based microsystem component. (MEMS stands for microelectromechanical systems.) As electronic and optical components reach the micro- and nanoscales, efficient assembly and packaging require the use of adhesive bonds. This work focuses on resolving several fundamental issues in the transition from macro- to micro- to nanobonding. A primary issue is monitoring surface properties of parts to be bonded. At submillimeter scales, traditional means of evaluating surface energy cannot be applied. We are using contact mechanics to evaluate surface properties of micron-scale parts. Another issue is that, as bondline thicknesses decrease, knowledge of the stability and dewetting dynamics of thin adhesive films is important to obtain robust, void-free adhesive bonds. While researchers have studied dewetting dynamics of thin films of model nonpolar polymers, little experimental work has been done regarding dewetting dynamics of thin adhesive films, which exhibit more-complex short-range interactions. Our investigations into the dewetting dynamics of thin adhesive films have already had an impact on manufacturing processes. We continue to investigate the fundamental limitations of current adhesive-bonding technology and how these size limitations can be overcome. The areas of contact mechanics, capillary fluid flow, surface energetics, and wetting have all been investigated. The focus areas that we selected—evaluating the surface properties of micron-scale parts and minimizing adhesive bondlines without sacrificing bond quality—will result in development of techniques and models for the next generation of micron-scale devices. By resolving these adhesive-bonding issues, we are allowing significantly smaller devices to be designed and fabricated. Simultaneously, we are increasing the manufacturability and reliability of these devices.

(1) Define smallest probe that can be used in the contact mechanics technique. We developed a method of making hemispherical probes that gives us more control over the size of the hemisphere. Minimizing the size of the hemisphere will allow us to evaluate surface properties of smaller areas. We select a glass rod with a diameter equal to the desired diameter

Silicon probe for analysis of micron-sized areas.

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of the hemisphere. We bring the tip of the rod into contact with the uncured liquid silicone or epoxy. The liquid adheres to the rod by surface tension. We then hang the rod vertically during cure. We are currently in the process of making smaller hemispheres, between 250 μm and 500 μm . This size hemisphere allows us to evaluate the surface properties of a 100–200 μm area using the JKR (Johnson, Kendall, Roberts theory) contact mechanics technique.

(2) *Extract relevant surface energetics parameters to be used in wicking transport model; model wicking transport in micrometer-size gaps.* We developed a new technique to evaluate the capillary wicking behavior of liquids in micrometer-size gaps. Rather than setting the desired gap between two parallel plates, as was done previously, we measured the flow of liquids in fused-silica capillary tubes. This allowed much better control of the gap spacing. As a result, the error in the measurements is significantly lower than those obtained previously. Using this technique, we made measurements using capillary diameters down to 7 μm . Measurements in 2 μm -diameter capillaries are in progress. Measurements in gaps below 2 μm are dependent on being able to obtain smaller capillaries.

To validate the Washburn equation down to micrometer-size scales, we calculated the surface tension of the liquid based on experimental values of flow versus time. The experimental data agreed with the literature values of the surface tension within a few percent for all capillary sizes studied. We conclude that the Washburn equation is valid in capillaries with diameters down to 7 μm . We will continue to investigate the flow behavior in smaller capillaries.

(3) *Extend dewetting analysis to include three adhesive/substrate combinations and correlate results with “spinodal dewetting” mechanism observed in model polymer films.* Two adhesive systems, Epon 828/T-403 and Epon 828/PACM, were spin-coated onto silicon (Si) wafers and five metal-oxide-coated wafers, for a total of 12 adhesive/substrate combinations. Since 828/T-403 dewetted from silicon dioxide (SiO_2) and 828/PACM did not, we chose the 828/T-403 as a model system for further investigation to determine the critical parameters driving the dewetting process. In all cases where dewetting occurred, the process was controlled by a nucleation and growth process, not by the spinodal dewetting mechanism observed in model polymer films. The T-403 molecule is asymmetric, while the PACM molecule is symmetric. We believe that this difference in chemical structure of the two cross-linkers explains the difference in dewetting behavior. We

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observed a strong correlation between humidity and the time required for films to dewet. Upcoming work includes efforts to quantify the effect of humidity on dewetting behavior.

(4) *Build a model that can predict droplet size for at least three adhesives of interest.* We tested four dispensers for their suitability in applying adhesives. From these options, the Picospritzer by Stoelting appeared to give the best results. The Picospritzer basically gives a millisecond-duration pressure pulse through a tube to the headspace above a liquid column in a capillary. The pulse does not dislodge a droplet from the tube, but it causes the meniscus to bulge far enough from the capillary opening to be wicked onto the surface. We developed a model of the system to show the interplay between parameters such as the column diameter and length, fluid properties, and pulse duration. We performed parametric studies with the model and are designing experiments for verification.

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Refereed

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38605

Microfabrication with Femtosecond-Laser Processing

M. L. Griffith, P. Yang, T. S. Luk, D. E. Reckaway, G. R. Burns

Numerous Sandia and Department of Energy initiatives require components having micron-size features. One example is nuclear weapons in which subminiature stronglinks and neutron tube micromechanical screens are components that production either needs today or would like to have in the near future. Various sensors (biological, optical) would benefit from new techniques to fabricate complex waveguides in glass that are currently not possible. Miniaturization will dominate future hardware designs, and technologies that address the manufacture of these microscale features will be in demand. In particular, the design community requires techniques that, at minimum, complement existing processes such as photolithography/etching, LIGA (the German term Lithographie, Galvanoformung, und Abformung, for lithography, electroforming, and molding), microelectrodischarge machining (micro-EDM), and excimer laser drilling. If possible, these techniques should have the flexibility to fabricate complex three-dimensional shapes in various materials, therefore significantly improving designs in terms of new, one-of-a-kind components.

Femtosecond-laser processing has the potential to fulfill design demands and material issues while expanding and improving fabrication of microcomponents. One of the unique features of femtosecond lasers is the ability to ablate material without transferring heat, and therefore damage, to the surrounding material. A femtosecond ($\text{fs} = 10^{-15} \text{ s}$) is less than the electron-phonon coupling time in metals.

This research investigates the special characteristics of femtosecond-laser processing for microfabrication. Sandia will explore the basic mechanisms of femtosecond-laser ablation, gain a science-based understanding of the process, and determine the process parameter space for laser processing of metals and glasses. We designed and assembled a femtosecond-laser manufacturing system. We initiated our study into the effects of laser and environmental parameters on removal rate, feature size/definition, aspect ratio, and material structure. For photonic devices, we selected glass compositions to understand the mechanisms of refractive index modification in waveguide formation. We implemented the first edition of the computer-aided design (CAD)-to-part software and fabricated metallic components. We will address manufacturing requirements for compo-

Stainless-steel component with 100 μm fingers.

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nent fabrication, including precision and reproducibility. Success will permit us to miniaturize multiple components.

We designed and assembled the femtosecond-laser microfabrication system. We performed preliminary studies on metal ablation, showing ablated hole diameters as small as 4 μm . With very preliminary studies on the effect of scan velocity on ablation depth, we produced various geometric shapes in stainless steel (SS). We fabricated one such shape, an intricate comblike pattern, in 125 μm -thick SS with 100 μm features and 100 μm spacings. Initial work on miniaturizing an impeller body looks promising. The initial CAD/computer-aided manufacturing (CAM) interface allowed for the layered manufacture of a steel tool that was used to room-temperature vulcanizing (RTV) mold a silicone replica of the impeller, where features were on the order of 200 μm .

For photonic devices, we selected eight glass compositions to understand the mechanisms of refractive-index modification in waveguide formation. We selected glasses with varying amounts of glass modifiers, a low anneal temperature, a wide working-temperature range, and different thermal properties to verify the local densification and the thermal stress mechanisms on the local refractive-index change. In addition, we selected glasses that possess large amounts of transition metals to study the effect of defect formation on refractive-index modification.

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38606

Mesoscale Controlled Motion for a Microfluidic Drop Ejector

P. C. Galambos, M. T. Ensz, S. S. Mani, R. J. Shul, B. Jokiel, Jr.

A class of mesoscale devices is enabled by integrating a microfluidic drop ejector (MDE) with a mesoscale micron-precision, motion-controlled platform. Applications include biochemical analysis (e.g., proteomics), “intelligent ink” patterning, mesoscale rapid prototyping, adhesive deposition, and direct writing of circuits. The MDE, originally designed for inkjet printing, is capable of ejecting chemical analytes, evaporatively self-assembling solutions, ultraviolet (UV)-curable polymers, liquid adhesives, and conductive inks. The MDE ejects fluid via a variable positive displacement pump, unlike bubble jet. Superior performance specifications include drop-size variation, no satellite drops, and no thermal effects. By integrating the MDE with precision motion control, precise volumes of two or more different solutions can be deposited at the same target location.

This project leverages Sandia-owned property such as the MDE, electromicrofluidic packaging methodology, LENSTM (laser-engineered net shaping)—developed motion-control software, and mesoscale linear magnetic actuators. The approach will be to use mesoscale machining capabilities to integrate the MDE into a device. Mesoscale parts to be machined are a housing, guides, and rare-earth magnets (REMs). The approach includes the assembly and demonstration of one or more devices such as the “intelligent ink” patterning system or the mesoscale rapid prototyping machine. The “intelligent ink” patterning-system demonstration would involve the deposition of drops at precisely defined locations. During evaporation, self-assembly within the “intelligent ink” drops would result in precisely patterned functional nanostructures on the target substrate. Mesoscale rapid prototyping machining would be capable of building parts out of a UV-curable polymer having 20 μm or smaller linewidths.

Early in the project we concentrated on the design of a “sideshooter” ejector that is compatible with a variety of liquids, can eject small volumes (0.5 fl), is capable of on-the-fly drop-size adjustment, and is mass producible utilizing SUMMiT-VTM (Sandia Ultraplanar Multilevel MEMS [microelectromechanical systems] Technology). The baseline design and parametric variations are completed and in fabrication (RS349). The design utilizes a bidirectional high-

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performance electrostatic comb drive (6 μm and 10 μm actuator travel) that can produce forces on the order of hundreds of mN to rapidly advance a piston into an ejection chamber. The chamber contains an exit hole (nozzle) out of which drops are ejected. Reverse-direction actuation allows the piston to be rapidly withdrawn for fast chamber refill. The longer (10 μm) stroke and bidirectional drive are new actuation features. Parameters include nozzle hole size (2, 5, 10, and 20 mm diameter), piston width (7, 25, and 50 μm -wide pistons), and sealing and filling flow geometries.

We performed the finite-element analysis of the drop-ejection process using Sandia's GOMA code to size the actuator (determine the force required to eject a drop). The analysis indicated that a force of hundreds of mN would eject a drop and that the leakage around the piston would not prevent drop ejection. Pressures on the order of two to three atmospheres would be generated, compatible with the strength of the polysilicon cover layer. The actuators in fabrication were oversized to account for unforeseen effects.

Because this is mechanical ejection only (no field or heat is applied to the liquid), the ejector should be compatible with any solvent that does not corrode silicon (Si). We investigated the compatibility of the ejection system with chloroform and toluene because they are the solvents used on the Chem-Lab-on-a-Chip project to deposit coatings on surface acoustic-wave sensors. The Si ejection system chip can be mounted on a stainless-steel (SS) or PEEK (polyether ether ketone) manifold (inert to most solvents) that contains two or more wells, allowing two or more liquids to be fed to different ejectors on the chip. The adhesive used to attach the Si to the SS manifold is potentially susceptible to solvent attack. For this reason we chose a Teflon-filled bismaleimide (BMI) adhesive that is resistant to most solvents, including chloroform and toluene.

The other assembly issue for this project is the method of mounting the target onto rapidly positionable stages. We chose two commercial stages that meet the requirements of 1 m/s motion with micrometer accuracy over 1 mm^2 of travel area.

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38608

Science-Based Sensing of Phase Transformations in Steels

F. J. Zutavern, C. V. Robino, P. S. Duran, M. W. O'Malley, M. Reece

The ability to control microstructure and residual stress distribution in forgings, welds, and structural materials is fundamentally based on control of solid-state phase transformations. However, the ability to directly sense and monitor the progress of phase transformations in real time under steady-state and transient thermal conditions is lacking. Recent advances in experimental and numerical approaches to the study of solid-state transformations in steels provide a basis for developing new sensors for phase-transformation kinetics. Advances in high-speed dilatometry and high-speed, high-resolution, hot-stage microscopy provide accurate data for comparison with electromagnetic (EM) and laser ultrasonic (LU) sensor results. Advanced numerical models, including a model for interpretation of dilation data and validated EM modeling of ferromagnetic materials, are also key to understanding the sensor output and sensitivity. Sandia is investigating the use of advanced active and passive EM sensors and LU methods to directly sense and monitor the progress of phase transformations in ferromagnetic steels during steady-state and transient heating conditions. Miniature inductive sensors are sensitive to magnetic permeability and resistivity changes caused by changes in temperature and related directly to the phase transition from ferrite to austenite. Short-pulse LU sensors are also sensitive to temperature and microstructural variations related to the ferrite-to-austenite phase transition, as well as stress, defects, and dimensional variations. Applications for these sensors include forging, welding, and thermomechanical processing of steels and other materials. The sensor analysis will utilize the computational models to benchmark the sensitivity of the methods and results. Success in this has broad applications to optimization of thermomechanical processing and joining of steels and other materials for the national manufacturing community.

The vacuum heat-treating and -sensing test apparatus (Gleeble) has been adapted for magnetic sensors and their respective data-acquisition equipment. We outfitted the Gleeble with a precision x-y-z positioner and high-bandwidth, low-noise signal feed-throughs to accurately locate and monitor the magnetic sensors. We designed, fabricated, and tested five types of thermally protected sensors with steel samples heated to

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950°C: water-cooled, and four types of radiation shields—thin foil, graphite, glass tube, and palladium-coated glass tube.

We programmed the Gleeble for several magnetic sensor tests. We wired control signals (voltage, current, and synchronizing trigger) from the control system to the data-acquisition system to synchronize the magnetic sensor data with the information from the control system (time, temperatures, voltage, current, and power angle) for both heating and cooling processes. We thoroughly tested the Gleeble to verify signal accuracy and timing precision with the data-acquisition system and the control signals.

We tested six magnetic sensors (radial, azimuthal, and coaxial magnetic-field orientations in vacuum and ferrite-coupled configurations) in the passive mode, where magnetic fields generated by the heating current are detected. The fast-rise, short-pulse heating current was spectrally analyzed to assess its impact on passive and active sensing. We have already identified some of the characteristic properties of the magnetic phase transition in the initial data from the passive sensors. We programmed the Gleeble to scan repeatedly across the Curie point (770°C) over a 50°C range. We acquired data for the different sensors and are analyzing it to extract magnetic phase-transformation effects.

For the active mode, where the sensor supplies a higher-frequency signal to generate magnetic fields, we designed and fabricated high-pass, high-power, analog electronic filters. These filters reduce the low-frequency heating signal generated at the sensors and protect signal generators, amplifiers, and digitizers. This is not an insignificant issue, because more than 10 kA of current can flow through the sample in 1 ms-wide pulses. The sudden rise and fall of this heating current within a few millimeters of the magnetic sensors can easily produce spikes that are greater than 1 kV. We assembled a variety of steels with a range of phase-transformation behaviors for testing. Previously unavailable data for steady-state, high-temperature, EM properties have been contracted with a professional laboratory that specializes in these measurements. They are extending the temperature range of their measurements to include the magnetic phase transition (770°C). In preparation for correlation with the sensor measurements, we developed and implemented significant improvements in Gleeble dilatometry.

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52173

Micromechanical Spectrum-Analyzer System

D. R. Adkins

There is a growing recognition that a large array of simple sensors may have advantages over a small array of more-sophisticated sensors. Often the signal that clearly identifies a threat is rapidly attenuated with distance. This is particularly true when the acoustic radiation from a source is in a frequency band above the audio range, and a simple sensor in close proximity to the threat could provide the best identification of the source. Sandia's goal in this project is to reduce the size and power consumption of an ultrasonic spectrum-analyzer system for threat detection and alarm in an underwater environment.

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A basic monitor device would perform several functions: sense noise, discriminate if noise is a threat, and notify personnel of the threat location. The challenge is to manufacture the monitor device so it is small enough to be covert and cheap enough so that thousands can be used to cover a large area while maintaining close proximity to the source. Power requirements sometimes dictate size, and digital signal processing affects both power and cost. Our work helped reduce the need for digital signal processing by employing a microfabricated acoustic spectrum-analyzer (MASA) that mechanically processes the signal and discriminates threats. The MASA device can process the signal in real time and consume almost no power.

Our proposed tasks were as follows: (1) integrate a hydrophone with the spectrum-analyzer and signal processor into a compact package, (2) incorporate a pattern-recognition (PR) program into the signal processor and provide a visual display of the results of the pattern correlation, (3) minimize the power consumption and component size for the integrated system, (4) test the system in an aqueous environment at signal frequencies above the audio range, and (5) perform

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environmental tests to determine the influence of temperature and vibration on system performance.

We purchased two piezocomposite hydrophones. One hydrophone was driven like a speaker to produce ultrasonic pressure waves at frequencies between 40 kHz and 60 kHz. We used the second hydrophone as a pickup to sense the pressure wave and transfer an electrical signal to the spectrum-analyzer. The spectrum-analyzer consisted of four flexural plate-wave (FPW) devices, each of which resonated at a specific frequency between 50 kHz and 60 kHz. At resonance, the FPWs produce a back electromotive force (emf) that is measured with a root-mean-square (RMS)-to-direct-current (DC) converter integrated circuit (IC).

We immersed both hydrophones in a pool of water for the tests and routed the measured signal to a single resonator. The output signal from the RMS converter peaked at a drive frequency of 53,430 Hz. The half-height bandwidth for the system was on the order of 40 Hz. As the drive voltage to the speaker increased by a factor of 10, there was a linear response in the output of the RMS converter. Because of the high Q of the resonator, the signal-to-noise ratio was very good; however, we did not make a quantitative measurement. This signal can be used easily in a PR routine.

The temperature dependency of the FPW did prove to be a problem in the tests. The resonant peak of the FPW would drift approximately 2000 Hz per degree Centigrade of temperature change. We also performed thermal tests on a second type of resonator where a plate rocks about two pivots. This teeter-totter resonator had a resonance frequency of 38 kHz, and it drifted only 20 Hz per degree Centigrade.

Our test system required about 0.5 W for one channel of the spectrum-analyzer, but it was not designed for low power consumption. We designed a revised circuit that will cut the power consumption by a factor of 10. The new circuit uses the power-down features of the ICs to lower power consumption, and it also has a programmable IC for PR routines. We ordered circuit boards for this second-generation design.

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Biotechnology

The Biotechnology investment area enables Sandia research efforts that develop targeted biotechnology capabilities in support of national security missions. Biotechnology will integrate Sandia's core capabilities in the physical, informational, and engineering sciences and augment them with new biotechnical capabilities at the cellular/molecular levels. These core capabilities will also provide a unique platform from which Sandia can make significant contributions to the biomedical needs required by our mission responsibilities. The focus is on tools and capabilities to build informational and physically based systems. These models will facilitate improved toxin-detector systems and improved microinstrumentation.

Sandia is using chlorophyll-like molecules to harvest photons and direct the light energy to a reaction center for the photosynthesis of high-energy fuel molecules to power microelectromechanical applications. Light energy is converted by the biomimetic chloroplast component into a chemical that can be used in the dark and replenished when the chip is again under illumination. These structures can provide power sources for integrated microelectronic and microelectromechanical systems that will support national security missions.

“Biomimetic Chloroplasts: An

Integrated Microdevice Power Source” uses light energy to produce a fuel source. This project has filed a patent disclosure and a patent application and has obtained one patent.

10746

Predicting Function of Biological Macromolecules

L. J. D. Frink, S. A. Means, M. J. Stevens, M. G. Martin, M. P. Sears, H. P. Hjalmarson, P. S. Crozier, S. L. Rempe

While sequencing technology has been a major thrust in computational biology for the last decade, there is now considerable interest in predicting protein structures from their amino-acid sequences, understanding the interactions and functions of proteins in their native environments, and understanding cellular response to stimuli. This increased understanding is expected to lead to a revolution in medicine in the next century. Sandia's focus in this project is to develop and demonstrate the applicability of a variety of computational tools to biophysical problems. This involves applying and extending massively parallel (MP) molecular simulation, molecular theory, and engineering codes to model a diverse set of problems, including deoxyribonucleic acid (DNA) condensation, DNA interactions, protein-protein interactions, drug docking, ion-channel protein-mediated transport across membranes, electroporation, effect of intracellular calcium and sodium in neurotransmitter release, and studies of xenopus oocyte fertilization. The project involves both developing code needed for biology applications and applying the codes to real problems.

We studied many different systems because the goal of this project was to develop biophysical modeling expertise at Sandia. Furthermore, since Sandia has a variety of unique computing capabilities utilizing MP computers, the secondary goal was to leverage those tools to solve difficult biophysics problems.

- *Simulation of biological macromolecules.* One primary emphasis of our work was simulation of biological macromolecules. We focused on ion-channel proteins (in particular, the gramicidin A channel), DNA, and unstructured proteins. We performed both molecular-theory calculations and molecular-dynamics (MD) simulations on these systems. We showed the important role that multivalent ions can play in the formation of special DNA assemblies (e.g., torroidal assemblies). Furthermore, we applied the molecular theory codes to study potentials of mean force experienced by ions as they traverse the channel. These calculations lay the foundation for many more detailed studies of ion transporters. Finally, we built a theoretical framework that can and will be used to study protein and ion solvation.

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- *Simulation of cells and cell membranes.* In addition to studying biological macromolecules, using molecular modeling tools, we developed coarse-grained models for lipid bilayers. The coarse-graining strategy should allow investigation of longtime phenomena such as fusion and vesicle simulations. Furthermore, we applied Sandia's finite-element simulation capabilities to several relevant cell-biology problems, specifically calcium dynamics in excitable systems (neurons, cardiac cells, etc.). This application included exploration of spatial distributions otherwise intractable in the experimental laboratory. Finally, we performed several investigations of electroporation in the context of this project.

- *Methods development.* We completed detailed investigations of biological force fields and implemented these force fields in our molecular modeling codes. We also developed new, faster molecular-theory algorithms and specialized nonequilibrium molecular-theory codes to treat protein solvation and ion-channel transport.

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10774

Biosensors Based on the Electrical Impedance of Tethered Lipid Bilayers on Planar Electrodes

R. C. Hughes, D. Y. Sasaki, S. M. Brozik, D. W. Branch

Impedance-based, planar chemical microsensors are the easiest sensors to integrate with electronics. The goal of this project is a several-orders-of-magnitude increase in the sensitivity of this sensor type. Sandia recently developed novel chemical sensors based on planar, interdigitated microelectrodes coated with thin films of polyelectrolytes. The ion conductivity of ions doped into these films is sensitive to a wide range of volatile organic compounds (VOCs), including nerve-agent simulants. We believe that the mechanism of detection involves reversible plasticization of the polymer chains, allowing faster ion motion detectable by simple alternating-current (AC) impedance at low frequencies (10 to 1e5 Hz). We achieved parts per million (ppm)-level sensitivities with these new devices, but to achieve orders-of-magnitude increases in sensitivity, we are exploring ion motion (impedance) in very thin lipid-bilayer capacitor membranes that are chemically tethered to our planar electrodes. The basic idea is to mimic biological-chemical sensors that rely on changes in ion transport across very thin organic membranes for the sensing. The large increase in sensitivity over polyelectrolytes will come from molecular-recognition (MR) elements like antibodies that bind the analyte molecule. The MR sites can be tied to the lipid-bilayer capacitor membrane, and a number of mechanisms can be used to modulate the impedance of the lipid bilayers. These include coupled ion channels, pore modification, and double-layer capacitance modification by the analyte molecule.

We built on previous successful work to learn how to fabricate a rugged, planar biosensor. One of the major problems was in developing a consistent recipe for the fusion of unilamellar lipid vesicles onto the lipid-chip electrode surfaces. There are many variables, including the choice of lipids in the mix, the use of cholesterol, the use of extrusion or sonication to form the unilamellar vesicles from the multilayer ones, and the role of temperature. The preparation of the lipid-chip surface is also fairly crucial. We found that an ultraviolet/ozone clean just prior to vesicle fusion is important, probably because of the transient hydrophilic nature of the surface just after the cleaning step. Using a consistent method to form the lipid bilayers, we found that they were very stable compared to free-standing

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black lipid membranes, which are good for rugged biosensors. We then tried several methods for improving the seal between the lipid bilayer and the electrode substrate. Many other researchers in the field of supported bilayers have had this problem. We tried a new set of lipid chips with a capping of silicon dioxide (SiO_2) over the silicon nitride (SiN) that forms the barrier to ions around the rim of the electrode. We also tried gold (Au) electrodes instead of platinum. Neither modification improved the seal. We also tried a new method of forming a templated sol-gel scaffold over the electrode area. To form a seal, we mixed photoresist with the sol-gel precursors and then patterned the area of the electrodes with a shadow mask. Once we cured the sol-gel, we could open the unexposed area of photoresist to the metal by dissolving out the undeveloped photoresist. The exposed areas should have all the pores in the templated sol-gel blocked. This has not worked completely yet since the process has not yet yielded a pinhole-free film, but further changes in the process should give a better seal. We also tried a completely different configuration on flat Au electrodes, by using an "O"-ring seal to the electrode surface with the templated sol-gel as a scaffold on the surface. This gave very fast vesicle fusion, but the seals were no better than the best lipid-chip results. Our hybrid bilayers still yielded very good stability with functional gramicidin channels, in one case lasting for three weeks with repeated washing of different solutions. We made one attempt at using gramicidin that was derivatized with biotin. The concept is that biotin has a very strong affinity for the protein avidin. We showed that the labeled gramicidin was functional (that is, conducted cesium ions), and we hoped that the introduction of the protein avidin would disrupt the ion-channel conduction by tying up the gramicidin in the top leaf of the bilayer. This first attempt was unsuccessful, but we anticipate that further work with labeled gramicidins will lead to biosensors with great selectivity.

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10780

Nanostructured Materials Integrated in Microfabricated Optical Devices

D. Y. Sasaki, A. R. Burns, M. E. Warren, S. M. Brozik, M. B. Sinclair, S. A. Kemme, C. J. Brinker

This project combines the emerging strength of nanocomposite materials at Sandia with the recognized expertise and processing capabilities involving microfabricated optical-device structures for the development of microsensor arrays and unique tunable microoptical devices. The project involves the design, development, and characterization of molecular (nanoscale) to micron-scale structures to achieve desired material and device function. At the core of the material is a liquid crystalline (LC) lipid bilayer that mimics the properties of a biological cell membrane. The bilayer is functionalized with molecular receptors for specific recognition of chemical and biological species, and optical reporters that signal the occurrence of the recognition event. These molecular and supramolecular structures will be supported on a structurally oriented, mesoporous, inorganic matrix. The matrix offers structural stability and physical protection of the LC materials and provides a platform for forming dense LC structures for greater signal output. Together, the materials form a unique nanocomposite with molecularly dynamic organic components for rapid optical response to specific analytes coupled to a robust inorganic scaffold with highly defined and tunable surface area and pore volume. Integration of the nanocomposites to microfabricated optical devices will occur in two stages. In the first stage, we will couple the materials onto substrate-mode platforms for combinatoric sensing arrays. The second stage will then further the materials integration by forming the material into an optical structure yielding devices that can tune their properties through chemical signaling. Multiple materials and optics issues must be addressed to successfully merge these disparate research areas. Results from this work alone will make great strides in creating new micron-scale sensing arrays for biopathogens and combinatorial approaches to materials and drug discovery, and unique microfabricated optical structures with rapid and tunable switching properties.

Our achievements were in materials and optical-device development. We (1) prepared functionalized lipids for selective binding and detection of proteins, > 50 nm mesoporous silica sol-gel materials for lipid-bilayer immobilization, (2) completed studies on the reversible

Results from this work alone will make great strides in creating new micron-scale sensing arrays for biopathogens and combinatorial approaches to materials and drug discovery, and unique microfabricated optical structures with rapid and tunable switching properties.

chromatic shift of polydiacetylene (PDA)/sol-gel hybrid materials, (3) characterized reversible nanoscale structure changes in functionalized lipid bilayers as they respond to chemical recognition events at the membrane surface, (4) developed a diffraction grating for 548 nm light on a silica substrate, and (5) tested the optical properties of sol-gel hybrid materials on the microoptical device.

For the development of protein-selective lipid bilayers, we prepared three new glycolipids functionalized with mannosyl, glucosyl, and galactosyl moieties. The glycolipids were also labeled with a pyrene fluorescent probe on the hydrophobic tail of the lipid to allow a monitoring of lipid reorganization in response to protein binding. When placed in a bilayer of distearylphosphatidylcholine, the glycolipids tended to aggregate, causing the pyrene groups to fluoresce as excimers (emission of 470 nm) upon excitation at 346 nm. In the presence of micromolar quantities of the lectin, Concanavalin A, in pH 7.0 buffer solution, the mannosyl-functionalized liposomes responded with a large change in fluorescence emission. Apparently, upon protein binding, the glycolipids disperse due to the steric interactions between the bound proteins and the spatial placement of binding sites on the protein's structure. The lipid bilayers were highly selective, showing no response to serum proteins or to the structurally similar lectin, Dolichos Biflorus.

We were also successful in the preparation of large-pore silica sol-gel materials, prepared by using polyethylene glycol-polypropylene glycol-polyethylene glycol copolymer micelle structures. The pores were of wormlike structure with open ends at the edges of the silica gel, offering a promising route to lipid-bilayer immobilization via liposome delivery into the pore structure. The average diameter of the pores was 50–60 nm, providing adequate size and shape for small unilamellar vesicles of 30–40 nm to travel into and fuse to the internal voids of the silica surface.

We found that PDA/silica sol-gel materials, which offer unique calorimetric changes in response to chemical and physical triggers, responded rapidly and reversibly to thermal fluctuations. We conducted complete characterization of these materials with regard to chromatic changes, modeling of the PDA self-organized assembly, and overall structure of the hybrid material, and described the results in a manuscript submitted to the *Journal of the American Chemical Society*.

In an effort to understand the changes in the supramolecular structure of the lipid bilayer as it responds to the chemical-recognition event on the membrane surface, we conducted

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atomic-force microscopy (AFM) experiments to examine nanoscale structure changes in the functionalized membranes. We found that, initially, receptor molecules in a phosphocholine lipid matrix formed nanoscale dendritic structures that spanned throughout the membrane. Upon chemical recognition with metal ions, the receptor molecules dispersed in the matrix, causing the structures to diminish in size and intensity. Removal of the metal ions induced a reformation of the receptor aggregates to structures near their original size and shape. The results of this work were published in the *Biophysical Journal* and *Langmuir*, and will appear in a special issue of *Langmuir* dedicated to the biomaterial interface.

We coupled the PDA/silica materials to microoptical device platforms to test the optical properties of the materials-mated platform. We designed the microoptical structure in a fused-silica wafer to diffract 548 nm light at 45° to the incident source, and the light was to reflect off the sensor material surface on one side of the fused silica, and a gold coating on the opposite side. We achieved good light intensity off three reflections, and the PDA/silica material gave good fluorescence from the light intensity provided by the light-impinged sites.

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26581

Molecular-Scale Studies of Single-Channel Membrane Pores

A. R. Burns, G. D. Bachand, B. S. Swartzentruber, J. G. Fleming, D. Y. Sasaki, K. O. Evans

Translocation of large biomolecules (e.g., proteins, deoxyribonucleic acid [DNA]) through single-ion channel protein pores in membranes is an emerging technology that promises new rapid detection and sequencing approaches. However, it is presently not possible to fully interpret the modulated ionic current signals because too little is known about the molecular-level details of translocation. Sandia seeks to introduce a new experimental approach, based on proximal scanning-probe microscopy (SPM), to study the molecular-level structure, energetics, and kinetics of biomolecule interactions with membrane pores during translocation. By implementing the proximal probes, we will supplement the existing macroscopic-ion current-detection approach and be able to (1) characterize the size and shape of a selected pore, (2) correlate local molecular interactions with ion currents, (3) directly measure the forces on translocating molecules, and (4) monitor atomic-scale movement of transmembrane pore proteins during translocation. This project will provide important new insights for molecular translocation through membranes that are critical for emerging biotechnologies. We also plan to apply our approach to robust solid-state nanopores, created with silicon micromachining techniques.

We demonstrated important biophysical capabilities that will continue to be important for biotechnology at Sandia.

We demonstrated important biophysical capabilities that will continue to be important for biotechnology at Sandia. We demonstrated the ability to create stable, free-standing lipid-bilayer membranes and to measure ion currents through a single active protein channel in that membrane. We demonstrated the ability to detect the translocation of individual single-stranded DNA molecules through that membrane pore. We acquired atomic-force microscope (AFM) images of proteins in membranes under fluid conditions with a molecular resolution (± 1 nm). We demonstrated our ability to manipulate and acquire force curves for individual biomolecules. Finally, we developed a new technique to make 2–5 nm solid-state pores, and we are very close to testing them in the ion-channel apparatus.

Once we establish a good procedure for incorporating protein pores onto supported membranes, we will be prepared to begin the following: (1) single-molecule force studies of

translocation with single-channel ion pores, (2) correlation of single-channel ion current with translocation forces, and (3) observation of pore/membrane movement with fluorescence and scanning probes.

26582

Efficient Massively Parallel Techniques for Protein Structure Generation

M. D. Rintoul, M. G. Martin, M. P. Sears

This project focused on providing a comprehensive suite of massively parallel (MP) algorithms for determining protein structure given a minimum amount of experimental information. Early in the project, Sandia worked on building efficient algorithms for crude candidate structures from data obtained by such means as nuclear magnetic resonance (NMR) and cross-linking mass-spectrometry (MS) experiments. This work included studying the effect of the imprecision on the number of structures and how one could most efficiently build these candidate structures. In conjunction with this work, we have begun to investigate the most promising molecular physics techniques that could be used to then refine the candidate structures and find the minimum-energy configuration associated with the specific topology of the candidate structures. Early on, this focused primarily on studying the required force fields and potential general techniques that would accomplish this best in a parallel manner. Since then, we have focused on developing a parallel tempering algorithm that is based on an existing Sandia molecular dynamics code (LAMMPS [Large-Scale Atomic/Molecular Massively Parallel Simulator]). Future work will focus on real-world application of the codes developed earlier and applying them to problems of interest at Sandia. This includes energy minimization of proteins within a membrane and related to computer design of drugs needed to defend soldiers against chemical weapons (CW).

The primary focus of our work was to investigate the most promising methods of finding a minimum-energy conformation of a protein using an MP simulation. The reason for this focus is that previous work was directed primarily at obtaining candidate structures based on experimentally, and perhaps theoretically, determined distance constraints. The work with distance constraints on this project was largely successful, and the next logical step is to create a method by which the structure or set of structures that fit specific distance constraints can be energetically minimized.

The energy-minimization calculation is inherently a molecular physics calculation of some sort, and we must consider some means of calculating the energies at the molecular level in all but the crudest calculations. There are a number of different techniques for doing the energy

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minimization, including molecular dynamics (MD), Monte Carlo (MC), and density-functional theory (DFT). We investigated the literature, spoke with local experts in all of these areas, and finally decided to implement a relatively new hybrid method known as *parallel tempering* or *replica-exchange*.

Parallel tempering solves the problem of exploring a complex energy landscape by creating multiple copies of a specific configuration and evolving them simultaneously at different temperatures. The configurations in each box are evolved by any of the energetic methods mentioned previously. Then, periodically, a special type of MC move is performed where two boxes are chosen at random, and the energy difference after swapping the two configurations between different temperature boxes is calculated. The move is either accepted or rejected, based on a typical MC technique such as Metropolis sampling.

This technique has become very popular over the last couple of years for two reasons. As discussed previously, it is a very clever way of searching the configurational space for minimum-energy configurations. But perhaps more importantly, the algorithm is very easily adapted for MP computing. The individual “replicas” that are held at specific temperatures can be distributed among different processors. The amount of communication between the different processors is practically negligible if each box is limited to an individual processor.

Our work focused on adapting LAMMPS, a longtime workhorse MD code for Sandia, as the core of a new parallel tempering code. An advantage for using LAMMPS is that we are using a code that already is very efficiently parallelized. Our ability not only to parallelize across replicas, but also to parallelize the replicas themselves, gives us a significant advantage over the codes that can only be parallelized across replicas. We have begun this initial implementation and anticipate completing it soon.

Molecular physics simulation work is nearing completion. There was also a goal of understanding the role that imprecise distance constraints played in reconstruction of protein structures. We developed a mathematical model of how the effect of imprecision on distance constraints affected the number of potential structures that solved the distance constraints.

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26583

Mapping Membrane Protein Interactions in Cell-Signaling Systems

M. M. Young, S. A. Datwyler, J. M. Faulon, C. B. Troup, R. Behrens, Jr., J. S. Schoeniger, A. K. Singh, R. B. Jacobsen, G. H. Kruppa, M. J. Ayson, J. Hong

Sandia will develop and apply a novel high-throughput experimental and computational technique to map the self-organization of membrane protein (MP) complexes. The cell membrane is the interface between the external world and the machinery of life. The thirty percent of proteins that are MPs regulate the flow of information into and out of the cell through signaling cascades that stimulate cellular responses. Signaling cascades depend on the molecular details of specific MP-protein interactions. Little is known about these critically important complexes because standard structure-determination techniques (x-ray crystallography and nuclear magnetic resonance [NMR]) can rarely be applied to characterizing protein-protein interactions within the membrane.

Recently, a technique called MS3D (tandem MS/MS [mass spectroscopy/mass spectrometry method]) was validated for low-resolution structure determination of soluble proteins. We will adapt the MS3D technique to determine the structures of MP complexes, specifically the structure of the rhodopsin-transducin complex (RTC). The RTC is a particularly suitable test case for structure-function studies, as large quantities of protein and several high-resolution crystal structures of both rhodopsin and transducin are available. However, the structure of the RTC is still unknown. We will obtain experimentally derived distance constraints from this complex using molecular cross-linking, proteolysis, and MS. We will then use the distance constraints, in conjunction with genomics, proteomics, and structural information derived for rhodopsin and transducin, to solve the structure of the complex. The solution of the RTC structure will represent a major scientific advance and will address a major challenge in the post-genomic era, which is to understand how the tens of thousands of gene products (proteins) encoded by the genome interact with each other to perform essential cellular functions.

Sandia made significant progress during the past year in extending the initial work on bacteriorhodopsin (BR) to rhodopsin. The accomplishments can be divided into experimental progress, which has primarily focused on the adaptation of the MS3D technique to rhodopsin, and

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computational progress, in the areas of experimental design, data analysis, and protein-structure modeling.

- *Experimental progress*

- *Protein purification.* We successfully purified all components of the RTC from bovine retinas. We isolated the rod outer-segment membrane (ROS) from the retina by homogenization, followed by separation on a sucrose density gradient. Rhodopsin represents > 95% of ROS protein after a series of washes performed in the dark removes soluble and membrane-associated proteins. Transducin, which consists of three subunits (*a*, *b*, and *g*), was purified by light-induced binding to rhodopsin in the ROS, followed by elution with guanosine triphosphate (GTP), which causes the RTC to dissociate. We separated the individual subunits into *a* and *bg* fractions by column chromatography.

- *Separation of monomeric rhodopsin following cross-linking.* After cross-linking of rhodopsin in ROS and reduction/alkylation of cysteine residues using tris(2-carboxyethyl) phosphine (TCEP)/4-vinylpyridine, we separated monomeric protein from multimeric cross-linked products using preparative gel electrophoresis. Protein was loaded onto an 11% acrylamide gel and eluted in a sodium dodecyl sulfate (SDS) running buffer. We collected fractions and checked them for protein using analytical gels. Recovery of monomeric protein was as high as 90%. We pooled the monomer-containing fractions and removed SDS by extraction in chloroform:methanol:water (1:2:2).

- *Functional assay of RTC.* We prepared an assay to determine whether we have functional RTC. The assay consists of (1) mixing purified transducin with light-exposed ROS, (2) washing off the unbound transducin, (3) eluting the bound transducin with GTP, and (4) running a gel on the eluted transducin. We determined that purified transducin binds rhodopsin in a light-dependent manner and can be GTP-eluted, indicating that the purified proteins are functional.

- *CNBr digestion of rhodopsin.* We developed CNBr digestion conditions for rhodopsin. Fourier-transform ion cyclotron resonance–mass spectroscopy (FT/ICR–MS) of the resulting proteolytic fraction shows 89% sequence coverage. The missing N-terminal fragment has two N-glycosylation sites, making its mass difficult to predict, and has not yet been identified in the MS spectra of CNBr digests.

- *BS3–cross-linked rhodopsin.* We cross-linked rhodopsin with the homobifunctional amine-specific reagent BS3 and the heterobifunctional amine/carboxylic acid-specific reagent EDC. We are in the process of optimizing the stoichiometry of these

We successfully purified all components of the RTC from bovine retinas. We isolated the rod outer-segment membrane (ROS) from the retina by homogenization, followed by separation on a sucrose density gradient.

reactions and have already identified one BS3-labeled peptide in monomeric rhodopsin.

- *Computational progress*

- *Data reduction.* We developed a macro program to be used within the XMASS MS spectrum-analysis program. The macro automatically processes spectra acquired from liquid chromatography/MS (LC/MS) or direct-infusion MS experiments and picks monoisotopic peaks for further analysis.

- *MS spectrum assignment.* We developed a new version of the spectrum assignment program, ASAP, to process the output files from the macro program. Improvements to ASAP over the past year consist of (1) an option to output the entire theoretical list of cross-linked species, (2) support for multiple proteases, (3) protease-specific missed cleavage sites, and (4) an option to force a global amino-acid modification.

- *Simulated annealing transmembrane domain builder.* An MC/SA transmembrane domain builder program is currently under development. The program supports distance constraint-based structure modeling at the backbone level. Additional work is required to validate and refine the scoring function and to incorporate other experimental constraint types.

- *Light-adapted rhodopsin model.* We constructed a backbone-level model of the light-adapted rhodopsin structure using the known dark-adapted structure as a starting point. The seven transmembrane helices from the dark-adapted structure 1f88 and the all-trans form of the rhodopsin chromophore, retinal, were represented as rigid objects in a distance geometry (DG) calculation. We included 24 distance constraints in the DG calculation, along with additional constraints imposed by the topology of the rhodopsin structure. The resulting light-adapted structure is consistent with the helical movements proposed in the literature.

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32574

High-Throughput Instruments, Methods, and Informatics for Systems Biology

D. M. Haaland, J. A. Timlin, M. B. Sinclair, K. W. Boyack, W. C. Sweatt, B. N. Wylie, S. B. Martin

Cell scientists, medical researchers, and security organizations working on biothreat assessments require deeper understanding of cellular mechanisms. Better instruments, informatics, and knowledge-management methods are essential tools in this search for mechanism. The needs are especially critical when working with the new high-throughput technologies, including gene and protein expression arrays. In this project, Sandia will research both instrumentation and algorithms that directly address improved data collection and new analysis techniques suitable for dealing with such large datasets, and the tools for integration with other Web-accessible databases and literature. Current microarray technology allows only binary comparisons between the expression levels in control and treated cells in each experiment. Also, quantitative comparisons between microarray experiments are poor, thus limiting the information that can be gleaned from complex events. With the new scanner and the collaborative analysis tools developed in the project, we can investigate a variety of opportunities, such as the development of new biologically based biosensors for bioagents, protein detection, and understanding the genetic basis of cancer and its treatment.

After experiments with a hyperspectral spectrometer converted to microarray scanner yielded useful initial results, we designed, built, and tested a new hyperspectral scanner optimized for microarray experiments. We developed methods for preprocessing the data to remove curvature in the image that distorts the spectral image and to correct for nonuniform laser-line illumination. A critical finding of this new scanner was the presence of impurity emissions in commercial and in-house-printed microarrays. Commercial microarray scanners confuse this impurity emission with the emission of their labeled green fluorophore. This discovery has important implications for microarray research since the impurity emission is spatially located within the printed deoxyribonucleic acid (DNA) spots and is highly variable from spot to spot. Thus, commercial scanners are not able to compensate for the impurity emission. We used our new multivariate-curve resolution (MCR) algorithms to discover the pure spectrum of each emission source and to obtain quantitative image maps of each emitting

With the new scanner and the collaborative analysis tools developed in the project, we can investigate a variety of opportunities, such as the development of new biologically based biosensors for bioagents, protein detection, and understanding the genetic basis of cancer and its treatment.

species. We demonstrated improved gene expression accuracy with the new scanner in the presence of the impurity. In addition, we demonstrated the ability of the scanner to quantitate five emission sources simultaneously. These results confirm that the new scanner can operate in a much higher throughput mode than possible with commercial scanners. We also collaborated with biologists to perform designed experiments that identify and minimize sources of experimental error in the microarray experimental procedures. These experiments demonstrated that the major error was due to poor mixing of the solution with the array during the hybridization step. This investigation led to improvements in the hybridization geometry to greatly reduce this source of error. We also designed a new prism-based imaging spectrometer that should yield increased optical throughput and improved image quality. Finally, we contributed to the multivariate analysis of microarray data from our university collaborators to better understand the quality of the data and to achieve supervised classification of the microarray data from many microarrays.

In the bioinformatics portion of the research, we now (1) use robust nonparametric normalizations and robust nonparametric correlations for array data, (2) exchange data with multiple outside institutions, and (3) can simultaneously and automatically operate several tools in a coordinated fashion for data analysis. We found that parallel database servers are not yet required for the scale of these data and that naive use of natural language tools does not yield the text understanding that we require. We contacted computational linguists and expect to be able to make significant advances in upcoming work. Importantly, we worked closely with the University of New Mexico Medical School and made great progress by addressing actual problems; specifically, we have new statistical methods to detect important genes in cancer and a powerful database query and visualization research environment. We published in two leading journals, *Science* and *Genome Research*, and expect to publish important results concerning leukemia soon.

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Biomimetic Chloroplasts: An Integrated Microdevice Power Source

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Self-assembled, self-organized materials can provide mesoscale power sources for integrated microelectronic and microelectromechanical systems (MEMS) applications. A biomimetic chloroplast would use light energy to produce a gas or liquid for use as a fuel or chemical feed. For example, hydrogen (H) could be generated and stored on-chip for electrical power via an integrated fuel-cell component. A chloroplast is the biological structure that converts light energy to storable fuel for a living cell. Sandia plans to use chlorophyll-like molecules to harvest photons and direct the light energy to a reaction center for the photosynthesis of high-energy fuel molecules. Light energy will be converted by the biomimetic chloroplast component into a storable high-free-energy chemical, which could be used in the dark and replenished when the chip is again under illumination. The fuel or feedstock could be supplied as needed to a catalytic microreactor on demand. We are developing the photochemistry and catalysts required for producing H (the biomimetic photosynthetic reaction center) and also the self-assembling components of a light-harvesting apparatus required for a small, efficient, integrated power source. Self-assembled metal porphyrins form the integrated light-harvesting complex and reaction center; these are being self-organized and compartmentalized in porous silica nanocomposites and micellar nanoassemblies, along with platinum (Pt)-nanoparticle catalysts for generation of molecular H. The nanostructured silica and platinized liposomal environments permit access by small electron donors, acceptors, and water through small pores while maintaining microscale compartmentalization and organization of the functional molecular components.

We completed the following tasks: (1) demonstration of direct electron transfer from the tin (Sn) porphyrin to the hydrogenase and Pt catalysts under illumination by visible light in aqueous solution, (2) Sn-porphyrin photomediated H generation by Pt nanostructures, (3) incorporation of Sn porphyrin into pores of silica films and selective removal of the detergent templating molecules, (4) formation of Pt nanoparticles within the pores of silica films using photocatalysis, (5) growth of shells of Pt nanocrystals on the surface of micelles of sodium dodecylsulfate and Brij surfactants that contain the active Sn-porphyrin photocatalyst,

Platinized micelle nanoassembly.

Sandia plans to use chlorophyll-like molecules to harvest photons and direct the light energy to a reaction center for the photosynthesis of high-energy fuel molecules. Light energy will be converted by the biomimetic chloroplast component into a storable high-free-energy chemical, which could be used in the dark and replenished when the chip is again under illumination.

(6) selection of porphyrins for construction of light-harvesting arrays, and (7) assembly of rudimentary light-harvesting arrays. We completed the tasks using the platinized micellar nanoassemblies, except for the incorporation of true light-harvesting functionality. We altered this task because of the important discovery of the ability to fabricate platinized micellar nanoassemblies, i.e., micelles that contain the photocatalytic Sn porphyrin and that are coated with 3 nm Pt metal nanocrystals. The Pt nanocrystals on the micellar surface are joined to make the shell of nanoparticles a single crystal that is porous and resistant to mechanical stresses. These platinized micellar nanoassemblies efficiently photosynthesize H₂ from water by using the photocatalytic porphyrin to supply strongly reducing electrons to the Pt metal shell, which then catalyzes the reduction of water to H₂. These amazing nanoassemblies offer new and enhanced properties that should simplify the remaining tasks of incorporation of light-harvesting arrays. They also make possible our ultimate goal of producing a true biomimetic chloroplast by formation of a proton gradient across the bilayer membrane of a liposome containing the photocatalytic porphyrin within the bilayer. The light-harvesting array can be fabricated within the bilayer or in the interior of the liposome.

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38609

Physical and Electronic Changes Caused by Membrane Signaling as a Transduction Pathway in Affinity-Based Biosensors

S. M. Brozik, R. C. Hughes, P. Esherrick, G. D. Bachand

Despite decades of intensive research in the field of trans-membrane protein function, there is little understanding of the structure-function relationship at the atomic level. This is due to the difficulty of producing sufficient quantities of purified protein for crystallographic studies. To date, only a few integral membrane proteins (MPs) have been resolved at atomic detail. Single-molecule spectroscopic measurements, in combination with electrical detection of ion flux, offer an alternative method for obtaining structural and functional information on MPs. Sandia's goal is to develop tools that allow simultaneous optical and electrical measurements at the single-molecule level. In the past couple of years, the potential of combined optical and electrochemical measurements applied toward understanding the dynamics of single-ion channels has been realized, as illustrated by the recent surge of work on the Shaker potassium (K) channel. This project explores the development of unique experimental and computational capabilities for detailing structural and functional information of ligand-gated channels, specifically, the serotonin type-3 (5-HT₃) receptor. As we build Sandia's suite of experimental tools, we will use gramicidin as a model system since the helical structure of this peptide has been established and the mechanism of gating through dimerization is generally agreed upon. If we can optically detect dimerization at the single-molecule level and make this coincide with a change in ion flux, we can then begin to apply these capabilities toward understanding the 5-HT₃ receptor, a more complicated system. We will also apply molecular modeling tools to elucidate the mechanism of ion conductance at the atomic level and understand protein lipid interactions. We can then apply our findings to design appropriate mutant receptors for site-specific fluorescent labeling to verify experimentally the structural requirements needed for ion flux.

Our milestones were aimed at making separate electrochemical measurements in response to agonist binding and fluorescence energy-transfer technique (FRET) between donor- and acceptor-labeled receptor and agonist. This would then lead to combined electrochemical and single-molecule spectroscopic measurements of an ion-channel system. We set up the experimental system to take such measurements.

Sandia's goal is to develop tools that allow simultaneous optical and electrical measurements at the single-molecule level. ...This project explores the development of unique experimental and computational capabilities for detailing structural and functional information of ligand-gated channels, specifically, the serotonin type-3 (5-HT₃) receptor.

Specifically, we developed two separate single-molecule apparatuses to address our goals. The first is a Sandia/University of New Mexico (UNM)-built single-channel confocal microscope for the measurement of fast kinetic events ($\sim 100 \mu\text{s}$). The second apparatus is a single-molecule imaging microscope. We purchased a patch-clamp amplifier that will be interfaced eventually with the spectroscopic tools. We showed that we can successfully measure fluorescence of a single-probe molecule with our setup and measure single-channel electrochemical events. We are using fluorescent-labeled gramicidin as a model channel system to calibrate our experimental setup. We successfully synthesized two pairs of labeled gramicidin derivatives for the optical and electrical single-molecule studies. We obtained complementary deoxyribonucleic acid (cDNA) of a ligand-gated channel protein; specifically, UNM supplied 5-HT₃ receptor cDNA in the pCDM6x1 plasmid. Transformations of *E. coli* cells with plasmid DNA are being carried out by the method of Maniatis *et al.* We are also working on a mammalian expression system, specifically over expression and purification of the protein in hamster embryonic kidney cells. Currently we are establishing a viable expression system. Sandia will conduct the fast kinetic experiments of channel gating. UNM will conduct complementary experiments, including the use of FRET to monitor structural changes of the ion channel that either increase or decrease the distance between donor and acceptor, and single-molecule fluorescence anisotropy, which will be used to measure the changing polarization direction of an emitting fluorophore and can be used to determine torsional (twisting) motion of the 5-HT₃ receptor. Finally, we note that in a separate project, molecular-theory codes were successfully applied to treat ion-channel transport through the gramicidin A channel. Those calculations provided detailed information on the structural features of gramicidin that control the transport process. They also provided a quantitative estimate for energy barriers encountered by an ion traversing the channel. We will continue to apply molecular-modeling tools to gain insight into mechanisms behind ion transport through channel proteins.

We are using fluorescent-labeled gramicidin as a model channel system to calibrate our experimental setup. We successfully synthesized two pairs of labeled gramicidin derivatives for the optical and electrical single-molecule studies.

53340

Rapid Syndrome Validation Project (RSVP) Hypothesis Testing and Development

A. P. Zelicoff, S. A. Caskey

The U.S. is in a vulnerable position and its population at significant risk in the event that an unusual or dangerous disease emerges. The Rapid Syndrome Validation Project (RSVP) System is designed to lessen the consequences of an outbreak of an infectious disease by providing early detection. RSVP 2.0 software is ready for hypothesis testing and the inclusion of more-advanced detection algorithms.

To provide the confidence needed to validate the detection capabilities of RSVP, it is important that we conduct controlled hypothesis and concordance testing. Development of neural networks is also needed to improve the system's capability for early recognition of disease outbreaks based on the reported clusters of syndromes. This proposed effort will provide data essential to statistically testing several hypotheses and to assess the application's effectiveness and supportability.

As a biological early-warning system, RSVP would cue epidemiologists that something unusual is occurring in the community and cause early medical and protective responses. The neural network algorithms will enhance the system's ability for earlier recognition of "signals" and "early clusters" from the noise of routine illness in a particular population area.

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The RSVP made the following accomplishments:

(1) In this project, Sandia made moderate progress in developing a comprehensive beta-test program and identifying clinics that will participate in the beta-test. This project supported the installation and operational setup of six beta sites/clinics in the Lubbock, Texas, area with the Texas Regional Department of Health #5, and three sites in San Mateo, California. We also have commitments to install 22 more sites in New Mexico and ~ 40 more sites in Texas.

(2) We collaborated with Sandia specialists to determine the feasibility of adapting space-time cluster-analysis algorithms to the assessment of statistically significant clusters of syndrome reports in a geographic area. The data feeds from RSVP are compatible with the variables required for this analysis and include zip code centroid for the analysis, data history for syndromes by zip code, and a selectable range (distance) for the analysis to cover. This analysis technique and the associated animated display of information at one-day intervals will add an important new dimension to identifying disease outbreaks at the

earliest possible time. Preliminary analysis indicates that space-time cluster techniques will provide an additional 21–28 days of advanced notice on the outbreaks of infectious diseases like influenza. We will incorporate space-time cluster techniques into the RSVP software as soon as possible.

(3) We purchased and installed critical ARC/IMS and ARC/SDE software, which has accelerated the map query and response times for the system.

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Computational and Information Sciences

The goal of the Computational and Information Sciences investment area is to develop next-generation computing and information systems capabilities that will provide a strategic benefit to the nuclear weapons program and other important Sandia business areas. Recent advances in massively parallel computing technology are greatly expanding the usefulness of computer simulations. Computational and information sciences proposals focus on system software for computer clusters, emergent behavior, adaptive software, and parallel input/output (I/O) visualization. A theme of these efforts is manipulating and interacting with large datasets. Another important aspect of this work is creating technologies that make high-performance computers easier to use and thus broaden the impact of such computing on Sandia's programs.

The “Large-Scale Nonlinear Optimization Arising from PDE Models” project has made significant progress toward the implementation of successive quadratic programming algorithms, which will significantly reduce the computational requirements for large-scale applications. The parallel optimization methods that are being developed will solve high-fidelity, coupled-physics problems that are too expensive to solve with existing

optimization capabilities. Collaboration with academia was developed through the Computer Systems Research Institute (CSRI) to study large-scale transient PDE (partial differential equation)-constrained simulation. Two patent applications have been filed as a result of this effort.

10728

Algorithmic Advances in Computational Structural Biology

R. D. Carr, W. E. Hart, A. M. Johnston, M. J. Collins

The quantitative comparison of protein structures is a fundamental problem of computational biology. A “contact map” is a discrete representation of a protein folded in three dimensions. The maximum contact map overlap (CMO) problem is a combinatorial optimization problem that has been proposed as a measure of similarity between such structures. The goal of CMO is to find the largest substructure common to two given contact maps. This problem is known to be nondeterministic polynomial (NP)-complete. Sandia developed several computational approaches to CMO, based on linear programming (LP) and genetic algorithms (GAs). We analyzed our results on various proteins from the protein data bank (PDB). We also derived some mathematical results arising from these algorithms; these results cover numerical stability of the algorithms, relationships among the different methods, and efficient proofs that computations are correct.

We investigated a variety of computational approaches to the protein CMO problem, our measure of protein structure similarity. We implemented these algorithms and investigated some theoretical issues.

Using the AMPL (A Mathematical Programming Language) modeling language, we developed and tested an efficient, scalable realization of the CMO LP.

We developed powerful heuristics for obtaining both upper and lower bounds for CMO, including GAs (for lower bounds), Lagrangian relaxation (for lower and upper bounds), and local search. Lagrangian relaxation appears to be the best computational approach for large proteins.

Using these methods, we scored the structure similarity of many protein pairs of real biological interest.

We investigated issues of numerical stability and analyzed the sensitivity of our LP formulation to round off errors resulting from finite-precision arithmetic. In addition to obtaining bounds on these errors, we developed a procedure for transforming an almost-feasible solution (infeasible due to round-off error) into a truly feasible solution, changing the objective as little as possible.

We developed “implicit modeling,” a new method for solving a very large LP by transforming it into one with far fewer variables; the transformed problems can often be solved

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by efficient combinatorial algorithms. We showed that implicit modeling is essentially dual to Lagrangian relaxation and investigated the theoretical and computational consequences of this duality. We implemented implicit modeling for CMO.

We are continuing to develop efficiently checkable certificates that prove rigorously that a claimed solution truly is optimal or near optimal. These certificates are needed before we start the large amount of computation of clustering the PDB. We will launch this large-scale computation before submitting our final report.

Refereed

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10757

Large-Scale Nonlinear Optimization Arising from PDE Models

B. G. Van Bloemen Waanders, K. R. Long, P. T. Boggs, A. G. Salinger, R. A. Bartlett

This project will develop new parallel optimization methods for large-scale applications and use them to solve critical problems on Computational Plant (CPlant) and Accelerated Strategic Computing Initiative (ASCI) architectures. Sandia considers optimization problems with equality and inequality constraints defined by partial differential equation (PDE)–based simulation equations, which represent a wide range of design, control, and analysis applications. We will pursue the integration of three areas of research: (1) the coupling of the nonlinear simulation to the nonlinear optimization procedures, (2) the extension of powerful optimization techniques, and (3) the exploitation of parallelism in all aspects of this process.

We will explore several variants of the highly successful Sequential Quadratic Programming (SQP) methodology. Specifically, we will use reduced SQP (rSQP) and limited memory SQP to perform optimization with OLF, ALEGRA, and MPSalsa™. We will investigate various levels of coupling between the SQP methods and these simulation codes. This investigation will highlight the tradeoff between the level of coupling and the efficacy of the parallel optimization method. We will also extend current rSQP methods to handle nonlinear control and design constraints in addition to simulation constraints. Further, we will develop new Hessian approximations that employ low-fidelity Hessian evaluations combined with limited memory updates.

The results of this research effort will include a set of methods and techniques to apply modern optimization technologies to important design, control, and other Sandia applications. It will also result in recommendations on the development of advanced simulation codes to allow the tight coupling of these codes to optimization methods. Thus, this work will affect how large-scale optimization can best be integrated into frameworks such as SIERRA.

Large-scale PDE–constrained optimization (PDECO) comes in many forms, and the variety of algorithms and interfacing mechanisms presents a complex range of options for a heterogeneous simulation environment such as exists at Sandia. To achieve a general approach for simultaneous analysis and design (SAND) optimization for a large range of

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simulation codes is a lofty challenge because, by definition, SAND methods leverage the linear algebra of the simulation code, and therefore each interface needs to be custom-designed. This project addresses these interfacing problems through a variety of software tools and establishes a systematic nomenclature and approach for the consideration of SAND optimization.

Software is a major challenge in PDECO, and much of our work has been to develop software tools that will aid the exploration of research ideas in PDECO, provide guidance for future development of production-quality PDECO capability, and provide immediate PDECO capability for Sandia problems. We designed these tools from the start with PDECO and interoperability in mind. We developed the following:

- (1) A software framework (rSQP++) for solving reduced-space PDECO problems.
- (2) A software framework (Split/O3D) for solving full-space and inequality-constrained PDECO problems.
- (3) A PDE simulation component system (Sundance) that is capable of providing the additional operations required by the more strongly coupled levels of PDECO.
- (4) An interface between rSQP++ and an existing production PDE code, MPSalsa™.

We conducted numerical experiments to evaluate the different levels of optimization of PDECO. Coupling between the rSQP++ optimizer and a Sandia production code, MPSalsa™, resulted in an order-of-magnitude speedup relative to a black-box method. These experiments also gave us insight into the accuracy required in Jacobian calculations. We completed a survey of PDECO problems solved using rSQP++ and Sundance. Because of Sundance's very flexible nature, we were able to explore all levels of coupling for PDECO; as with MPSalsa™, going to the intrusive levels of optimization yields an order-of-magnitude speedup.

An interesting class of problems arose that we spent some time considering. In particular, it often occurs in applications that have more than one objective. The so-called *multi-objective optimization problem* has some special properties when the constraints are PDEs. Suppose, for example, one wants to drill a well into an aquifer to help prevent contaminants from entering a city water system. The primary objective is to reduce the contaminants in the system below a given threshold. Secondary objectives may include minimizing cost, minimizing the time to completion, and minimizing the amount of water taken out of the aquifer. There is no single way to handle the multi-objective problem, but building on work done in this area, we were able

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to show how a formulation called *hierarchical control*, which takes into account an ordering of the objectives, can yield solutions that are significantly smoother and thus more useful in many applications.

Refereed

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10777

Parallel Methods for Coupling Circuit- and Device-Scale Simulations

S. A. Hutchinson, E. R. Keiter

The focus of this project is to study coupling issues between parallel device and parallel circuit simulation. To that end, Sandia completed several tasks necessary for this type of work. The code used in this is the XYCETM parallel electronic simulator. Previously, we performed an initial study with a simple one-dimensional (1-D) device, in which we were able to use only one type of coupling between the circuit and device simulations. Recently, we implemented a much more sophisticated (2-D non-structured meshes) device-simulation capability within XYCETM. Additionally, we also implemented new options for coupling between the device and the circuit. One of the main goals of the project was to implement a two-level Newton scheme, in which for each Newton iteration of the circuit simulation we perform an inner-loop Newton solve on the device-simulation level. This two-level Newton scheme has been implemented within XYCETM and functions in both parallel and serial. We showed that this scheme is more robust for coupled circuit-device problems than the more obvious conventional Newton method.

The goal of this work was to investigate algorithms for coupling device- and circuit-level simulations. Circuit-level problems, which are based on a network of coupled ordinary differential equations (ODEs), and device-level problems, in which a single semiconductor device from a circuit is simulated on a mesh as a system of partial differential equations (PDEs), are very different numerical problems. The numerical approaches best suited for each type of problem are different on both the linear and nonlinear solver levels.

Generally, there are two methods used to solve a coupled problem. One is the “full Newton” method, in which both the circuit and device problems are solved simultaneously in the same Newton loop. This approach results in one Jacobian matrix per Newton iteration for the entire problem and preserves tight coupling between the two simulations, but is not very robust numerically. The other approach is referred to as the “two-level Newton” method, in which the circuit problem and device problem(s) have separate, but coupled, Newton solves. In this approach, each subproblem has its own Jacobian matrix and its own Newton loop. The circuit problem is the outer control loop for the entire problem. This approach typically

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does not maintain as tight a coupling between the two solvers but has better convergence properties.

We used the XYCE™ parallel circuit simulator, developed at Sandia, in this effort.

(1) *Implementation of a sophisticated device-simulation capability in XYCE™.* Previously, the PDE device simulator in XYCE™ could solve only 1-D problems, and these did not pose much difficulty to the linear or nonlinear solvers. We needed a larger capability (2-D) to challenge the various algorithms under study.

The new capability in XYCE™ allows for 2-D nonstructured device simulation. This allows simulation of a device with arbitrary geometry, an arbitrary number of electrodes, and an arbitrary 2-D doping profile. Additionally, multiple material types can be handled (including oxide layers); we added a displacement current calculation, which allows for simulation of metal-oxide semiconductor field-effect-transistor (MOSFET) structures.

(2) *Implementation of two-level Newton scheme in XYCE™ as an option for coupled device-circuit problems.* This required some ingenuity, as the original conception of the two-level Newton was fairly complex in its implementation. The two simulations were considered to be completely separate entities, with separate Jacobian matrices, separate data structures, etc. This type of approach is problematic, as it results in a loose link between the two codes. In fact, many problems of interest (single-event upset, for example) to Sandia involve very fast transients, and for that case, such an approach is not appropriate.

Fortunately, it was possible to implement two-level Newton in a manner that preserved tight coupling between the two simulations. In this approach, a single Jacobian matrix is constructed, in much the same manner as for the full Newton method. However, at different phases of the calculation, different sections of the linear system are “turned off.” For example, in a device phase of the calculation, the matrix rows associated with the circuit problem are essentially removed from the calculation by simply putting a “1” on the diagonal of those rows, and by putting a “0” into the corresponding residual vector location. The outer loop of the nonlinear solution method has the entire problem “turned on,” and we use this loop to determine if the overall problem has converged or not. Using such an approach allows maintenance of the tight coupling needed by fast transients, but has more robust convergence properties than the traditional “full Newton.”

The new capability in XYCE™ allows for 2-D nonstructured device simulation. This allows simulation of a device with arbitrary geometry, an arbitrary number of electrodes, and an arbitrary 2-D doping profile. Additionally, multiple material types can be handled (including oxide layers)....

(3) Development of a test-bed of circuit-device coupling problem for use in parameter studies.

(4) Comparison of conventional full Newton and the two-level Newton for a variety of problem types.

10778

A JAVA™-Based Tool for Multifidelity Modeling of Coupled Systems

D. R. Gardner, G. L. Hennigan, J. P. Castro, M. F. Young, M. A. Gonzales, E. S. Wong

Significant effort has been invested in developing high-fidelity models for nuclear weapon (NW) components, e.g., the neutron generator. However, comparatively little effort has been invested in developing computer-modeling tools to examine interactions among weapon subsystems. Computer tools for modeling complex subsystem interactions in an NW in varied environments and over a wide range of time scales (from nano-seconds to years) at multiple levels of fidelity can enable designers and safety analysts to perform their jobs “faster, better, and cheaper.”

Sandia developed a method for coupling models of differing spatial fidelities for thermal radiation. Specifically, we coupled a three-dimensional (3-D) finite-element model (FEM) of a component to a 0-D (lumped-parameter) system model for thermal-radiation problems. We compared temperatures predicted by this mixed-fidelity system model to those predicted by a full 3-D FE system model and a 0-D system model.

We encapsulated this mixed-fidelity method within a JAVA™-based framework. Users of the framework can select modules from a library, modify them, and connect them into a system. One of the modules may be represented by a 3-D FE module; the others are represented by 0-D models. In addition, users can loosely couple electrical circuit and thermal models. For example, a user can couple temperatures from a 3-D FEM of the arming, fuzing, and firing system (AF&F) to 0-D models for the remainder of the weapon and can model electrical-circuit functions in the AF&F.

We are currently working to use these methods and the software to couple neutron and electron/photon radiation models to electrical-circuit models, thus providing an enhanced capability to model systems of NW modules in abnormal environments.

The primary accomplishments of recent work were the refinement of the mixed-fidelity thermal-radiation algorithm, and the improvement of the JAVA™-based architecture to support multifidelity and multiphysics models in a more flexible and general way.

We refined the algorithm for linking a 3-D FEM of a system component to a 0-D (lumped-parameter) system model for thermal radiation. We assessed the performance of the

Prototype Entero GUI (thermal-electrical modeling).

The primary accomplishments of recent work were the refinement of the mixed-fidelity thermal-radiation algorithm, and the improvement of the JAVA™-based architecture to support multifidelity and multiphysics models in a more flexible and general way.

algorithm using three models for a prototype system consisting of an aero-shell enclosing an AF&F and two other modules. The three models were a 0-D system model, a mixed-fidelity system model, and a fully 3-D model.

In the 0-D system model, each component was represented by a 0-D model for temperature, i.e., each component had a single temperature.

In the mixed-fidelity system model, the AF&F was represented by a 3-D FE mesh. We used a modified version of the COYOTE heat-transfer code to calculate average temperatures for the mesh.

In the fully 3-D system model, each component was represented by an FE mesh.

The average temperatures predicted by the mixed-fidelity model more closely approximated those predicted by the 3-D system model than those predicted by the 0-D model and, in addition, provided internal temperatures for the AF&F. This is important because the functioning of a temperature-dependent circuit in the AF&F will depend on its location within the AF&F if the temperature varies with location. Temperature as a function of position can be predicted in the 3-D and mixed-fidelity system models, but not in the 0-D model.

For equivalent system models, the mixed-fidelity model ran more than 25 times faster than the 3-D model on a 1.2 GHz engineering workstation (under 3 minutes compared to more than an hour), indicating that optimization studies with mixed-fidelity models are feasible even though they may not be feasible with 3-D system models.

In summary, the mixed-fidelity model ran sufficiently fast with sufficient accuracy to enable design-optimization studies for coupled thermal/electrical modeling. Further studies to verify this conclusion are warranted.

We designed but did not test an extension of the algorithm to conductive heat transfer. The concept is to connect modules in a 1-D system with constructs called a “thermal wire.” Conduction occurs only along its length, and its cross-sectional area as a function of length is specified. This construct can be connected to a 3-D FE mesh using either the surface-average temperature or an average surface temperature for the area of contact.

We enhanced the JAVA™-based software architecture to incorporate the mixed-fidelity thermal algorithm and the multiphysics coupling in a more flexible and general way. The improved architecture is based on a software entity called a *module*. Some of the module types and their functionality are described here.

Improved Entero GUI (thermal-electrical modeling).

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- The Primitive Module provides characteristics and functionality based on the module's type and attributes. A Primitive Module may be extended to provide a more specialized functionality.
- The Composite Module provides containers for all other modules, including other Composite Modules, and represents how an engineer views a system. Modules may be added or removed dynamically from a Composite Module during the execution of the software.
- The Application Module is an extension of the Primitive Module that provides wrappers for external applications, such as COYOTE or the XYCETM parallel electronic-circuit simulator. It automatically adds any modules that the application requires.
- A Port Module provides the communication and data-transformation mechanism between modules. In particular, the multifidelity algorithm for thermal radiation is implemented in the software as a Port Module.

To demonstrate the software, we conducted a mixed-fidelity, coupled thermal-electrical simulation of the LM-185 voltage reference circuit embedded in the AF&F.

In work funded by the Computational Sciences Research Foundation (CSRF), we used the improved software architecture to couple XYCETM to the Neutron Gamma Energy Transport (NuGET) code to begin the development of a flexible environment for electrical designers to model the effects of radiation on circuits. We proposed additional work to extend this coupling, to include the Integrated TIGER Series photon-electron transport codes.

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26512

Parallel Atomistic Computing for Failure Analysis of Micromachines

P. M. Gullett, S. J. Plimpton, M. G. Martin, A. Slepoy

To quantify microstructure-property relations related to weapon microcomponents, Sandia is developing atomistic algorithms for parallel computers that quantify continuum quantities relevant to design and finite-element (FE) codes. With these and other serial computing tools, we are performing atomistic simulations of various sizes, geometries, materials, and boundary conditions (BCs). Currently, no capability exists that can handle the different size-scale effects required to predict failure. Nonlocal continuum models have been proposed to address this problem; however, they are phenomenological in nature and are difficult to validate for microscale components. Our goal is to separately quantify damage nucleation, growth, and coalescence mechanisms to provide a basis for macroscale continuum models that will be used for micromachine design. Because microcomponent experiments are difficult, a systematic computational study that employs Monte Carlo (MC) methods, molecular statics, and molecular dynamics (MD) (Embedded Atom Method [EAM] and Modified Embedded Atom Method [MEAM]) simulations to compute continuum quantities will provide mechanism-property relations associated with the following parameters: specimen size, number of grains, crystal orientation, strain rate, temperature, defect-nearest-neighbor distance, void/crack size, chemical state, and stress state. This will be the first foundational study to quantify size-scale effects from nanometers to micrometers in terms of damage progression and thus potentially allow for optimized micromachine designs that are more reliable and have higher fidelity in terms of strength. To accomplish this task, we must develop and evaluate several atomistic methods to cover the range of defects, strain rates, temperatures, and sizes that a material may see in micromachines. As such, we are providing a complete set of tools for large-scale atomistic simulations that include preprocessing of realistic material configurations, processing under different environments, and post-processing with appropriate continuum quantities. By running simulations with these tools, we are able to determine size-scale effects that correlate microstructure and defect configurations with mechanical properties of materials.

We developed some algorithms for preprocessing, processing, and post-processing for atomistic simulations, but

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have not completed the tool kit. For preprocessing, a code (PREWARP) developed at Johns Hopkins University can be used in a straightforward manner to vary crystal orientations, specimen sizes, defects, grains, and grain boundaries. We used PREWARP to construct meshes and grains with different sizes to evaluate plasticity of the nickel (Ni) (LIGA [the German term *Lithographie, Galvanoformung, und Abformung*, for lithography, electroforming, and molding] weapon material). For processing, we modified WARP, a parallel version of an EAM potential MD program, to account for multiaxial states of stress. We ran torsion simulations of Ni to compare with simple shear results from a previous project. For post-processing, we determined stress, strain, deformation gradient, and misorientation tensors for both the EAM and MEAM simulations. One critical result arose when comparing EAM and MEAM stresses. Near a defect that engenders anisotropy, the MEAM simulations generate an asymmetric stress tensor, whereas the EAM simulations generate a symmetric stress tensor. As the distance from the defect increases, the stress values converge for the MEAM and EAM results. The asymmetric stress near the defect is more physical, which implies that if one were to use EAM results near grain boundaries, the stress tensor would be incorrect. Therefore, we have just begun to parallelize MEAM with the post-processing quantities: stress, strain, deformation gradient, and misorientation tensor. We also examined four different BCs related to biaxial loading conditions to observe the phenomenological void growth response: one with periodic conditions and the other three with different finite BCs. The phenomenological void growth results are very similar regardless of the boundary type, which makes comparison to FE results convenient.

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Implementation of Fault Tolerance in Scientific Simulation Application Software

R. R. Drake, R. M. Summers

The ability for scientific simulation software to detect and recover from errors and failures of supporting hardware and software layers is becoming more important because of the pressure to shift from large, specialized, multimillion-dollar Accelerated Strategic Computing Initiative (ASCI) computing platforms to smaller, less-expensive interconnected machines consisting of off-the-shelf hardware. As evidenced by the CPlantTM experiences, fault tolerance (FT) can be necessary, even on such a homogeneous system, and may also prove useful in the next generation of ASCI platforms.

Sandia will study, implement, and test the feasibility of various FT mechanisms controlled at the simulation-code level. That is, errors and failures will be detected by underlying software layers, communicated to the application through a convenient interface, and then handled by the simulation code itself. Targeted faults include corrupt communication messages, processor node dropouts, and unacceptable slowdown of service from processing nodes. We will consider recovery techniques such as resending communication messages and dynamic reallocation of failing processor nodes.

The goal is to determine a practical solution to such faults and the ability to retrofit existing simulation codes. We will consider (visible) layers of communication under message-passing interface (MPI) that allow detection and adjustment of catastrophic failures like a node dropout. The local-area multicomputer (LAM) implementation of MPI is an example, providing dynamic process spawning, some level of FT, and standard support for many platforms and operating systems. Complementary to the MPI implementation will be a robust fault-detection and -delivery signal-handling interface that will provide to the application the ability to recognize and act on platform errors.

There are many layers associated with detecting and recovering from errors in the communications of a simulation code. The larger pieces are the MPI, the communication engine, and the parts of the operating system itself. This research taught us that all parts of this communication must be integrated to perform FT to be useful.

From the beginning, we focused on detecting and recovering from a lost compute node. The big issues are how to

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detect when node loss has occurred, how to synchronize all processes, spawn replacements, and then backtrack to a state saved off in some manner. With the current software available, the problem is the MPI layer. Although there is significant research in this area, we were frustrated by the lack of implementations of MPI that are close to providing production fault recovery of an error such as the loss of a compute node.

This created a bottleneck for the project because we cannot code to an interface that does not exist, much less test possible implementations of simulation-code-level FT. The signal-handling and synchronization code that we wrote earlier in the project cannot be extended to distributed processes without an underlying communication mechanism, which would not be portable because it is not standard.

The work we did on the LAM/MPI was a very good start to a difficult problem. Unfortunately, much work remains to produce a version of MPI that would support capabilities of FT of the form needed to recover from the loss of a compute node. The researchers thoroughly defined the issues involved with FT at different layers and described how an application might interface to an MPI implementation that had some FT capabilities, while still compiling and working with an MPI implementation that did not have FT. The paramount goal is to find an acceptable interface that can eventually be written into a standard.

We are a bit premature in developing an application to do FT at the simulation-code level. If applications do not ask for FT, the MPI and communication layer developers have no impetus to write FT code, but if there are no implementations of FT MPI implementations, then the application developers will not write code to take advantage.

We believe that significant progress has been made regarding understanding the issues involved and gathering interest and research power.

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26514

Smart-Sensor Technology for Joint Test Assembly Flights

K. D. Marx, D. A. Sheaffer, Jr., N. M. Berry, C. M. Pancerella, R. C. Armstrong, A. B. Doser, E. P. Parker, J. Dimkoff

The world relies on sensors to perform a variety of tasks from the mundane to the sophisticated. Currently, processors associated with these sensors are sufficient to handle only rudimentary logic tasks. Although multiple sensors are often present in such devices, there is insufficient processing power for situational understanding. Until recently, no processors that met the electrical-power constraints for embedded systems were powerful enough to perform sophisticated computations. Sandia performs many expensive tests using sensor arrays. Improving the efficacy, reliability, and information content resulting from these sensor arrays is of critical importance. With the advent of powerful commodity processors for embedded use, a new opportunity to do just that has presented itself.

We seek to bring the software and expertise gained from our work in commodity parallel computing to the general field of sensor technology and sensor arrays. As a result of this work, sensor-array tests of practical importance to Sandia will increase the amount of usable information derived from those tests by an order of magnitude while improving the believability of the data. While this work is applicable to the emerging vision of ubiquitous computing generally, we will focus on a system of importance to Sandia: Joint Test Assembly (JTA) for intercontinental ballistic missile (ICBM) warheads. This work will improve the fidelity of the transmitted data by increasing the information throughput of the telemetry using information-filtering and fault-detection algorithms that are borrowed from high-performance computing (HPC). The morphology of distributed-sensor arrays is close to the more familiar case of cluster computing and can benefit from our expertise and software already developed. Latency hiding, fault tolerance, and real-time distributed steering are all concepts previously absent from sensor technology that will dramatically increase the information content, fidelity, and believability of the resulting data.

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(1) We acquired a vibration shaker with signal generator and power amplifier to drive it.

(2) We mounted an aluminum bar on the shaker and instrumented it with two strain gauges, a pickup coil, and a temperature sensor.

(3) We designed and fabricated a signal-conditioning board to process and amplify the signals from the sensors. These constitute a simple electromechanical system, called the “JTA mockup,” which captures many of the features of hardware existing in JTA flights. The JTA mockup has proven to be invaluable in acquiring ground truth regarding the viability of this work for instrumentation development and, ultimately, for JTA flights.

(4) We are continuing the activities begun in earlier work. We set up a PC104 processor running the LINUX operating system as the smart-sensor central processing unit (CPU). We connected it to a data-acquisition board to implement analog/digital (A/D) conversion of signal data and to make the data available to decision-making software.

(5) We tested the JTA mockup and sensor system to understand their behavior under normal conditions and some abnormal conditions.

(6) Based on the test results, we revised and augmented the computer model that describes the behavior of the system.

(7) We wrote preliminary software to detect normal and abnormal behavior and to report back to observers.

(8) We designed and implemented a sensor framework component.

(9) We integrated the framework with other JTA software sensor components.

(10) We revised our preliminary design of the integrated intelligent agent smart-sensor architecture.

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26515

Multilevel Methods for Nonlinear Structural Mechanics

C. R. Dohrmann, M. W. Heinstein

Robust and scalable parallel algorithms for solving nonlinear partial differential equations (PDEs) are essential for Accelerated Strategic Computing Initiative (ASCI) modeling and simulation to have a significant impact on weapons programs at Sandia. Computational models with millions of unknowns are becoming commonplace in the engineering sciences. A major challenge with these models is to obtain solutions in reasonable amounts of time. For example, the critical time-step used in explicit transient dynamics decreases with mesh refinement and can increase runtimes significantly. Implicit dynamic formulations are not constrained by a critical time-step, but they do require the solution of large systems of equations.

We seek to complete our investigation of multilevel solver strategies and to implement select ones into general-purpose computational frameworks. In particular, we will make the multilevel solver work available to various applications through the TRILINOS solver framework being developed at Sandia. Access to TRILINOS and SIERRA applications will be made through the finite-element interface (FEI). In addition to our implementation plans, we hope to make further progress in the areas of solvers for indefinite systems of equations arising from mixed FE formulations of elasticity.

(1) *Improved a two-level preconditioner developed previously.* We recently demonstrated the effectiveness of the preconditioner on ASCI Red with up to 512 processors. We applied the code to an elasticity problem recently used to demonstrate the parallel scalability of the finite-element tearing and interconnecting/dual primal (FETI-DP) solver within the parallel structural dynamics code SALINAS. The code developed under this project could solve the same problems in less time and with fewer iterations than the FETI solver in SALINAS. We also made comparisons with Sandia's AZTEC iterative library for problems dealing with elasticity and conduction heat transfer. We observed that the number of iterations, solution times, and condition numbers remained nearly constant for the project preconditioner. The same was not true for the preconditioners considered in AZTEC, as evidenced by increasing numbers of iterations and solution times for larger problems. Results from other numerical studies indicated that

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condition numbers remain bounded independently of the number of subdomains and magnitudes of material-property jumps. We developed both serial and parallel versions of the preconditioner. The preconditioner is applicable to both elasticity problems and Poisson equation problems such as conduction heat transfer.

(2) *Extended a two-level preconditioner developed in previous work to a multilevel setting.* The preconditioner combines a node-coarsening strategy and the solution of constrained-energy minimization problems to obtain optimal performance. In particular, we observed that condition numbers remained nearly constant as problem size increased for problems in two and three dimensions. In addition, the performance of the preconditioner was not affected significantly by large material-property jumps in the problems. The multilevel preconditioner will be useful either as a stand-alone code or as an approximate solver within a two-level method like the one described above.

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Algorithmic Support for Commodity-Based Parallel Computing Systems

V. J. Leung, R. E. Riesen, C. A. Phillips, J. R. Johnston

Effective scheduling on commodity-based supercomputers like Computational Plant (CPlant) must account for factors that have not significantly impacted Sandia's Accelerated Strategic Computing Initiative (ASCI) Red machine: central processing unit (CPU) heterogeneity, bandwidth limitations, irregular interconnection topology, and reduced hardware reliability. Existing schedulers make strong assumptions about the uniformity of network connectivity and resource availability (e.g., node memory), and consequently these tools will not perform as well on more heterogeneous computing platforms.

Sandia seeks to develop efficient algorithms for managing resources in parallel computers, focusing on scheduling for processor allocation. This work will directly impact the utility of CPlant via improved batch and interactive schedulers. Additionally, our work will provide a characterization of the jobs that are run on CPlant and JANUS (e.g., communication load/pattern of network congestion), which is needed to make smart decisions for scheduling.

We will evaluate the performance characteristics of jobs running on CPlant and evaluate the throughput of the CPlant scheduler. Given this analysis, we will develop new schedulers for CPlant that improve the throughput of this machine, and, in particular, we will develop schedulers that exploit users' guidance to tailor the schedule to problem characteristics.

In earlier work, we found that contiguous node allocation resulted in the best performance for communications-intensive jobs. Shortest-path routes should give the best communication performance when CPlant nodes are allocated contiguously. However, the Myrinet router does not guarantee shortest-path routes. Based on our previous generalization of Dally and Seitz routing for Siberia, a three-dimensional (3-D) extension of our work provided shortest-path routes for Antarctica.

We then built an event-driven CPlant simulator, which tests allocation strategies. The objective of the simulator is to exhibit tendencies rather than to predict running times precisely. Our simulations suggest that 1-D allocation strategies coupled with space-filling curves yield processor locality in higher dimensions. The simulation results were sufficiently promising to justify implementing the allocation algorithms on CPlant.

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We performed a limited number of experiments on Zermatt. This pilot study demonstrates a proof of the concept that both careful 1-D ordering and allocation to preserve locality within this 1-D ordering improve system throughput. We implemented these new allocation strategies in the new release of the CPlant System Software, Version 2.0. We phased this version into the CPlant systems at Sandia.

Previously, we found that the CPlant scheduler will drain the machine when a job has been waiting for more than 24 hours. During the time that CPlant is being drained, many processors can go idle while jobs that can fit on the machine are waiting. To increase processor utilization and decrease job waiting times, we added backfill to the CPlant scheduler.

Refereed

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26517

Parallel Repartitioning for Optimal Solver Performance

K. D. Devine, M. A. Heroux, B. A. Hendrickson, E. G. Boman, R. T. Heaphy

The partitioning of data and work for distributed-memory solver packages is typically established by the application that calls the solver. However, the best distribution of data for the application is often not best for the solver. Overlapping Schwarz preconditioners, for example, may have very unbalanced workloads, due to work required in the overlap regions, even if the data distribution is balanced for other phases of the solver computation. Robustness and performance of linear solvers can be greatly improved by developing partitioning strategies that are optimized for preconditioners and solvers.

By combining the parallel data redistribution tools in ZOLTAN with state-of-the-art preconditioning and linear-solver technology in TRILINOS, Sandia seeks to develop partitioning strategies that enable improved performance and robustness for preconditioners and solvers. This project focused on the following tasks:

- (1) Incorporate ZOLTAN into the TRILINOS framework.*
- (2) Develop meaningful cost functions that give good parallel data redistribution for solvers.*
- (3) Develop the algorithmic theory and implementation that allow us to compute data distributions with the best properties for preconditioners and, specifically, overlapping Schwarz preconditioners.*

We made significant progress toward developing repartitioning strategies for optimal solver performance. We improved our ZOLTAN-TRILINOS coupling to allow greater flexibility, utility, and performance in both libraries. In TRILINOS, parallel redistribution capabilities were made available to all TRILINOS data objects. Development of an abstract redistribution class in Epetra was key to this extension; the redistribution class provides all TRILINOS objects with methods for importing and exporting objects. In ZOLTAN, we implemented a distributed-data directory tool that simplifies location of off-processor data after redistribution. The directory is scalable in both memory and performance; look-ups of off-processor data can be done with $O(1)$ communication costs.

We developed cost functions that should lead to more effective graph-based decompositions for preconditioning. Assuming that a problem is modeled as a graph, graph

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partitioners balance nodal weight while attempting to minimize the weight of edges cut by subdomain boundaries. Our cost functions incorporate information from the application into the edge weights so that partitions can be generated that, for example, follow the streamlines of a fluid-flow simulation. Such subdomains have greatly improved properties for preconditioners, allowing greater robustness and effectiveness.

We continue work on multiconstraint partitioning, which should allow generation of a single partition that is effective for both the preconditioner and the solver. We began new work on hypergraph partitioning, which provides more accurate communication-cost models than graph partitioning and allows partitioning of nonsymmetric and rectangular systems. We also continue our parallelization of the iterative improvement partitioning strategy for overlapping preconditioners for which we obtained promising results (in serial) last year.

Refereed

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Graduated Embodiment for Sophisticated Agent Evolution and Optimization

M. B. E. Boslough, P. G. Xavier, R. J. Pryor, F. J. Oppel, III, M. J. McDonald, C. E. Lippitt

Many problems in intelligent systems can be approached using evolutionary methods, but require thousands of generations of thousands of individual entities to evolve desirable solutions, and the simulation cost to evaluate every individual is high. This severely limits the ability of evolutionary methods to find high-fidelity solutions, even on massively parallel (MP) computers.

Sandia is attempting to avoid this limitation by developing methods for graduated evolution and fitness testing for embodied agent optimization. Our concept is to evolve agent behaviors in a hierarchical fashion by staging fitness evaluation through multiple levels of fidelity. Behaviors evolve through progressively higher-fidelity worlds, up to and including those with real robots and humans in real environments.

We started with low-fidelity simulation environments to separately evolve behavior strategies along a hierarchy and will combine and test evolved behaviors in increasingly higher-fidelity environments. We are using the UMBRA simulation environment for its heterogeneous fidelity simulation capabilities and are creating and optimizing behaviors using various evolutionary methods on the Computational Plant (CPlant).

We will now utilize simulation and genetic-programming tools that we developed previously to generate new graduated evolutionary algorithms for various applications. We will expand upon the evolutionary programming methods that we developed for generating flight-control algorithms with two main problems. The first will be to develop high- and low-level behaviors for flying robots. A particular focus will be on soaring, but other behavior components will also be considered. The second will be in cooperative algorithms. We will combine these two problems to develop swarming robots that harvest their energy from atmospheric turbulence and realistic time-dependent wind fields.

Work progressed along two fronts: (1) development of a modeling and simulation environment based primarily on UMBRA, the Sandia framework for development, analysis, experimentation, and control of systems and networks of intelligent machines, and (2) development of genetic-programming methods that can be integrated into the UMBRA

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modeling and simulation framework to provide behavior algorithms that are evolved within a high-performance MP computing environment using low-level building blocks that can be engineered and written by hand or evolved in an earlier stage of development.

We are using UMBRA to model devices and the environments within which they operate as embodied agents with fine- and coarse-grained physical effects models. UMBRA's low computational overhead provides efficient computer runs for modestly complex problems. Brain, sensor, and physical-state variables can be output at any time-step to monitor the instantaneous state of the vehicle. We developed a high-fidelity glider model with a six-degree-of-freedom (6 DOF) flight dynamics model and an engineered and hand-coded autopilot system. The terrain is from a model developed for the Army's Joint Virtual Battlespace. UMBRA has been used to simultaneously simulate hundreds of vehicles.

The overall architecture of the initial low-fidelity and high-fidelity UMBRA models can be generalized for any autonomous robotic behavior. A brain module captures the behavior algorithm that includes both a low-level autopilot program and a high-level goal-seeking behavior. This module provides a formal interface that can be reused in a variety of applications. It compiles and executes programs in the form of a decision tree that can be stored in an ASCII (American Standard Code for Information Exchange) file for platform independence. While the brain program was evolved using a genetic program on the CPlant, these programs can be hand-coded or evolved from hand-coded programs.

Physics modules contain the method for integrating from one physical state to the next. In the simplest low-fidelity model, it can be a simple stepping function to move an agent around on a discrete two-dimensional (2-D) grid with functions such as "turn right," "turn left," and "move ahead" that are returned from the brain module based on state variables stored in the registers. In the higher-fidelity model, the flight physics module executes a full flight dynamics equation for all 6 DOFs by integrating the equations of motion using real aerodynamic and mechanical coefficients.

Sensor modules simulate the function of transducers that allow the flight controller to determine the physical state of the vehicle. In the low-fidelity model, the sensor module outputs the state data that are directly input from the physics module, thereby modeling a vehicle with perfect situational awareness. In the higher-fidelity model, sensors are built in a way that includes noise, drift, calibration errors, and instrument failure.

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We also generalized a version of a genetic-programming tool. The data structure of the tree that contains the flight-control algorithm consists of multiple arrays that keep track of state variables (for flight simulation), calculated variables (for high-level situational awareness and decisions), calculated integers (for policy table flags), registers (genetically calculated values), and pointers (for multiple decision trees that depend on policy flags). Array dimensions are determined at compile time and depend on the evaluation function, the number of DOFs of the flight vehicle, and whether the flight space is discrete or continuous. By generalizing the genetic programming, behaviors for any environmental rules can be developed with the same code, from the most basic (4 DOFs, discrete space, simple flight rules, fixed lift zone) to the most advanced (6 DOFs, continuous space, full aerodynamics, turbulent boundary layer). We demonstrated the fastest convergence that approaches the best solution we have ever found for the benchmark problem.

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38611

Stochastic Programming for Enterprise Modeling—Optimization for Nondeterministic Simulation

P. D. Hough, M. M. Johnson, D. A. Jones, M. L. Martinez-Canales

In recent years, optimization has become an increasingly valuable tool for solving a wide range of problems in areas such as aerospace engineering, computational chemistry, environmental management, manufacturing, health care, transportation, and stockpile stewardship. In most of these applications, it is assumed that all information needed to formulate and solve the optimization problem of interest is known and that the final solution is not only optimal, but is also reliable in some sense. As a result, these problems are formulated and solved as deterministic problems.

With the continued growth in the use of computer modeling and simulation, treating the related optimization problems in a deterministic fashion has become inadequate. This is a direct result of the uncertainty that arises in the models that are used. In this situation, the question of how reliable the results of the simulation are becomes important. The response to these questions has been a growing effort to understand, quantify, and take into account the various uncertainties that arise in the computational models. To continue to be effective, optimization algorithms must follow suit.

The goals of this project are to develop robust and scalable optimization algorithms that will effectively solve mission-critical optimization problems in which uncertainty arises and to incorporate them into software tools that will enable analysts to make use of them. Sandia will base these algorithms on stochastic programming, which encompasses both the evaluation of functions defined by deterministic models with well-characterized sources of uncertainty and the evaluation of functions defined by stochastic models. The work is motivated by and will be demonstrated on two classes of applications: enterprise modeling and parameter identification.

We completed a survey of the literature in nonlinear stochastic programming and found a number of areas that require attention. In short, there is a lack of nonlinear optimization algorithms that take advantage of uncertainty quantification techniques (e.g., statistical analysis), and there is a corresponding absence of software that allows close cooperation between optimization algorithms and models of uncertainty. Examples of where such interaction is required

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include evaluating sufficient decrease requirements and evaluating stopping criteria. Based on our findings, we spelled out specific tasks that are intended to address these shortfalls in nonlinear stochastic programming.

We identified the Weapons of Mass Destruction Decision Analysis Center (WMD-DAC), a homeland defense initiative, as the enterprise modeling problem to which we will apply newly developed stochastic programming methods. WMD-DAC applications seek to provide tools to analysts that will allow them to make policy decisions in the event of a biological or chemical attack. The models used will be nonlinear and include random variables. We defined optimization problems that evaluate various scenarios of tradeoffs between costs and casualties. Modifications of the WMD-DAC system for use with optimization algorithms are nearly complete.

One aspect of uncertainty quantification is local sensitivity analysis. An obvious way for nonlinear optimization algorithms to take advantage of sensitivity analysis is in the computation of finite-difference (FD) gradients. Such computations are required when solving simulation-based problems, as analytic derivative information is usually unavailable. In collaboration with uncertainty quantification researchers, we developed an approach for making use of local sensitivity analysis (based on statistical sampling) in gradient-based optimization algorithms. When performed in the neighborhood of the solution, such analysis provided great benefit to a nonlinear interior-point method. In particular, it was able to run to completion on a parameter identification associated with an extreme ultraviolet lithography thermal analysis problem where it was previously unable to make progress.

Another aspect of uncertainty analysis is quantifying the variability in both the simulation and the data against which it is being calibrated. When solving a parameter identification problem, therefore, it is desirable to take these variabilities into account. We are in the process of evaluating the effectiveness of a variability measure, the Overlap Shortfall Index (OShI). We implemented an OShI-based objective function for some simple test problems to evaluate its effectiveness. Results indicate that while OShI measures the desired effect, improvements are required to make it a useful objective function for optimization. In particular, an appropriate normalization scheme must be incorporated.

Interactions with the computer code FUEGO development team revealed an opportunity to establish a working relationship with their model validation efforts.

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Robust Message Routing for Mobile (Wireless) Ad Hoc Networks

M. M. Johnson, H. Y. Chen, M. E. Goldsby, H. R. Ammerlahn, A. S. Yoshimura, B. P. Van Leeuwen

As nodes in mobile ad hoc networks come to be used as operational units, performing distributed computations under program control, it will be desirable to provide an effective programming model for them. Such mobile nodes communicate over an asynchronous wireless-communication channel, and communication protocols used for mobile ad hoc networks typically provide only best-effort message delivery. Protocols, such as Transmission Control Protocol (TCP), that provide reliable, in-order delivery in wired networks are unsuitable for ad hoc or other wireless communication. In this project, Sandia will implement reliable, ordered message delivery on top of an ad hoc communication protocol.

We will use simulation to assess the performance of the transport and routing protocols under different network conditions, and we will implement the transport and Virtual Geographic Routing (VGR) protocols on the wireless test-bed.

We designed and implemented a reliable transport protocol that provides reliable message delivery, message fragmentation and reassembly, and single-source first-in-first-out message ordering.

We developed a novel *ad hoc* routing scheme called VGR. VGR has the advantages of conventional geographic routing (scalability, efficiency, and high message-delivery ratio) without the requirement for global positioning system (GPS) or other positioning technology. VGR assigns to each node a fictitious or virtual location consistent with local node connectivity and uses the fictitious location to do geographic routing. We developed an algorithm for virtual location assignment.

To simulate the reliable transport protocol under the conditions of a wireless *ad hoc* network, operating network (OPNET) models of the IEEE 802.11 link layer protocol and *Ad Hoc* On-Demand Distance Vector (AODV) routing protocol were obtained and altered to make them suitable for this project. A two-node simulation is now operational.

To simulate the routing protocol, we developed a VGR model for use with a general-purpose simulator developed at Dartmouth College.

We designed and implemented a reliable transport protocol that provides reliable message delivery, message fragmentation and reassembly, and single-source first-in-first-out message ordering.

We obtained and configured hardware for a multinode wireless test-bed. Each node consists of a single-board computer (SBC) mated with an 802.11 radio-frequency (RF) spread-spectrum modem.

With the implementation of the transport protocol, development of the routing protocol, and the establishment of simulation and implementation test-beds, we have laid the groundwork for completing the evaluation and implementation of the components required for reliable messaging in *ad hoc* networks.

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Scalable Fault-Tolerant Algorithms for Linear-Scaling Coupled-Cluster Electronic Structure Methods

M. L. Leininger, I. B. Nielsen

Coupled-cluster theory has enabled the computation of molecular properties with an accuracy often exceeding that of experiment. Despite the tremendous progress in computer architectures, the high-degree polynomial scaling of this method represents the greatest obstacle in the accurate theoretical treatment of mainstream chemical problems. Although it has long been recognized that this super-linear scaling is non-physical, the development of efficient reduced-scaling algorithms to massively parallel (MP) computers has not been realized. Sandia is addressing this high-scaling cost of the coupled-cluster method by implementing locally correlated linear-scaling algorithms in a way that will enable the iterative solution of the nonlinear coupled-cluster equations involving several billion unknowns and scaling to thousands or millions of processors. Fault tolerance will be essential in allowing these distributed-memory applications to run on the next-generation Accelerated Strategic Computing Initiative (ASCI) machines, such as the Sandia Red Storm computer. We will implement the code in a modular fashion, developing general components for the distribution of large datasets across memory and disk, the solution of nonlinear equations, and the handling of faults in distributed-memory applications. These components will be made available to other Sandia projects. Programmatically, this work will benefit those modeling the molecular structures and the chemical reactions of central importance to Sandia programs in materials modeling and biochemistry. The ability to accurately describe large chemical systems is critical in validating models used in Sandia's ASCI materials-aging efforts and in providing accurate scoring functions for evaluating protein ligand-binding affinities.

We completed initial implementations of the proposed sparse representation for distribution of the coupled-cluster amplitudes and the proposed sparse generalized contraction routine. The sparse data representation handles sparse multidimensional arrays, storing only the nonzero elements. Data are blocked, and only blocks containing elements larger than a given threshold are stored. Variable block sizes are supported, and we use generic programming to provide features required to support the generalized contraction routine. The

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implemented generalized contraction routine provides the ability to contract arrays of arbitrary dimensions using the sparse data representation. We made preliminary performance analyses to investigate whether high computational efficiency can be obtained in the contraction routing using the relatively small block sizes that are required to reduce data storage for large, sparse systems. We implemented a pilot atomic-orbital (AO) basis second-order Möller-Plesset algorithm for implementation of the coupled-cluster doubles equations. In addition to the AO-based coupled-cluster approach, we investigated a local correlation model using a combination of AOs and localized occupied molecular orbitals. We wrote a program to perform the orbital localization and investigate the sparsity of the resulting array (T2) of double substitution amplitudes. We measured the sparsity of T2 for different classes of molecular systems, including linear systems, sheets, and globular molecules. We implemented a pilot local common constraint situation display (CCSD) program. This program does not utilize sparsity for computational savings, but it does project intermediates into the reduced solution space, and thereby provides a reference point for future sparse implementations.

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Micromagnetic Suspension

L. Romero, T. R. Christenson, W. E. Hart, A. A. Giunta

Sandia's goal is to apply robust optimization techniques to the problem of micromagnetic suspension. We developed a theory on how to achieve passive stable magnetic levitation with alternating magnetic fields. We say the levitation is passive because we specify the time variation of the field ahead of time, rather than adjusting it with feedback.

Although we proved that this can theoretically be accomplished, it is a different matter to actually find a configuration that allows us to do this robustly. The main thrust of this project is to develop an objective function that characterizes the robustness of a given configuration and to use optimization tools to minimize this objective function.

Our original proposal involved finding robust configurations for a new type of spin-stabilized magnetic levitation that we developed. However, early in our work we came up with the idea of passive (no feedback) alternating magnetic-field levitation (PAMFL). Our accomplishments are in three major categories.

- *Theoretical developments.* We developed the theory for PAMFL, which shows how to suspend a rotor containing a system of permanent magnets using a system of permanent magnets in the base, along with a system of magnetic coils in the base. We find an equilibrium position where the rotor experiences no force from the alternating magnetic field and so the force of gravity balances the steady magnetic force. The alternating magnetic field does not cause the rotor to move in its equilibrium position, but is used to stabilize the equilibrium position. We developed an analysis that uses linear stability theory to analyze the stability of arbitrarily complicated systems of magnets both in the base and on the rotor. We submitted this theory to the *SIAM Journal of Applied Mathematics*, as well as our theory on horizontally spin-stabilized magnetic levitation.

We also developed an objective function that characterizes how sensitive a stable configuration is to imperfections in the system. For example, it characterizes how large a percentage change in the magnetizations of the magnets we can tolerate before our stable configuration becomes unstable. We also developed a simulation code that allows us to simulate the motion of the rotor in the magnetic field. This is different from the stability code in that it allows us to put in finite-amplitude

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perturbations and to analyze the effect of many different sorts of imperfections in the system.

- *Linking with DAKOTA.* We linked our objective function with the optimization package DAKOTA (Design Analysis Kit for Optimization and Terascale Applications). The initial attempt to use DAKOTA was unsuccessful due to DAKOTA 2.0's inability to handle nonlinear equality constraints. This was remedied by DAKATO 3.0.

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Sensitivities for Large-Scale Simulation Codes

B. G. Van Bloemen Waanders, C. C. Ober, R. A. Bartlett, E. R. Keiter

The primary objective of this research is the development and implementation of algorithms for efficient sensitivity analysis in key, large-scale partial- and ordinary-differential (PDE and ODE) equation-based simulation codes. This capability would enable the creation of a unified design environment consisting of optimization, uncertainty quantification, and error analysis techniques, in addition to the traditional forward solution. There is a growing demand for sensitivity information from the PDE/ODE simulation community to support design tools. Such tools are available in the form of powerful optimization and uncertainty quantification (UQ) algorithms, which are accessible through general frameworks (i.e., DAKOTA [Design Analysis Kit for Optimization and Terascale Applications]). Without sensitivity information from the PDE simulation codes, these black-box approaches use finite-difference (FD) techniques to calculate gradient information; this expensive approach limits optimization and UQ from considering anything but a small number of design parameters.

Among a multitude of research issues, the most important ones consist of formulation design, transient simulations, and nonsmoothness. The formulation design issues depend on the simulation and the problem type. In the case of compressible fluid flow (PREMO), Sandia's final goal is shape optimization, which requires an investigation of discretized versus continuous formulations and low-level derivative methods. Nonsmoothness is a critical issue in electrical simulation (XYCETM), which could be caused by device modeling and time integration. Both areas need to be investigated.

Our goal is to provide general tools to the simulation community through SIERRA. We will attempt to generalize as many components as possible, such as the use of automatic differentiation tools, complex step, and the identification of sensitivity parameters. In addition, we will conduct some of our prototype design studies within the SIERRA framework.

We investigated several state-of-the-art methods to address sensitivities and time integration. A considerable number of methods are available, and each is applied for different reasons and applications. Low-level sensitivity techniques to calculate derivatives consist of finite-differencing, automatic differentiation, and the complex step. In addition to these low-

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level calculation approaches, we reviewed different ways of formulating sensitivities for simulation codes, and derived and are in the process of implementing the most appropriate method for shape optimization.

We reviewed automatic differentiation tools, including automatic differentiation of Fortran codes (ADIFOR), automatic differentiation of C codes (ADIC), automatic differentiation of library of C++ codes (ADOLC), and fast automatic differentiation (FAD). We concluded that FAD, which is a lightweight automatic differentiation library, can be efficiently used to calculate the operators of the analytic adjoint formulation for the steady-state Euler equations. We developed a complete tensor library coupled with the FAD lightweight automatic differentiation library. This capability is a new hybrid approach, combining an analytic adjoint derivation and the calculation of its operators through automatic differentiation.

We added direct sensitivity capabilities to an electrical simulation code (XYCE™) for the steady-state case and identified two possible sources of nonsmooth behavior. We conducted some studies to identify the nature of the nonsmooth behavior, and more detailed investigations are under way. We extended the XYCE™ input structure to include “meta-data,” which can be used to identify sensitivity or optimization parameters.

We implemented prototype sensitivities for transient simulations in a chemically reacting fluid-flow simulator (MPSalsa™) in preparation for extending sensitivity methods in both PREMO and XYCE™ to the transient case, if appropriate. We developed modifications to the code to manipulate the finite elements associated with the boundary conditions.

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Differentiating Technologies

The Differentiating Technologies investment area focuses on research activities that accelerate the development of novel sensing, microsystems, and cybersecurity technologies. Investments are being planned for advanced, remote infrared (IR) optical sensing; novel microchip designs for sensor networks; and advanced cybersecurity countermeasures. New materials are being investigated for IR sensing applications that will enable the realization of very high sensitivity and highly wavelength-specific detection schemes. In addition, researching and developing “adaptive countermeasures” has the potential to produce new methods of defeating cyber attacks.

The utility of many small electronic devices is limited by the power supply. Sandia is developing a “Microengine for Advanced Power Generation” capable of producing 10–20 W of electrical power using a liquid hydrocarbon fuel. This engine will provide an order-of-magnitude reduction in weight compared to standard lithium ion batteries. The project includes design and integration of a combustor and an engine, and fabrication using

LIGA (the acronym for the German words for lithography, electro-forming, and molding) technology. Successful completion of this project will lead to important technical advances in microcombustion, miniature-engine design, micro-fabrication of LIGA metal and ceramic parts, and the application of advanced diagnostics at small scales.

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Adaptive Network Countermeasures

J. Vanrandwyk, T. J. Toole, J. A. Hutchins

For most attackers, conducting accurate system or network reconnaissance is the critical first step of the attack process. If a defender can thwart an attacker's reconnaissance efforts, it will be considerably more difficult and time-consuming for that adversary to successfully attack the network.

Traditionally, protocol stack implementations (e.g., Transmission Control Protocol/Internet Protocol [TCP/IP]) provide, rather than limit, information to attackers. This includes providing information about what addresses on the network are active, what services are running on systems, and possibly enough information to deduce what operating systems (OS) are running on networked computers. With this information, an attacker can tailor a specific attack to a computer, thus not wasting time or risking detection of himself/herself by attempting attacks that may not succeed.

Some measures used to thwart reconnaissance activities include perimeter defenses (e.g., firewalls and routers) to limit information available to attackers. Defenders have also used "honeypots" as a method of attracting, then distracting, an attacker. These approaches leave large gaps in the scope of their protection.

If we can provide attackers with information that suits our ends rather than their ends, we can greatly increase the time and skill required to map our networks, computers, and available services.

Sandia proposes a new area to examine: adaptive network countermeasures (ANC). We will develop software that a defender can use to watch unused subnets and reply to attackers answering for all addresses and all ports. Then we will study how such a system can identify, then mislead or confuse, a widely used reconnaissance tool. Finally, we will simulate protocol stacks and applications to distract an attacker without offering the vulnerabilities found in real honeypot systems.

We developed prototype network countermeasures to respond to common network scans just as the actual IP stack of an OS would respond. We used common scanning tools such as "nmap" and "xprobe" to test our countermeasures. This approach works extremely well in an environment where the attack tools being used are those that are commonly employed today.

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We improved our ability to characterize attackers' levels of sophistication. This is done simply right now via human judgment.

We identified potential problems in implementing network countermeasures. Processing network traffic and responding to it appropriately could be very difficult on a high-bandwidth network such as Sandia's.

We investigated different hardware and OS options on which to build our software. We determined that FreeBSD with its very efficient kernel and widespread support in the security community will be our OS platform. We also investigated our hardware options and utilized "embedded PCs" manufactured by NEX COMputers that offer several important features. These boxes are compact and lightweight, allowing the end-user to place the computers in utility closets in various places on a given site to tap different points in the network. At the same time, these computers are powerful enough to provide the level of processing that we require.

We found software (honeyd) already written to aid in our countermeasure development. We worked with the author to improve and extend his software package, making it suitable for integration into our project.

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Microengine for Advanced Power Generation*B. L. Haroldsen, G. J. Fiechtner, A. M. Morales, M. A. Bankert, J. H. Chen, T. N. Raber*

The utility of many small electronic devices is limited by the power supply. Sandia is developing a mesoscale Stirling engine capable of producing 10–20 W of electrical power using a liquid hydrocarbon fuel. We expect the engine to provide an order-of-magnitude reduction in weight compared to standard lithium (Li) ion batteries. The project includes design and integration of a combustor and an engine, fabricated using LIGA (the German term Lithographie, Galvanoformung, und Abformung, for lithography, electroforming, and molding) technology. Although other engine designs perform better at macroscales, we believe the Stirling engine concept is better suited to small-scale applications. Most microengine designs suffer from scaling effects such as limited combustor performance owing to excessive heat loss and quenching of reactions. Since the Stirling engine uses external combustion, the combustor and engine can be scaled and optimized semi-independently. Continuous combustion minimizes issues with flame initiation and propagation. It also allows us to consider a variety of techniques to promote combustion that would be difficult in a miniature internal combustion engine. The ideal Stirling cycle requires efficient heat-transfer and isothermal processes. Consequently, unlike other thermodynamic cycles, the high heat-transfer rates that are inherent to miniature devices are an advantage for the Stirling cycle. Our design approach includes both modeling and testing. We are developing the combustor and engine individually and will integrate them into a complete system. The initial engine prototype uses a rotary piston design. Materials of construction are nickel and ceramic. The combustor uses an excess enthalpy design with a catalyst to start and promote combustion. Successful completion of this project will lead to important technical advances in microcombustion, miniature-engine design, microfabrication of LIGA metal and ceramic parts, and the application of advanced diagnostics at small scales.

We performed an extensive review and analysis of the engine and combustor design, including development of detailed computer models. From this, we selected concepts for prototype designs. For the combustor we selected an excess enthalpy design with a platinum-iridium catalyst. In this design, we use the exhaust gas to preheat the reactants. This allows combustion at conditions where the flame would otherwise be

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quenched, and it provides a large heated surface to enhance heat transfer to the engine. We used CFD Research Corporation's computational fluid dynamics (CFD)-ACE code to model the combustor. This is a finite-volume code in which various complexities of surface and homogeneous chemistry and transport models may be implemented. We used the CHEMKIN (chemical kinetics) library (which is used in CFD-ACE) to specify the chemistries and transport properties of gas-phase species. Variables included the diameter and length of the combustor, the fuel-air ratio, and the inlet velocity. We fabricated a simple tube-in-tube prototype combustor for testing and are now fabricating a second prototype, with a planar geometry that lends itself to microfabrication, using alumina nanoparticle casting and sintering. The prototype combustors use a linear heat exchanger geometry with methane as the fuel. We selected the geometry primarily for convenience in testing.

For the engine, we selected two concepts for prototype fabrication. The designs are complete, and fabrication is under way. One design uses rotary pistons while the other uses cylindrical pistons. The planar geometry of the rotary design is more compatible with the LIGA fabrication process that we are using. The cylindrical piston design will use conventional machining techniques. For this reason it is slightly larger than the rotary design. The rotary design has two epitrochoidal chambers, one at the hot end of the engine and one at the cold end. The two rotors are out of phase, so the working gas is alternately forced from the hot to the cold region and back again while being compressed and then expanded to extract work. We can easily couple the rotary motion to an electrical generator; the motion is inherently smooth, eliminating the need for a flywheel. The planar geometry also enhances heat transfer to the working gases, and we can easily separate the hot and cold sides of the engine by a long regenerator to minimize parasitic heat transfer. The cylindrical piston design works in a similar manner with multiple pistons in the hot and cold regions that move the working gas back and forth. Connecting rods couple the pistons to a rotating shaft that is connected to a small generator. Since it uses more conventional machining, we can fabricate this design more rapidly. The simpler geometry also makes it more amenable to modeling so we can quickly and easily study some important scaling issues. The materials of construction for the combustor and the engine are nickel/manganese and ceramic.

These materials are compatible with LIGA, provide high-temperature compatibility, and provide acceptable heat-transfer properties.

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Particle “Front End” for Compact WMD Threat-Detection Systems: Integrated Microsystem Concepts for Intelligent Particle Collection, Separation, Preconcentration, and Processing

K. Wally, E. B. Cummings, M. P. Kanouff, D. J. Rader

An objective of this project is to develop concepts for the direct impingement of collected aerosols into microliter-scale collectors for interface to microfluidic analysis systems. One goal is to experimentally demonstrate an inertia-based microseparator device that can focus airborne particles and deposit them into a narrow stripe. By particle-focusing, we mean that the deposited particle stripe is significantly narrower than the nozzle width. Ideally, the device would collect particles in a user-selectable size range (nominally 1–5 μm) with a low-pressure drop (nominally < 2 in. of water). Sandia tested two such inertial focusing/collecting prototype designs in this work: the focusing impactor (FI) and the opposed-flow virtual cyclone (OFVC). A second goal modeled the complex interactions that affect the electrokinetically pumped microfluidic micro-impinger. We compared the results obtained with these models to some experimentally obtained results. In addition to these reported results, the project also developed methods and materials for fabrication of deep, narrow microchannels, and methods of experimentally measuring fluid pressure in open microchannels through optical measurement of meniscus curvature. We also pursued work on microscale dielectrophoretic particle concentrators.

- *Particle-focusing.* The FI accelerates air and suspended particles as they flow into a two-dimensional converging wedge-shaped slit. We aligned the two plates with a full-angle θ between them and separated them by a distance W at their closest approach. Particles aligned with flow streamlines and thereby experienced size-dependent particle-focusing. At the converging exit, inertia prevented large particles from changing direction, so air turned while particles continued toward impaction. Ideally, geometry and operating conditions can be designed so particles within a desired size range are effectively focused.

We tested particle-focusing capabilities of a prototype FI with monodisperse oleic acid droplets. The increase in particle-focusing with increasing particle size was clearly evident;

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deposition width decreased tenfold as particle size increased fourfold. These tests demonstrated the size-dependent, particle-focusing capabilities of the FI geometry at low-pressure drop (measured at ~ 1.4 in. of water).

Similar tests of an OFVC prototype provided mixed results. Although we observed strong particle-focusing, the stripe sometimes exhibited sinusoidal behavior instead of the desired straight line. For certain geometries and flows, this behavior was sometimes suppressed and straight-line deposit recovered. Thus, although the OFVC appears promising, additional work remains to identify conditions under which sinusoidal behavior can be reliably suppressed.

- *Capillary and electrokinetic (EK)-flow modeling.* The FI will deposit particles into a liquid-filled, electrokinetically driven, open microchannel. There are complex interactions with this scheme. The air velocity in the FI promotes evaporation, and aerodynamic pressure affects liquid flow. Capillary forces are significant. We used modeling to understand these coupled phenomena.

In a nondimensional form of the momentum equation, using representative properties and geometries, the relative importance of terms in the equation can be assessed. Specifically, capillary-induced pressure gradient and viscosity dominate gravity, and inertia is least important. Neglecting inertia makes the equation linear, allowing superposition of pressure and EK flows, yielding a combined solution. We used this superimposed solution with a one-dimensional form of the continuity equation to describe microchannel flow.

With negligible inertia, pressure flow can be approximated as fully developed, with average flow velocity proportional to pressure gradient, square of channel width, inverse of fluid viscosity, and a proportionality constant depending on channel geometry and free-surface shape. We performed finite-element (FE) calculations to obtain proportionality constants as a function of these parameters.

We obtained the evaporation rate and the aerodynamic pressure on the microchannel by finite-element model (FEM). We calculated evaporation assuming equilibrium between vapor and liquid, with rate determined by diffusion and advection. We express evaporation rate as volume evaporated, per time, per unit area of surface, giving units of velocity. Evaporation rate depends on air-flow rate. To further test the model, we simulated an earlier unsuccessful dry-running microchannel geometry. Flow-reversal can occur in microchannels through evaporation and capillary wicking, and dry-out can result if wicking cannot sustain evaporation.

We obtained the evaporation rate and the aerodynamic pressure on the microchannel by finite-element model (FEM).

We calculated evaporation assuming equilibrium between vapor and liquid, with rate determined by diffusion and advection.

We identified three approaches for maintaining forward flow. One applies a forward-pressure differential along the channel. Another is to taper the microchannel. The taper inhibits would-be flow-reversal while promoting forward EK flow. A third approach parallels the open channel with an interconnected closed channel. The EK and pressure flow in both channels interact, with the closed channel replenishing open-channel evaporative losses and promoting forward flow by suppressing flow-reversal.

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Electronics and Photonics

The Electronics and Photonics investment area explores innovative solutions to national problems that build on Sandia's existing strengths. Advances in the realization of small, low-power, integrated microsystems and concepts that advance silicon and compound semiconductor science and technology support Sandia's mission needs. Research focus areas have included microdevice concepts that enable advances in microelectronics, photonics, microelectromechanical systems, and sensors. Other important research includes using semiconductor fabrication techniques to combine electronic, optical, mechanical, and chemical functions into integrated systems; new approaches to integration, packaging, and micropower systems are being investigated.

High-performance micro-fabricated electromagnetic (EM) devices are difficult to integrate. "Microfabrication of Electromagnetic Devices" seeks solutions to these processing issues that will enable batch microfabrication of a large class of EM devices. These devices include powerful millimeter-scale actuators. The resulting generic magnetic microactuator platform technology is well suited for applications involving microrobotic propulsion, high-reliability and relatively high-power handling optical and radio-frequency

switching, low-leakage gas and liquid valves, gas- and liquid-flow regulators, precision microoptical positioning stages, and micro-generators. Two patents have been filed on the microfabrication and multiple-angle x-ray exposure techniques.

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Radiation-Induced Prompt Photocurrents in Microelectronics: Physics

P. E. Dodd, G. Vizkelethy, D. E. Beutler, W. Beezhold, D. L. Buller, D. S. Walsh, B. L. Doyle

The goals of this project are to study the physical phenomena underlying prompt photocurrents in microelectronic devices and circuits, and to develop a dose-rate radiation source capable of irradiating devices at the microscale. These microscale dose-rate experiments provide data on the fundamental response of single transistors that can be used to validate device-level simulation tools. Da VINCI, a three-dimensional (3-D) numerical device simulator used at Sandia primarily for cosmic-ray upset analysis, had not been applied previously nor validated for the study of x-ray and gamma-ray photocurrents.

Previously, we found that the transient radiation microscope (TRM) developed in this project did not simulate more usual x-ray or electron linear accelerator (LINAC) data well for devices with thick active layers. Using Da VINCI, we traced this discrepancy to the limited range of the ions used to simulate dose-rate effects. A major thrust of this year's effort was to prove or disprove that Da VINCI was correctly interpreting the results and to determine whether the TRM could accurately reproduce LINAC results for thin devices more typical of modern microelectronics. Therefore, we performed TRM experiments on a number of microelectronic devices of interest to potential Sandia weapons applications.

A second thrust of this work was to further improve the TRM system to achieve 10 ns pulsewidths and dose rates on the order of 1 Trad(Si)/s.

We believe the TRM can be a valuable tool to study hostile-threat photocurrent effects in current and future weapon electronics. In addition to proving that the TRM can replicate electron LINAC test data, we showed that the physical models in Da VINCI correctly described the physics that led to anomalous storage time effects in devices with thick active regions.

We successfully set up and are now using the "Mark IV" version of the TRM. This final version of the TRM can operate in either a short-pulse or long-pulse mode. In the long-pulse mode, the ion beam is swept into the slits, stays there for from 250 ns to microseconds, and is then deflected away from the slits. In the short-pulse mode, the ion beam is swept from one

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side of the slits to the other side, passing through the slits only very briefly (~ 10 ns). In long-pulse mode we are able to achieve dose rates in excess of 1 Trad/s. In short-pulse mode it becomes very difficult to measure the dose rate because the pulse contains so few ions. An additional complication is that because so few ions are contained in the pulse, the pulse reproducibility is poor. In future work, it may be possible to further improve the system by using beam-blanking directly on the ion source rather than by controlling the accelerated beam. This method would have the further benefit of reducing beam noise at the end station.

We also performed further experiments to conclusively prove whether the storage-time mechanism determined by Da VINCI simulations in previous years' work was correct. We performed TRM experiments on two different fast PIN (positive-intrinsic negative) diodes, one with a thin depletion layer and one with a thick one. As predicted by Da VINCI, the thin diode did not show a storage-time effect, while the thick diode showed a storage time due to the ions "ranging out" within the depletion region. While not typical of devices used in electronics systems, the PIN diode results were an excellent vehicle for studying the accuracy of the physical models in Da VINCI.

To be a useful hardness assurance tool, it is essential that the TRM reproduce transient photocurrent results obtained in more usual broad-beam dose-rate sources such as flash x-ray or electron LINACs. We tested three different devices being considered for system use in the TRM and compared the results to data taken at the electron LINACs at the Idaho State University Accelerator Center. We obtained very good agreement between the TRM and the LINAC data, validating the use of the TRM as a dose-rate source that can emulate more traditional methods.

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SOI-Based High-Aspect-Ratio Si Bulk Micromachining for MEMS Applications

R. J. Shul, C. P. Tigges, M. A. Polosky, C. T. Sullivan, T. R. Christenson, O. B. Spahn, M. J. Cich

Nearly all microactuator types rely on elastic suspension for reliable and effective operation. The exceptionally high yield strength and linear mechanical response possessed by single-crystal silicon (Si) renders it an appropriate material for the fabrication of springs, particularly if they can be patterned into arbitrary prismatic geometry. Using a deep reactive-ion etch (DRIE) process and silicon-on-insulator (SOI) wafers, Sandia will fabricate released, movable, single-crystal Si structures 10–100 μm thick with lateral dimensions $< 5 \mu\text{m}$. The integration of these structures with surface-machined microelectromechanical systems (MEMS) or LIGA (the German term Lithographie, Galvanoformung, und Abformung, for lithography, electroplating, and molding) enables considerable design leverage in diverse applications such as clasps, sensors, inertial resonators, microengines, acceleration switches, and position actuators. The attraction of high-aspect-ratio Si is that the parts can have relatively high longitudinal (out-of-plane) stiffness and mass. With this technology, we expect to fabricate thick actuators with increased force and comparable throw as compared to surface-micromachined (SMM) MEMS. Additionally, we will use a multimask lithographic process to form thick comb drives and stators (providing high force) with thin springs (low spring constants) on a single device. This technology also will enable us to fabricate high-mass structures with micrometer resolution for accelerometers or gyros and extremely rigid, lightweight, high-strength structural components for systems applications. The development of this technology also will allow fabrication of a simple and robust microdiscriminator/optical redirect design. The simplicity is a direct consequence of the use of thick Si, which reduces the number of required levels for the device structure and permits a simpler configuration of the optical redirect elements and interconnect.

We recently achieved several advances in process development, device fabrication, and new applications for bonded SOI wafers. Process development reported for earlier work resulted in the fabrication of mechanical devices including acceleration switches, actuators, and mechanical springs. This progress has generated interest in the fabrication of high-mass mechanical structures using bulk single-crystal Si.

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We fabricated single-level and multilevel single-crystal Si actuators using a new mask design that increases device yield. Earlier mask layouts resulted in low yield due to lengthy overetch times necessary to completely etch the Si from the “honeycomb” wet-etch release holes. As a result, many of the thin spring structures ($< 2 \mu\text{m}$) were etched laterally. This compromised the critical dimensions of the springs and, in some cases, completely lifted the springs from the Si carrier substrate. This phenomenon is often referred to as *aspect ratio-dependent etching* (ARDE). Features with different lateral dimensions often etch at different rates and therefore to different depths. To resolve this, we designed a new mask set that increases the diameter of the honeycomb wet-etch release holes to reduce the required DRIE overetch time. In addition to these changes, the new mask design of the multilevel actuators included higher-resolution alignment marks to improve alignment tolerance to better than $0.5 \mu\text{m}$. We completed fabrication runs with promising results and are continuing testing to evaluate voltages required to actuate both single- and multilevel structures.

Fabrication of SOI devices was also extended to environmental sensing devices. We designed and fabricated low-G and high-G microacceleration switches on $> 100 \mu\text{m}$ -thick SOI wafers and etched them using the DRIE. The structures were released using buffered-oxide etch (BOE) and dried using supercritical carbon dioxide (CO_2). To minimize undercut of the springs, we included additional structures (some anchored to the handle wafer and some that were “dropouts”) in the design. Post-fabrication inspection showed that in some cases the dropouts interfered with the functionality of the device and reduced yield. At this point, optimization of the DRIE process is necessary to eliminate these structures but maintain dimensional control of the springs. On low-G devices, we etched a via into the backside of the wafer for wet chemical release. This eliminated etch-release holes from the shuttle, increasing the mass, reducing the complication of ARDE, and improving dimensional control of the springs. We delivered functional devices and prepared them for a flight test.

We demonstrated wafer-to-wafer integration using DRIE and bonded wafers in the fabrication of a MEMS safing and arming device in the microfuze program. The fabrication sequence begins with patterning and etching a thick handle wafer using the two-level mask process and front- and backside processing. The backside processing defines a large through-hole and alignment marks, while the two-level mask process creates features on the front side at three levels: anchor level,

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support level, and cavity level. We then bond the preprocessed handle wafer to a blank device wafer using a direct fusion bonding process. The device wafer is subsequently lapped to the desired thickness ($\sim 100 \mu\text{m}$). We align the device structures to the etched cavity in the handle wafer using backside alignment. We etch a large, proof-mass shuttle with springs and anchors into the device wafer using the DRIE process. The etched structures are separated and thus released from the handle wafer by the depth of the underlying cavity. Device yield was greater than 50% on the first two wafers processed with the dominant failure mechanism due to the dropout features.

We completed a process sequence and mask layout for the electromagnetic SOI devices. We expect DRIE development runs shortly. If successful, this device could provide a solution to the need for a damped acceleration switch in future weapon systems.

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Defining the Frontiers of Vertical, External-Cavity, Surface-Emitting Lasers

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Sandia's goals in this project are to develop electrically pumped, near-infrared (NIR), vertical, external-cavity, surface-emitting lasers (VECSELs) and to use nonlinear optical techniques to shift their wavelengths to the blue/ultraviolet (UV) and to the IR. The nonlinear conversions include intracavity frequency doubling and intracavity optical parametric oscillators. The challenges in developing this technology are to control the laser wavelength, increase the laser mode area, reduce the optical absorption of the laser light, and efficiently remove heat from a bottom-emitting VECSEL so the laser power and efficiency can be dramatically improved. We also plan to explore nitride-based vertical-cavity surface-emitting lasers (VCSELs) as an alternative blue/UV source.

VCSELs have many attractive properties, including narrow linewidth, wavelength selectable by engineering the semiconductor-layered structure, good efficiency, and good beam quality. One shortcoming is their relatively low power, a limit imposed by their typically small transverse dimension of a few micrometers. The goal of our project was to increase this power by increasing the aperture of the gain region from a few micrometers to over 100 μm . This requires the use of an external mirror (hence, the name *vertical external-cavity surface-emitting laser*) as the output coupler. It must be spaced many millimeters from the wafer. This space can be used to insert nonlinear optical crystals for frequency conversion, via frequency doubling or optical parametric oscillation. With optical pumping by an edge-emitting laser at 815 nm, we were able to increase the VECSEL power to 100 mW at 980 nm and, using an intracavity-doubling crystal, we generated 5 mW at 490 nm. The limit to the power of the optically pumped VECSEL was heat removal. As we increased the pump power and the mode area, the wafer overheated, shutting off lasing. We improved heat removal by optically contacting a sapphire window to the top of the wafer, which allowed us to increase the lasing power to 2 W with 20% optical conversion efficiency.

For many applications, it is necessary to electrically pump the VECSEL. The problem we encountered was pump current nonuniformity over the aperture. The current tended to be concentrated around the aperture rim rather than in the center,

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as needed for the lasing mode. Adding a current-spreading layer to the top of the wafer helped, but was inadequate. This led us to develop a bottom-emitting VECSEL that uses the thick substrate to spread the current. This gives a uniform gain, but light absorption in the substrate limits efficiency and power. This problem is the subject of further design and testing.

Refereed

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10749

Growth and Characterization of Quantum Dots and Quantum-Dot Devices

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There is a clear systems need for the development of alternative short-wavelength (ultraviolet [UV]) as well as 1.3 μm infrared (IR) lasers on gallium arsenide (GaAs) for use in vertical-cavity surface-emitting lasers (VCSELs). To meet this need, Sandia will develop efficient, self-assembled quantum-dot (QD) emitters. Confinement in three dimensions (3-D) will minimize the degradation of output power with increasing temperature and improve overall efficiency. Enhanced 3-D confinement should aid in the development of shorter-wavelength UV/visible VCSELs as well as produce ultralow threshold currents. The 3-D carrier confinement will decrease lateral carrier diffusion, thereby increasing the internal quantum efficiency (IQE). Additional benefits of QDs within VCSELs include polarization control and the ability to tailor the emission wavelength by accessing material compositions with greater strain than permitted in quantum wells (QWs). To maximize device performance, we will develop a microscopic theory that combines photonic and quantum kinetic aspects so that optical properties of the QD/extended-QW system can be predicted and compared to the observed characteristics. Using metal-organic chemical vapor deposition (MOCVD) and molecular beam epitaxy (MBE), we will examine the effects of surface orientation and strain on the size and position distribution of self-assembled QDs. We will use a combination of surface orientation, strain effects, and substrate or mask patterning with electron-beam lithography to grow QDs with controlled size, shape, and spatial distribution. We will explore development of stable QD formation by argon (Ar) ion-beam etching of various substrates as an additional preparation technique. We will prepare QD light-emitting diodes (LEDs) and lasers using the techniques developed in this investigation for use in existing and future Sandia projects.

We used MOCVD to grow indium arsenide (InAs) and gallium antimonide (GaSb) QDs on GaAs and indium antimonide (InSb) QDs on GaSb. The QDs are uniform in size, varying from 2 nm to 30 nm in height and 20 nm to 100 nm in width with densities of $0.5^{-5} \times 10^{10} \text{ cm}^{-2}$. The size and position uniformity varies depending on the growth conditions. The

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photoluminescence (PL) intensity and linewidth are also dependent on growth technique and conditions, including temperature and growth rate. We observed PL intensity at both low temperature (77 K) and room temperature. We achieved a linewidth of 19 meV for indium gallium arsenic antimonide (InGaAsSb) QDs in a GaSb matrix, which suggests a low, inhomogeneous broadening. InGaAs QDs show emission between 1.1 μm and 1.3 μm , and InGaAsSb QDs show emission between 1.6 μm and 1.7 μm . We observed a “surfactant” effect, which reduces the surface energy for nucleation when Sb is added to InAs QDs. We also observed a complementary effect when As is added to InSb QDs on GaSb, interpreted as a reduction in the In adatom diffusion length. We produced QD multilayers, which overcomes limitations due to saturation of the active region. We are incorporating InGaAs QD multilayers into GaAs-based edge-emitting diode laser structures.

We initiated an investigation into the dynamics of excitation-energy (e.g., exciton) transport in multidot-well structures. We theoretically showed that the two dominant mechanisms by which an exciton hops between widely separated states are dipole-dipole and photon-exchange coupling. We found that for dot-to-dot coupling, the photon-exchange interaction can compete with the dipole-dipole coupling only for long-distance ($> 400\text{ nm}$) transfer. We are currently formulating multiphonon-assisted hopping transfer rates between dots.

We computed gain spectra using a theory that was developed for a QD laser using a self-consistent treatment of the coupled QD/QW system, including many-body Coulomb effects. Our approach involves adapting the semiconductor Bloch equations in the screened Hartree-Fock approximation to describe a shallow QD surrounded by a QW region. This picture describes both strain-induced dots and dot-in-a-well structures. The solution of the semiconductor Bloch equations gives the optical spectra. We extended our theory of QD optical properties to address beam-quality issues in InGaAs QD lasers and investigate III-nitride QD active regions. We showed that QD active regions exhibit an anomalous dependence of the refractive index on excitation, which is drastically different from other laser active materials. In agreement with experiments, we find that the tendency for degradation of the output beam quality by filamentation effects in QDs is eliminated. For III-nitride QD active regions we augmented our existing models to describe the charge separation in the QDs due to piezoelectric effects.

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Refereed

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10766

Heterogeneous Integration of Optoelectronic Arrays and Microelectronics

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Integrated microsystems provide the benefits of small size, low-power consumption, robustness, and potentially inexpensive manufacture. However, multifunctional, advanced microsystems often require a combination of microelectronic and photonic technologies. For example, high-density, two-dimensional (2-D) integrated optoelectronic arrays are the basic components necessary to construct real-time electrooptical signal-processing and analog information-processing microsystems. In corresponding applications such as digital and neural computing, data mining, and data communication switching, there is a critical need to provide local electronic processing in each optoelectronic pixel. Moreover, to achieve the required functionality in these systems, highly sophisticated devices, often with state-of-the-art performance, are necessary. Thus we need combinations of dense numbers of high-performance devices originating from disparate technologies to achieve the next generation of information-processing, interconnect, and intelligent sensing microsystems.

As the integration density increases, heat dissipation becomes a critical issue. Thus, tailoring the properties of the substrate material independently from the epitaxial material is desirable. Transfer of the epitaxial material to a foreign host by low-temperature appliqué bonding allows this independence. We extended the appliqué technique to bonding functional devices onto substrates designed for thermal management.

An alternate form of device integration is homogeneous integration where more than one type of device is fabricated from the same epitaxial material. This integration has many benefits, and we demonstrated a 64x64 array of interleaved vertical-cavity surface-emitting lasers (VCSELs) and photodetectors on a 55 μm pitch. This integration path is synergistic with our other programs, and the 4096-element arrays provide the high-density 2-D arrays required for imaging or neural computing applications.

Heat dissipation from VCSELs limits the light-output power possible from any given device. By increasing the thermal conductivity of the VCSEL substrate, we can achieve higher powers. We successfully demonstrated high-power gallium-arsenide (GaAs)-based VCSELs bonded to silicon (Si) heat sinks. We bonded the VCSEL epitaxial material to Si using

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an indium (In)-metal thin film. The GaAs substrate was partially removed, leaving approximately 100 μm to aid in spreading current across the large-aperture devices. We achieved the process using electron-beam–evaporated In and a flip-chip bonder modified with a nitrogen purge to allow melting of the In without oxidation, which prevents bonding.

VCSELs are uniquely suited for massively parallel interconnects and scannerless imaging applications due to their small size, high efficiency, and amenability to formation of high-density, 2-D arrays. We successfully fabricated 4096-element arrays (64x64) containing alternating rows of selectively oxidized 850 nm VCSELs and resonant-cavity photodetectors (RCPDs) on a 55 μm pitch monolithically integrated on semi-insulating GaAs substrates. We employed a matrix-addressable architecture to reduce the input and output electrical connections to the array, where all the VCSELs (or RCPDs) in each row are connected by a common metal trace at the base of their mesas. The columns are connected by metal traces that bridge from mesa top to mesa top, connecting every other row (i.e., only VCSELs or only RCPDs).

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10775

Miniature Sensors for BW Agents Using Fatty-Acid Profiles

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*Sandia made progress toward the demonstration of biological detection using Sandia-fabricated microfabricated devices. The miniature biological weapons (BW)-agent detector relies on an established technique of identification based on fatty-acid (FA) profiles. These biomarkers are used to distinguish bacteria at the gram-type, genera, and even species levels. Recent work demonstrates that fatty-acid methyl esters (FAMES) can be obtained from whole bacterial cells in an in situ single-step pyrolysis/methylation/mass spectrometry (MS) analysis. Derivatization and detection occur rapidly (in less than 1 minute) with little sample preparation. This method can also detect dipicolinic acid (DPA, a biomarker for sporulated *Bacillus anthracis*, the causal agent of anthrax), amino acids, and oligopeptides. This project focused on demonstrating that microfabricated components can perform the same pyrolysis technique as well as gas-phase separation and detection of FAMES.*

Sandia made progress toward the demonstration of biological detection using Sandia-fabricated microfabricated devices. ...This project focused on demonstrating that microfabricated components can perform the same pyrolysis technique as well as gas-phase separation and detection of FAMES.

We worked on the following tasks:

(1) *Demonstrate pyrolysis/methylation of individual types of bacteria using manual loading of sample, miniaturized pyrolyzer and gas chromatography (GC) columns, and standard detector (MS).* We performed successful pyrolysis/methylation of two types of bacteria and produced methylated FAs from whole-cell bacteria, without sample preparation.

(2) *Demonstrate selective detection of at least three types of bacteria using same system as in the previous accomplishment.* The FAMES produced from two types of bacteria were selective enough to allow differentiation of the bacteria. The patterns produced from each bacterium were distinct.

(3) *Characterize the detection ability for at least three bacteria using manual loading of sample, miniaturized pyrolyzer and GC columns, and miniature surface acoustic-wave (SAW) array or alternate detector.* This task was unmet due to problems with SAW detector performance.

(4) *Integrate modified miniature bioaerosol collector.* We did not attempt this task because of delays in meeting previous milestones and because of test fixture difficulties.

(5) *Optimize chemically selective detector and FAME concentrator.* Initial tests regarding secondary FAME concentration were unsuccessful. In addition, the coatings currently used for chemical selection of gas-phase species are not stable at the high temperatures required to keep the FAME species in the gas phase. Further work on higher-temperature coatings is required to allow for selective detection of FAMEs using SAW technology.

(6) *Fabricate test fixture and breadboard with full-up liquid dispenser and microfluidic conduits.* We met this milestone with the exception of the fluidic conduits. We designed and fabricated a new test fixture and successfully tested a combination of all three major devices—micropyrolyzer, microGC, and SAW detector.

(7) *Demonstrate combined breadboard system incorporating aerosol collection, reagent dispensing, pyrolysis/methylation, FAME chromatography, and detection.* Because this was a follow-on to the first milestone, which was not met, we did not meet this milestone either.

(8) *Micropyrolysis/methylation of DPA and methylated DPA (mDPA).* We completed this task.

(9) *Microchromatography of DPA and mDPA.* We achieved microGC analysis of mDPA. We determined that performing the analysis of the unmethylated form of DPA was irrelevant because of the success of the first task.

(10) *SAW detection of DPA and mDPA.* We met this milestone with mDPA only. The difficulty in achieving SAW detection for mDPA suggested that attempting SAW detection of the less volatile DPA would not be productive.

(11) *Preconcentrator coatings specific to DPA/mDPA.* We evaluated current preconcentrator coatings.

(12) *Micropyrolysis/MS analysis of spores at Colorado School of Mines (CSM).* We placed a contract with CSM and provided micropyrolyzers. We successfully pyrolyzed spores and detected mDPA-specific peaks.

We designed and fabricated a new test fixture and successfully tested a combination of all three major devices—micropyrolyzer, microGC, and SAW detector.

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10776

Enhanced-Sensitivity Acoustic-Wave Biosensor Arrays

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This project proposes to develop enhanced-sensitivity biosensors utilizing acoustic platforms with biorecognition layers. The resulting sensors will be capable of detecting both chemical and biological agents in aqueous media and have application in nonproliferation, military scenarios, environmental monitoring, intelligence, law enforcement, medical diagnostics, and food processing. Accomplishments to date include scientific and technical advancements in the field.

The sensor approach is based on resonant response enhancement that occurs in acoustic sensors when the shear wavelength produced by the oscillating device is four times the mean thickness of the surface layer. In this case, the viscoelasticity of the layer can dominate the response mechanism and be significantly larger than that due to the mass. Sandia is investigating several acoustic platforms (thickness shear mode [TSM] resonators, guide shear-horizontal surface acoustic-wave [SH-SAW] devices, and flexural plate-wave [FPW] devices) that cover a wide range of operating frequencies and therefore a wide range of analyte molecular weight, size, and bilayer viscoelasticity. Results from collaborative and preliminary investigations verify the ability of shear acoustic sensors to detect pathogens and proteins. Work in this area demonstrates the higher sensitivity of SH-SAW sensors over TSM devices in liquid and the potential for FPW devices to offer superior detection of lower-molecular-weight analytes in low-viscosity fluids. Progress to date demonstrates our ability to assemble sensitive bioreceptor layers on the acoustic-wave devices.

We made significant progress in the following areas:

- We developed acoustic and capacitance models to screen potential waveguiding materials.
- Diffusion and gravimetric settling analysis indicates that a flow system is essential to minimize nonspecific attachment of large particles (1–2 μm).
- We applied suitable chemistries to conjugate antibodies and fragment antigen-binding (fab) fragments to polyimide 2613 and polystyrene.
- We showed that Love-wave devices detect an anthrax simulant B8 *Bacillus thuringiensis* spores below noninfectious levels (~ 1500 spores/ml).

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Crucial to low-level detection of biowarfare agents in aqueous environments is the mass sensitivity optimization of Love-wave acoustic sensors. Recent work is a theoretical and experimental study of Love-wave devices based on 36-degree YX-cut LiTaO₃. Given that the detection limit (DL) of Love-wave-based microsensors is a strong function of the overlying waveguide, we developed several computer models to optimize the waveguide thickness. We used the computer models to study mass sensitivity, acoustic velocity, insertion loss, and interdigital transducer capacitance as a function of waveguide thickness. To date, we have investigated three waveguide materials, which include polyimide, polystyrene, and plasma-deposited styrene. To test the validity of the acoustic model using the Love-wave device, we injected bovine serum albumin (BSA) protein into the Love-wave test cell while recording frequency or phase shifts using a vector voltmeter or an in-phase/quadrature (IQ) demodulator. Polyimide had the lowest mass DL, with an estimated value of 1 ng/cm², as compared to polystyrene where DL = 2.5 ng/cm², and to styrene where DL = 6.4 ng/cm². We also developed suitable conjugation chemistries to tether antibodies and fab fragments to the waveguide. We measured the thickness of each film using ellipsometry, from which we calculated the surface concentrations. Preliminary capture studies used biotinylated latex beads. We used the monoclonal antibody BD8, which has a high degree of selectivity for anthrax spores, to capture the nonpathogenic simulant *B. thuringiensis* B8 spores. Using an optical counting method, we prepared spore samples, which contained a background of approximately 10,000 *B. subtilis* spores to determine nonspecific binding. This work demonstrates that Love-wave devices can be used to detect spores at concentrations below infectious levels. Currently, these newly developed modeling tools are being expanded to include viscoelastic waveguiding effects.

This work demonstrates that Love-wave devices can be used to detect spores at concentrations below infectious levels. Currently, these newly developed modeling tools are being expanded to include viscoelastic waveguiding effects.

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10783

Microfabrication of Electromagnetic Devices

T. R. Christenson, W. G. Yelton, C. P. Tigges, D. T. Schmale

Miniature electromagnetic (EM) devices profit from soft ferromagnetic materials with high-saturation flux density and the incorporation of permanent magnet material when appropriate. High-performance microfabricated EM devices, however, remain an integration challenge due to our lack of understanding in depositing high-quality, soft ferromagnetic materials, as well as our inability to cofabricate high-quality factor and high-density EM coils. In this work, Sandia addresses the microfabrication challenges associated with incorporating high-performance magnetic materials, including nickel iron cobalt (NiFeCo) soft magnetic alloys and samarium cobalt (SmCo) and neodymium iron boride (NdFeB) permanent magnet materials into microsensor and microactuator devices. The affected microdevice application areas include high-reliability and relatively high-power handling radio-frequency (RF) electronics, miniature gas and liquid valves, regulators and pumps, positioning microactuators, and miniature generators. The microfabrication techniques explored are based on deep x-ray microlithography and primarily use additive electroforming for the construction of EM features. We found that a repeated wafer-scale diffusion-bonding sequence has significant utility for realizing the complex and intricate geometry implied by EMs.

A number of reports in the literature describe the ability to electroplate high-saturation flux density magnetic material with saturation values up to 2.1 T while maintaining a low magnetostriction coefficient. The application of these films is largely for magnetic recording, and thus the corresponding film thickness is in the range of a few microns. The use of such materials for miniature EM devices, where the cross-sectional area that defines the magnetic flux may be several hundred to several thousand microns square, requires the extension to much greater thicknesses to over several hundred microns. With the use of experimental design technique, Sandia explored several electroplating bath chemistries over a variety of conditions to establish stable low-stress plating configurations amenable to thick electrodeposits of soft, high-saturation flux density ferromagnetic material. We achieved several hundred micrometer deposits of NiFeCo alloys with saturation flux density over 1.7 T with coercivity less than 2 Oe. Such

(a)

(b)

These pictures depict the model (top view) and scanning electron micrograph (bottom view) of a microfabricated eddy-current-damped accelerometer. The device provides one example of precision microelectromechanical devices that may be realized with this integrated approach.

We found that a repeated wafer-scale diffusion-bonding sequence has significant utility for realizing the complex and intricate geometry implied by EMs.

materials can sustain the direct generation of magnetic pressures in excess of 1 MPa or 150 psi.

We took various microfabrication approaches to realize EM coils or inductors. Ultimately, one of the most efficient geometries is one that closely approximates the helical winding of a wound spiral inductor. We developed a three-layer wafer-scale diffusion-bonding process to fabricate single-layer coils with several hundred micrometer sides and interwinding pitch of 35 μm with a magnetic axis parallel to the fabrication substrate. Thus, a one-mil single-layer coil has been closely approximated with a batch microfabrication approach. We found low-temperature ($< 400^\circ\text{C}$) bonding to be achievable, due in large part to the low roughness of the bond joints that we realized with precision lapping and polishing. To support this particular diffusion-bonding work, we developed a custom hot press that can apply a 50-ton load at up to 650°C in an ultraclean vacuum chamber.

Ultimately, packaging of miniature EM devices becomes a dominant manufacturing issue. The implementation of batch diffusion-bonded covers shows significant opportunity for improvements in this regard. We demonstrated another example of a packaging solution with a batch-fabricated eddy-current-damped microaccelerometer using embedded permanent magnets in a proof mass that alleviates the need for fluid packaging and yet provides precisely tailored damping over relatively long proof-mass stroke.

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GaAs MOEMS Technology

O. B. Spahn, J. F. Klem, E. J. Garcia, J. A. Johnson, T. Bakke, G. D. Grossetete, M. A. Polosky, J. L. Reno, C. P. Tigges, M. J. Cich

Use of compound semiconductors to realize microelectro-mechanical systems (MEMS) and microoptoelectromechanical systems (MOEMS) has several advantages. Due to epitaxial growth, they are monocrystalline and atomically flat and have extremely well controlled thickness and stress. Furthermore, use of direct-bandgap semiconductors allows for incorporation of optical functionality into mechanical structures, e.g., truly monolithic integration of lasers, MEMS, and detectors. In addition, there are numerous combinations of materials and release etches that can result in MEMS/MOEMS structures. Finally, the zinc blende structure allows for piezoelectricity as a result of lack-of-center symmetry (in contrast to silicon [Si]), which leads to interesting sensing applications.

Plan view of a 1x4 waveguide switch in operation.

(1) We demonstrated switching in a compound-semiconductor waveguide switch and fabricated these devices in a gallium arsenide (GaAs)/aluminum gallium arsenide (AlGaAs) material system.

(2) We characterized various properties of the compound semiconductor waveguide switch, such as resonant frequency and actuation voltage (mechanical properties), waveguide loss and coupling loss (optical properties), and its temporal performance, such as switching times and damping behavior. We observed novel light-sensitive behavior and advanced various hypotheses to explain it. Further experimental work is needed to fully understand this phenomenon.

(3) We characterized indium gallium phosphide (InGaP), a novel sacrificial material, for its suitability as a release layer for GaAs-based MEMS structures. We measured its crystallographic dependence and etch rates. InGaP is more desirable than AlGaAs as a sacrificial material because it allows for a hydrochloric acid (HCl)-based release, rather than hydrogen fluoride (HF)-based release. Consequently, materials that are attacked by HF can be used in the mechanical layers, such as oxides. This is significant for development of high-reflectivity structures, which rely on utilization of oxides in the alternating layers.

(4) We designed, fabricated, and tested high-reflectivity tilting mirrors (HiRTMs) and surface-normal GaAs-based MEMS structures.

We observed novel light-sensitive behavior and advanced various hypotheses to explain it. Further experimental work is needed to fully understand this phenomenon.

(5) We used analytical and finite-element modeling to understand electromechanical performance of both waveguide and surface-normal structures.

Refereed

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10785

Integrated Microsensors for Autonomous Microrobots

E. J. Heller, R. H. Byrne, D. R. Adkins, R. C. Hughes

The goal of this project is to develop a suite of new low-power integrated microsensor systems that will enable the development of networks of 0.25 in.³ autonomous microrobots. The focus of this work is on two primary sensor classes. The first class consists of microsensors that can be used as navigational and communication aids. Several possible devices in this class include, for example, micro-global positioning systems (GPSs), magnetometers, ultrasonic or optical detector systems (for proximity detection), and single-chip radio-frequency (RF) transceivers. Although a number of possibilities in this class will be considered, only those deemed most suitable to the microrobot application will undergo further development.

The second group of sensors consists of microsensors for environmental trace-chemical detection. There are a number of possible sensors to consider in this class, but microsensor systems based on chemiresistors and surface acoustic-wave (SAW) devices have already undergone the most substantial development and will be given priority. The primary emphasis is to develop microsensors that can take advantage of modern semiconductor manufacturing techniques to efficiently produce large numbers of essentially disposable microsensor systems. As devices are completed, they will be incorporated into microrobots being constructed by others. These microsensors will then be used to enable networks of autonomous microrobots. Several methods of network organization will be considered, but the primary focus is expected to be on "marsupial" systems. These systems use a larger mother robot to deploy and support a large group of networked autonomous microrobots.

Although small robots are typically built using off-the-shelf components such as batteries, motors, and conventional surface-mount electronics, we showed that it is possible to achieve a significant reduction in size by using custom-fabricated components with unpackaged bare-die microelectronics. The focus of this work is to create robotic microsystems that have essentially the same functions as much larger robot platforms.

- *New platform design.* The body of the microrobot is custom-fabricated in a lightweight epoxy resin using a stereolithographic process. An ultraviolet (UV) laser is raster-scanned over a pool of epoxy resin, building the robot body in a

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layer-by-layer process, a few mils at a time. Cavities can be built into the body to hold batteries, circuit boards, and motors. Components are held in the body using off-the-shelf 5-minute-curing epoxy. We adopted a modular design so that individual components, such as motors or circuit boards, can be removed for testing or to replace damaged devices.

- *Control board.* We redesigned the control board containing all of the control electronics for the microrobot for improved reliability and robustness. We moved most components to the underside of the board for better protection. This also allows additional space for microsensors on the front of the robot. Currently, there is space for up to about six microsensors on the microrobot. We used a new PIC microprocessor in a 28-pin metal lead frame to eliminate damage to wire bonds.

- *Wireless communications.* We developed a new, wireless, RF communications microsystem for the microrobot. The system is based on the reduced-fidelity model TR1000 transceiver module, which operates at 3.3 V and delivers a 115 kbps data rate, operating at 915 MHz. The first version of this system had a 30 ft communication range. A second revision, initially intended to offer several improvements, suffered a number of problems with loss and offered only a 3–7 ft communication range with a new chip antenna. We are developing a third revision with a ground plane to decrease noise and a wire antenna for greater communication range.

- *Remote control.* The microrobot remote control is based on the RF communication microsystem. We designed new remote-control boards to be compatible with modular design of the microrobot platform. A liquid-crystal display (LCD) module on a handheld remote-control unit enables reading sensor data back from robot.

- *Programming.* We moved the microrobot software from C-based programming language to PIC Basic Pro for ease of programming changes.

- *Microsensors.* We are adapting several new microsensors for use on the microrobot:

- *Temperature sensors.* We are using new temperature microsensors, linear over a temperature range of 10°–100°F. We attempted to send temperature data over radio link, but data errors resulted in erroneous characters. We are working to improve the integrity of the data transmission.

- *Gold nanoparticle chemical sensor.* Gold nanoparticle chemical microsensors were not stable, and coatings deteriorated over time, perhaps due to breakdown or dissolution of the coating upon the introduction of analyte. In addition, the

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power source must be pulsed to eliminate charge migration of the sensor and drift. This device is still being developed for better reliability.

- *Chemiresistor*. We attached a chemiresistor to the robot. The resistance is typically 1 K ohm in unchallenged state and up to 2 K ohm when challenged.

- *Microphone*. We are configuring a Knowles IM series hearing aid electret condenser microphone (1.3 V, 150 μ A) to send data back to the remote-control unit. An omnidirectional digital microphone from SonioMicrotronic may also be used.

- *Camera*. We are investigating a sample microcamera from Fujitsu. The camera operates at 3 V, 30 mW (15 frames/s). The camera could send images to an LCD module on a handheld remote control.

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Refereed

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10786

Silicon-Integrated Planar Microbatteries

S. H. Kravitz, D. Ingersoll, N. S. Bell

Sandia seeks a new microbattery concept that will be integrated into silicon (Si). By combining Si-micromachining with new cathode and anode materials, this concept will permit batteries to be built directly into integrated circuits (ICs) or micro-electromechanical system (MEMS) devices. The concept is to micromachine interdigitated reservoirs on a Si wafer to serve as containers for the battery materials. The reservoirs will be interconnected by microchannels that provide a means to pass electrolyte between the interdigitated reservoirs without allowing particles through. The reservoirs will be electrically isolated from each other by a thermally grown oxide. We will then add a conductive liner to the reservoirs. We will use stochastic techniques to fully model this device. As testing proceeds, the model will be validated and used to optimize geometries and boundary conditions and to predict reliability.

We will dispense the electroactive material into the reservoirs using MicroPen, a computer-aided design (CAD)-driven system consisting of a high-precision fluid-dispensing unit coupled with an X-Y table. To prevent clogging or migration between reservoirs, we will prepare spherical monodisperse powders with a narrow size distribution by co-precipitation of alkoxides or by flame pyrolysis of atomized chemical precursors.

We will design this device in two different ways. As a series-connected battery, it will supply 100 V to MEMS devices. In parallel connection, it will be a high-capacity/high-power 3 V battery capable of supplying high-current needs for communication or mechanical motion. With some battery chemistries, it will be possible to recharge using photovoltaic (PV) cells. The approach of making an integrated and co-packaged planar power source on a Si chip will reduce the size and cost of a battery-powered system.

We spent this year redesigning, refabricating, and trying to refill the microbatteries. The original design did not leave enough room around each battery compartment to ensure consistent sealing of the battery; the redesign provided better anodic bonding. The redesign corrected other problem areas encountered in the first design. All of these changes were successful, and we achieved good bonding and good yield.

We again tried filling the battery through the fill holes using the MicroPen. We tried various compositions and filling

The approach of making an integrated and co-packaged planar power source on a Si chip will reduce the size and cost of a battery-powered system.

procedures using different-sized needles on sealed devices. Eventually, some devices were filled, but none of these devices was functional. There were two different failure types. Some of the devices shorted. Other devices showed open. The devices were sawed in half and analyzed in a scanning electron microscope (SEM). The 3 μm -diameter separator posts in the shorted devices broke during the filling operation. None of the various compositional changes in viscosity or pressure could prevent one of the pastes from breaking the posts. We also analyzed the open devices in the SEM, which showed that little or no paste was present in one of the compartments. We concluded that we need to try filling the compartments before the lid is attached so that the compartments could be completely filled at low pressures. This should solve the problems of both post breakage and incomplete filling since we can now observe the filling.

We explored a new device and lid attachment sequence and concluded that the lids containing the electrode connection to the outside could be attached with adhesive. There are three criteria for this adhesive: (1) it must not be dissolved in the ethylene carbonate battery electrolyte, (2) it must not contaminate the battery materials, and (3) it must be able to flow between the Si compartments and the Pyrex lid with electrodes.

We achieved the first criterion using either ultraviolet (UV)-curable liquid epoxies or acrylates, which do not dissolve in ethylene carbonate. We achieved the second criterion by providing a deep-etched "moat" around each battery compartment, which prevents the adhesive from flowing into the compartment and mixing with the battery materials. We achieved the final criterion by using liquid adhesives that can wick into the space between the lid and the Si substrate, but that can be hardened by the UV light that passes through the transparent Pyrex glass.

We created a third mask design with deep-etched moats protecting the compartments of each device. We fabricated these devices successfully with high yields and presently are filling the devices with battery material. After filling and baking, we will temporarily clamp the lids to the compartments and measure voltage. Assuming that the batteries will be functional, we will attach the lids by adhesive.

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Refereed

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10796

High-Efficiency Optical MEMS by the Integration of Photonic Lattices with Surface MEMS

J. G. Fleming, S. Y. Lin, M. A. Polosky, S. S. Mani

Optical microelectromechanical systems (MEMS) are emerging as a key element of MEMS technology. However, despite the great interest in this area, the actual optical components employed—mirrors, simple lenses, and waveguides—are primitive. In this project, Sandia seeks a revolutionary advance in both MEMS and photonics through a combination of surface MEMS and the newly emerging field of photonic lattices.

Photonic lattices are the photonic analogues of semiconductors in which the photonic bandgap (PBG) arises as the result of a periodic array of regions of high and low refractive index. As a general rule, the pitch of the lattice corresponds to roughly half the wavelength of light at midgap. The properties of these engineered materials rely only on the index of refraction of the materials and their arrangement. These engineered materials have a number of novel properties, e.g., they can act as extremely efficient mirrors, and they can be “doped” to form very high- Q (quality) optical cavities and highly efficient 90-degree-bend waveguides. In many ways, it is natural to try to combine surface MEMS with photonic lattices. Silicon (Si), the basic structural material of MEMS, can also be used to form the lattice. Since the lattice properties rely on the repeat unit, which is small, small changes in dimension can result in large changes in optical properties of the lattice. Such small, well-defined displacements are readily obtained using MEMS processing.

We fabricated and tested one-dimensional (1-D) switching structures and fabricated the first iteration of large dielectric stack mirrors integrated with surface MEMS. In both cases, we identified the major fabrication problem as residual stress in the mirror stacks. We obtained useful switching-cavity data; however, the large integrated mirror structure required a redesign. The redesign involved the addition of a drumlike stiffening rim around the mirror combined with a series of stiff springs between the rim and the mirror, which can deform to relax the mirror stress.

We also fabricated hollow waveguides in which a 1-D mirror confines light in a hollow tube. These structures have been proposed sporadically by various groups since the 1960s; however, they are difficult to fabricate, especially on a small scale. These devices are structurally very similar to the channels

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being developed for bioMEMS/fluidics. There may be significant value to having a single platform, which can be used to channel both light and fluids. We demonstrated the waveguiding of light at 1.5 μm with 2–5 dB/cm loss, the efficient bending of light (0.35 dB/bend), waveguide splitting, and the guiding of light in visible wavelengths.

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Refereed

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26518

III-Antimonide/Nitride–Based Semiconductors for Optoelectronic Materials and Device Studies

G. M. Peake, S. R. Kurtz, E. D. Jones, N. A. Modine, J. G. Cederberg, K. E. Waldrip, J. F. Klem

Vertical-cavity surface-emitting lasers (VCSELs) operating at 1.3–1.55 μm would revolutionize communication technology due to the high efficiency, excellent beam quality, and manufacturability of VCSELs. Current promising materials are based on indium gallium arsenic nitride (InGaAsN) or gallium arsenic antimonide (GaAsSb), both grown on GaAs substrates where the superior thermal conductivity and index contrast of aluminum gallium arsenide (AlGaAs) distributed Bragg reflector (DBR) mirrors can be employed. However, because of poor valence or conduction band alignments, these systems do not satisfy the needed temperature stability. Sandia believes the GaAsSbN material system is a superior candidate for the 1.3–1.55 μm semiconductor laser system because it offers fewer difficulties with strain-layer growth and may be made to span a range of bandgaps from 0.8 to 1.2 eV (1.55–1 μm). However, lack of basic information concerning this alloy restricts its use in semiconductor devices. Therefore, we are thoroughly investigating the GaAsSbN alloy system. The growth of this material for laser applications is completely new and has not been investigated. The material properties of this alloy are poorly characterized, which affords an excellent opportunity for Sandia's world-class expertise in growth and characterization of novel semiconductors. This investigation will also enable us to expand the understanding of dilute nitride alloys beyond our existing world-class efforts in InGaAsN. We assembled a research team for this project that has demonstrated leadership in the research and device community through publications, invited presentations, and record device performance in developing new semiconductor alloys.

We performed band-structure calculations for GaAsSbN and InGaAsN to examine the effects of clustering. We found the configuration of the nitrogen (N) atoms to be the dominant mechanism for bandgap fluctuations in the mixed anion nitrides. We also performed band-structure calculations for AlGaAs and GaAsSb containing 16% Al (Sb) in a disordered configuration that confirmed our previous predictions on the small (20 meV) band repulsion in AlGaAs compared with more than 100 meV of band repulsion in GaAsSb. We performed

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preliminary calculations investigating N incorporation at Sb-covered surfaces. We concluded that the enhancement of N solubility at a GaAsN compared to a GaAs surface is due to the lower energy of the relatively small N atoms when they are substituted in compressively strained locations under the surface dimers of the reconstructed surface.

We produced organometallic vapor-phase epitaxy (OMVPE)-grown GaAsSbN material with room-temperature (RT) photoluminescence (PL) out to 1.29 μm and material with RT PL out to 1.25 μm that was incorporated into a laser structure and is currently in fabrication. We used x-ray diffraction (XRD) measurements of strained-layer superlattices to measure high-quality interfaces grown by OMVPE. We grew GaAsSbN by molecular-beam epitaxy (MBE) using reactive N species supplied by a radio-frequency (RF) plasma. We performed initial studies with low N concentrations (0.1%–0.2%), resulting in significant reduction in the RT PL relative to N-free samples; however, post-growth rapid thermal annealing produced a noticeable improvement in the PL. Samples grown with substantially higher N concentrations have correspondingly weaker RT PL characteristics; nevertheless, they exhibit relatively bright and narrow PL at low temperatures. We measured PL at 4.2 K out to 1.66 μm for unannealed GaAsSbN. We believe these quantum wells (QWs) to be among the smallest-bandgap type-I materials ever grown coherently on GaAs substrates.

We measured low-temperature (4 K) exciton diamagnetic shifts between 0 T and 33 T; upon comparing the results for two GaAsSb-strained QW samples, one with N and one without, we found that the conduction band mass is heavier for GaAsSbN than for GaAsSb. Similar results for InGaAsN have also been reported in the past. Thus, the anticrossing band model to successfully analyze the InGaAsN band structure is applicable to GaAsSbN. We plan future experiments that will provide exact mass enhancement values.

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26519

The Integration of Advanced Photonics and MEMS

J. G. Fleming, C. T. Sullivan, S. Y. Lin

There is considerable interest in optical microelectromechanical systems (MEMS). However, such devices typically do not take advantage of the full range of possibilities that arise from the wave nature of light. These devices typically consist of conceptually simple, but structurally complex, mechanical systems that are really just movable mirrors. One potentially interesting area of research is that of ring resonators and waveguide couplers. Physically, these are simple structures, but they have the potential of being able to act as narrow, high-efficiency band filters/drops couplers and switches. Progress in this area has been hindered by fabrication difficulties and difficulties in switching. The application of MEMS to this area potentially solves both problems. What is more, the size scale of such devices is almost ideal for MEMS; small displacements give rise to large changes in optical properties. Perhaps due to relatively recent rapid progress in fields that traditionally have not overlapped, there exists a window of opportunity to combine elements of the two fields to make significant technological advances. MEMS can offer to advanced photonics a simple, manufacturable "switch." On the other hand, advanced photonics offers the ability to not just reflect light in free space, but also to confine light within waveguides where it can be efficiently manipulated, switched, and filtered. This added functionality can not be realized by current MEMS technology. In this project, Sandia demonstrated switches, splitters, and attenuators. We fabricated, but have not yet optically tested, ring resonators. All of these devices were fabricated in a single run, and all are relatively small and intercompatible. The level of functionality that we already demonstrated would be very difficult to demonstrate in standard "mirror" MEMS processing. The functionality we believe we can achieve with ring resonator structures is completely beyond the capability of standard "mirror" MEMS.

Previously, we fabricated and actuated a single-crystalline silicon (Si) structure in which the waveguides were translated into proximity to create couplers, and into proximity to a ring to create switchable ring resonators. However, during testing of the devices, we found them to be too fragile to survive reasonable testing and processing, such as grinding end faces to improve input coupling. As a result, we moved on to dielectric

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waveguides integrated with a vertically actuated tungsten (W) plate onto which we attached various optical elements. This configuration is far more robust and offers a higher level of functionality. We developed a novel fabrication process to realize these structures. It involves silicon nitride (SiN)—based waveguides with a silicon-dioxide (SiO₂) lower cladding, a polysilicon (poly-Si) sacrificial layer, and a W actuation plate. Mechanically, the design is stable through its range of motion with actuation voltages between 40 V and 100 V, depending on the function targeted. It should be quite possible to lower the actuation voltage. The structures are currently stiff enough to allow air-drying, and we have observed no incidences of stiction during actuation. In the actuated state, these electrostatically based structures consume almost no power. The design allows for a continuous range of optical coupling. A wide variety of devices were laid out and fabricated in the same process flow. These include three types of broadband switch: splitters based on couplers, attenuators based on adsorption by a metal plate, and narrowband switches based on ring resonators. We demonstrated the broadband switch, attenuator, and splitter to work experimentally. We mechanically fabricated and tested the ring resonator-based narrowband switch.

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Aging Mechanisms in Dormant MEMS Structures

T. M. Mayer, B. C. Bunker, M. P. De Boer, D. R. Jennison

Thin organic films can render microelectromechanical systems (MEMS) surfaces hydrophobic, eliminating the catastrophic effects of capillary-driven interfacial adhesion. However, even treated surfaces can demonstrate strong adhesion and stiction after long-term environmental exposures due to aging and restructuring within the antistiction films. The physics and chemistry of interactions between micromachine components is poorly understood. Consequently, micromachine performance as a function of time and storage conditions ("dormancy") cannot yet be predicted. In this project, Sandia seeks to elucidate the mechanisms of property evolution in hydrocarbon and fluorocarbon coatings with an emphasis on self-assembled monolayers (SAMs). We employ a suite of in situ experimental probes to determine (1) how the molecular structures and compositions of MEMS surfaces change with time and environmental exposure, (2) how these molecular changes influence the interfacial adhesion between well-defined, nanometer-scale, single-asperity contacts, and (3) whether models based on molecular- and nanoscale experiments can be used to predict the evolving interactions between rough surfaces in model micromachine components. The result of this project will be the development of physical and chemical models for dormancy in MEMS that span molecular-, nanometer-, and micron-length scales. The models will provide a framework for evaluating MEMS environmental and packaging requirements and for developing more robust MEMS designs and antistiction coatings. This project will complement device- and system-level modeling efforts by providing experimental input to and validation of simulated interfacial phenomena for both molecular-scale dynamics of contacting surfaces and mechanical modeling of realistic MEMS structures.

We made significant progress in evaluating the stability of fluorinated alkylsilane films in humid environments, measured thermal decomposition of films in simulated packaging environments, and began to elucidate the mechanism and kinetics of film decomposition. We are evaluating adhesion energies of single-asperity contacts of freshly prepared and aged films and macroscopic tests of adhesion using cantilever-beam structures in a controlled-atmosphere environment. Highlights of recent work include interfacial-force microscope

The result of this project will be the development of physical and chemical models for dormancy in MEMS that span molecular-, nanometer-, and micron-length scales. The models will provide a framework for evaluating MEMS environmental and packaging requirements and for developing more robust MEMS designs and antistiction coatings.

(IFM) measurements of adhesion and friction of fluorinated alkylsilane films that are tightly bound to the surface. We showed that strong substrate binding leads to outstanding tribological performance, even after exposure to very high relative humidity for extended periods. We observed no film restructuring and no degradation of mechanical properties for tightly bound films. The alkylsilane films do exhibit a potential for thermal degradation under conditions of $> 300^{\circ}\text{C}$ in vacuum, a condition seen during packaging operations. X-ray photoelectron spectroscopy (XPS) measurements show that chain scission of the alkyl chain is the likely mechanism, and we measured activation energies for this process. In anticipation of problems associated with thermal stability of the fluorinated alkylsilane films, we began to investigate alternative films based on short-chain alkylsilanes or aromatic silane precursors. We spent considerable effort in preparation for more quantitative measures of film adhesion by IFM and cantilever-beam techniques. These measurements require careful preparation and characterization of IFM tips, and better control of environmental conditions than we were able to accomplish previously. Reconstruction of an environmental IFM and construction of a new environmental chamber for cantilever-beam studies of adhesion are nearing completion, and then we will perform planned measurements.

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32923

MEMS in μ Fluid Channels

C. I. H. Ashby, C. M. Matzke, T. L. Sounart, G. D. Bachand, S. S. Mani, M. Okandan

Microelectromechanical systems (MEMS) comprise a new class of devices that include various forms of sensors and actuators. Recent studies show that high-sensitivity MEMS cantilever structures, appropriately functionalized with chemically sensitive films or biological receptors, are able to detect a wide range of chemicals, biomolecules, or even single bacterial cells. In this approach, cantilever deflection replaces optical fluorescence detection, thereby eliminating complex chemical tagging steps that are difficult to achieve with chip-based architectures. A key challenge to utilizing this new detection scheme is the incorporation of functionalized MEMS structures within complex microfluid (μ fluid) channel architectures. The ability to accomplish this integration is currently limited by the processing approaches used to seal lids on pre-etched μ fluid channels. This project will combine Sandia's leading capabilities in MEMS processing with our newly developed low-temperature photolithographic method for fabricating μ fluid channels to construct MEMS-instrumented μ fluidic chips. We will initially apply this approach to immunospecific detection of bacterial cells in collaboration with Cornell University. We will also explore in situ cantilevers as a new approach to directly monitor fluid transport within μ channels. Cantilever-based detectors offer aN (10–18) force sensitivity that can be used to detect local flowrates and pressure gradients within μ fluidic channels. (Localized pressure and flow instruments currently are not available, but are critical to optimizing μ fluidic architectures.) Initial work will focus on passive MEMS structures; later in the project we will extend this new integrated approach to incorporate actuated MEMS that can be used to direct or otherwise modify μ fluidic-flow environments.

We measured the viscosity of a fluid in fully encapsulated μ fluidic channels using surface-micromachined, low-stress polysilicon (poly-Si) structures. These structures consist of a poly-Si plate clamped on three edges with one edge free to move, suspended above the surface of the Si wafer inside a hermetically sealed fluidic channel. The measurement of the angular deflection of the plate can be used to calculate the viscosity of an unknown fluid to an accuracy of 10%. We used fluids with viscosities in the range from 0.59 centi-Poise (cP) to

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2.3 cP at flowrates between 0.5 ml/hr and 8 ml/hr for the experiments performed.

Comb-drive resonators are being used to measure viscosities of polymer solutions in nonpolar solvents to begin the development of a MEMS microrheometer. The rheological behavior of complex fluids, such as polymer solutions, is modified when the fluid is confined to geometric length scales approaching a characteristic length of the fluid components (e.g., chain length). While preliminary measurements are being made with the resonators, we are designing a MEMS device to characterize complex non-Newtonian fluids in μ fluidic environments.

Dynamically driven μ fluidic sensors (e.g., for flow, viscosity, and chemical sensing) require electrostatic actuation in aqueous electrolytes. This, however, requires a better understanding of the electrochemistry and electrostatics associated with operating electrically driven Si devices in leaky dielectrics. For example, electrolysis, Debye screening, and anodization of the Si must be avoided to maintain device operability. We designed and are conducting experiments with comb-drive resonators to establish methods for electrostatic actuation of a Si device in water and other polar liquids. Using amplitude modulation (AM) drive signals up to 50 V, we successfully actuated resonators in polar organic liquids such as ethylene glycol and isopropanol. Current studies are aimed at driving the devices in water and realizing higher electric potentials.

We demonstrated the ability to adhere several different deoxyribonucleic acid (DNA) oligomers to silicon-dioxide (SiO_2) surfaces using divalent magnesium (Mg_2^+) to link the negative phosphate backbone of DNA to the surface. We used epifluorescence microscopy to confirm the presence of DNA, and atomic-force microscopy (AFM) to image the properties of the DNA films. The DNA remained attached to SiO_2 surfaces in the presence of aqueous buffers as well as organic solvents (e.g., acetone). Moreover, incubation of oligomers at temperatures characteristic of photolithographic processing (as high as 100°C) did not affect the integrity of the DNA. We recently demonstrated that DNA tethered on a Si/ SiO_2 surface through Mg_2^+ coupling is capable of hybridizing with the complementary strand of DNA as a probe. Current experiments involve adhesion of DNA to SiO_2 surfaces and subsequent formation of μ fluidic channels to test the compatibility of microfabrication processes with adhesion of DNA probes. DNA

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hybridization will confirm the presence and integrity of the DNA probes post-fabrication.

Refereed

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33602

Dispersive Photonics for Next-Generation Sensors and Microsystems

G. A. Vawter, S. A. Kemme, M. J. Hafich, W. J. Zubrzycki, C. R. Alford, S. Y. Lin, G. R. Hadley, J. R. Wendt

Artificially structured photonic bandgap (PBG) materials are commonly investigated for their unique ability to block and guide light. However, an exciting aspect of PBGs that has received relatively little attention is the extremely high refractive index distortion near the edge of the bandgap, but within the range of frequencies capable of propagating within the PBG material. In fact, it was recently proposed that a negative refractive index may be realized with the correct PBG configuration. Sandia proposes to investigate, both numerically and experimentally, the design and performance of such PBG materials intended to optimize the “distortion” of refractive index to realize new classes of photonic devices. For example, stripes of positive and negative refractive index form a planar “lens train” capable of guiding light much like a sequence of spherical lenses guides a Gaussian beam. Quadrants of positive and negative index will form a resonant optical cavity without mirrors or waveguides of any kind.

These optical properties of PBGs are expected to yield new and unexpected applications as understanding and fabrication technology develop in the next few years. It is feasible that guided light might be focused to extremely high intensity and used to probe micro- or nanocavities filled with organic material in a chemical or biological sensor role, such as cytology, or that refractive index of a fluid could be monitored with a very sensitive threshold wherein the strong index distortion effect would dramatically alter the optical properties of a waveguide or resonant cavity.

We conducted significant numerical investigation into the behavior of PBG structures with unique physical properties, culminating in the design of devices to experimentally demonstrate these properties and to ascertain the feasibility of possible applications. Fabrication of this design on a wafer is currently progressing, with mask design and wafer growth already completed.

We performed numerical modeling, indicating that interesting dispersive effects can be seen in devices that may be fabricated using Sandia’s current capabilities. Within structures comprising air holes in gallium arsenide (GaAs), we observed negative refractive behavior in the numerical modeling. This

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effect is present for angles ranging ± 10 degrees from the normal. At larger angles the effect gives way to diffraction into multiple beams and scattering. In addition, we simulated tightly focusing negative index lenses.

Ground-breaking simulations of propagation loss within PBG waveguides show that regions of reasonable low loss can be found in designs previously felt to be “nonguiding,” using older simulation tools and concepts. These observations led us to conclude that out-of-plane losses in row-defect waveguides occur as a result of resonant coupling between the fundamental slab eigenmode and its radiation modes as a result of the “corrugation” imposed by the hexagonal hole pattern.

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Engineered Superconductivity in Electron-Hole Bilayers

M. P. Lilly, J. L. Reno, J. A. Simmons, L. L. Stephenson, R. G. Dunn, D. R. Tibbetts, E. S. Bielejec, J. A. Seamons

Sandia seeks to fabricate and measure transport characteristics of an electron-hole bilayer (EHBL). Due to the strong attractive interaction between the oppositely charged carriers, we expect this system to make a transition to a superconducting state at low temperatures. We will implement the EHBL in gallium arsenide/aluminum gallium arsenide (GaAs/AlGaAs) heterostructures, where individual layers can be in close proximity to maximize the Coulomb energy. Additional critical features will be high electron and hole mobilities, low sheet densities, and independently contacted layers. Through use of bandgap engineering, these parameters can be tuned to optimize the device.

The success of this project relies on the integration of four techniques: molecular beam epitaxy (MBE) crystal growth, use of undoped heterostructures, dual-side lithography, and Coulomb drag transport measurements. Since the superconducting state depends on interactions between the layers, the high-mobility MBE heterostructures are required. To avoid problems that arise with doping bipolar systems, we will implement undoped heterostructures. We generate the carriers using self-aligned contacts in a field-effect transistor (FET) geometry; this technique is consistent with high mobility and low density. In the EHBL device, self-aligned contacts are needed above and below the bilayer. To achieve this, we will use the epoxy bond and stop etch (EBASE) technique developed at Sandia. Finally, to observe the superconducting state, we plan to use a transport technique, Coulomb drag, that is sensitive to electron-electron scattering between the layers. At Sandia we have demonstrated expertise in each of these areas. Using this expertise, we will fabricate EHBLs and search for the superconducting ground state.

Improvements to processing techniques have made undoped GaAs devices more reliable and reduced extrinsic modification to the two-dimensional (2-D) systems. Early efforts focused on fabrication of undoped single-layer devices, and we have been able to use the first generation of devices to address important physics problems such as the 2-D metal insulator transition (MIT) and weak localization.

In the EHBL device, self-aligned contacts are needed above and below the bilayer. To achieve this, we will use the epoxy bond and stop etch (EBASE) technique developed at Sandia.

Using the Compound Semiconductor Research Laboratory cleanroom, we fabricated single 2-D layers of both electrons and holes in a FET geometry. These samples, made from extremely high purity MBE undoped heterostructures, can be gated to world-record low density and exhibit a high mobility at all densities. Important advances in processing include reliable shallow contact to the n⁺ gate layer and improved ohmic contacts to the 2-D layer. We uncovered strain-induced density modulation in the early devices. Redesigning the device geometry greatly reduced the extrinsic strain effect and allowed record-low 2-D densities to be achieved. These processing techniques will be critical as we begin fabricating the more-complex bilayer devices in the coming year.

The successful fabrication of undoped heterostructures allows transport experiments in a new regime of dilute 2-D electron systems. We studied the temperature dependence of the resistivity of a dilute 2-D electron system for a range of densities. At high density, well-known phonon scattering dominates. At lower density and temperature, phonons freeze out, and a nonmonotonic resistivity is observed. Using both experimental results and theoretical calculations, we show that the nonmonotonic behavior is due to known temperature dependences of scattering from ionized impurities. Results from this experiment indicate that electron-electron interactions do not cause the 2-D MIT, a result of interest to the community studying this problem.

Our most recent experiments involve studies of weak localization in the high-quality 2-D electron and hole layers. Weak localization is a quantum correction to the resistance that arises from interference effect due to the wavelike nature of electrons. In electron systems, straightforward localization is typically observed. In hole systems, a more complicated combination of localization and antilocalization occurs due to hole-hole interactions. Both behaviors have been previously observed, but never in the same GaAs structure. Because we can create high-mobility 2-D electron and 2-D hole layers in the same undoped structure, with a single sample we will be able to directly compare the localization and antilocalization effect for the first time. Preliminary results are quite exciting, and the experiment is ongoing.

Advances in processing single-layer undoped structures have allowed transport experiments in previously unattainable regimes (low density and direct comparison of electrons and hole). We made significant progress toward creating and understanding the ultimate goal of this project, electron-hole bilayers.

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Silicon-Based RF MEMS Components

C. W. Dyck, J. G. Fleming, S. E. Allen, J. E. Stevens, C. E. Sandoval, M. S. Baker, C. D. Nordquist

Radio-frequency microelectromechanical systems (RF MEMS) is an enabling technology for the next generation of communications and radar systems in both military and commercial sectors. These devices have low insertion loss, low static power consumption, are lightweight, and are capable of high levels of integration with other components. Successful development of this technology would directly benefit strategic business units and the commercial sector for frequency ranges below 10 GHz. Historically, III-V compound semiconductor material has been used for RF communications components. However, preliminary concept prototypes in silicon (Si) show 10 GHz operation with 0.5 dB loss for Si-based, co-planar waveguide (CPWs). Based on these data, Sandia believes that it is possible to produce RF switches capable of efficient operation in the 10 GHz range with our novel and patented Si RF MEMS technology. Leveraging off of the RF switch development, we seek to prototype microdeployable antennas using actuation or fluidic approaches that allow for the flexibility in deploying antenna structures when needed for operation. In addition, we will design, fabricate, package, and test other low-loss RF MEMS components.

We evaluated high-resistivity (R) Si as an RF material by measuring the insertion loss of metal CPWs on high-R Si. The signal loss was 0.11 dB/mm below 32 GHz, similar to the insertion loss of thin metal CPWs on GaAs. Signal loss was dominated by the metal conductivity and not the substrate dielectric properties at these geometries. This was also the case for transmission lines that we fabricated using the Si standoff process. The limiting factor with high-R Si seemed to be process temperature.

We designed and fabricated RF switches using the Si standoff process. These devices were not RF functional due to a design error, but were nevertheless electrostatically actuated 1 billion cycles (tungsten [W] contact) without sticking. Currently, new devices are being processed that will solve the design error and that have improved RF responses over what the previous devices would have had. We added a dual damascene metal-deposition process to lower the series conductivity of the W CPWs and to add a second micromachining level. Initial development has already been

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successful on this part of the process, and we are close to releasing these structures.

We planned to fabricate an RF switch using the Si flip-chip process, then compare this process to the Si standoff process to determine the best approach. This happened much earlier than anticipated. High process temperatures caused the high-R Si wafers to severely warp, preventing us from pursuing a SUMMIT™ (Sandia Ultraplanar Multilevel MEMS Technology)-like surface-micromachining (SMM) process. We limited process temperatures to 800°C and observed no further warping.

We developed two new switches to compare to the Si stand-off process. The first switch consisted of aluminum CPW transmission lines. We suspended the center portion of the signal line above a shunt capacitor to the CPW ground lines. In the unactuated state, the incident RF signal on the CPW passed with minimal signal reflection, as the capacitive coupling between the signal line and the ground line was small. Application of a voltage between the signal and ground lines pulled the movable portion of the signal line down onto the capacitor dielectric, substantially increasing the capacitive coupling between the signal line and the ground line. At high frequencies this presented an RF short, causing most of the incident RF signal on the CPW to reflect. We successfully fabricated and tested these devices. They had good RF performance, but they suffered from unreliable operation due to pinholes in the dielectric material. This caused dielectric breakdown at the voltages required to actuate the structure.

We developed a second switch type to solve these problems. The general form of the switch remained unchanged; however, when we pulled down the movable portion of the signal line of this switch, it made contact to a second metal contact, which we then routed to a fixed capacitor. This change allowed us to better protect the capacitor dielectric from pinhole formation. We successfully fabricated and tested devices. These structures exhibited even better RF performance and were capable of more reliable operation. Current work on these switches focuses on improving the metal-metal contact and on redesigning the devices for easier implementation into switched filter and phase-shifter circuits.

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2-D Arrayed Resonant Subwavelength Gratings

S. A. Kemme, J. R. Wendt, G. R. Hadley, T. R. Carter, M. E. Warren, S. Samora, D. J. Rieger, C. L. Grotbeck

Sandia seeks a novel optical device that produces a dense two-dimensional (2-D) array of wavelength- and mode-selective reflectors. The resonant subwavelength grating (RSG) acts as a photonic crystal (PhC) as it reflects any specific spectral, spatial component from a wideband light beam. All of the light is transmitted straight through the device, except for the 100%-reflected narrow-wavelength (0.01–20.0 nm) and angular (~ 1 mrad) band of interest. This new concept of an RSG was first theoretically proposed in 1990, but fabrication efforts were undertaken only recently.

This unexplored component addresses the anticipated needs of the remote-sensing and data-communications communities such as (1) miniaturization of synthetic-aperture radar (SAR) and (2) small satellite research. Because this component can perform in both sensing and communications functions, the RSG is an enabling technology for a distributed and interconnected sensor web. Currently, a comparable technology for 2-D arrays does not exist.

As a narrow-band notch filter, the RSG is an optimal multiplexing/demultiplexing component for optical-communication and -sensing applications. Unlike thin films, RSG characteristics may be abruptly altered from one lateral position to the next to realize a 2-D array of wavelength filters or oriented polarizers.

RSGs are advantageous for secure wideband communications where free-space, broadcasted information could be spectrally encoded or polarization-encoded and covertly detected over narrow angular bands.

In the 2-D-array configuration, RSGs can be matched to an array of detectors or chem/bio cells for integrated optical sensing. Applications include narrowband filter arrays for fluorescence detection or single-chip integrated spectrometer detection arrays.

We conducted significant numerical modeling of the behavior of RSGs, culminating in a final design of a first-generation device with a narrow linewidth and extremely low sidebands. Testing of fabrication processes for the purpose of characterization and calibration is ongoing.

We conducted significant numerical modeling of the behavior of RSGs, culminating in a final design of a first-generation device with a narrow linewidth and extremely low sidebands.

The modeling indicated that a higher refractive index for the waveguide layer resulted in a narrower resonance; thus, we selected a thin film of titanium dioxide (TiO_2) ($n=2.4$) for this material. We then needed a lower-index material for the grating layer; this layer will act as an antireflection coating for wavelengths outside the resonance condition. The chosen thicknesses are optimized values that minimize reflectivity for all wavelengths in the range 700 nm to 1000 nm, except for the reflectance peak at 850 nm. The reflectivity across this wavelength range shows a full-width half-medium (FWHM) of 1.6 nm and a peak reflectivity in the sidebands of less than 0.035, with a reflectivity of unity at the central wavelength.

To form an array of these devices without requiring additional processing implies that one of the device parameters that is determined by the photolithographic mask must be changed. The optimum duty cycle for low sideband reflectivities was 0.4. Variation of the period of the grating, with all other device parameters held constant, results in linear change in the reflected wavelength with little detriment to sideband suppression. The change is virtually linear, and the sideband reflections are not enhanced by changing the period over this range. These changes in period may be made on the mask easily.

We performed characterization and calibration of fabrication processes. We grew TiO_2 on fused silica substrates at Sandia. In parallel, we ordered TiO_2 thin films on fused silica from CVI Laser. We measured the refractive indices of these layers, which are approximately 2.4 ± 0.1 . We plan to accommodate this variation by first characterizing the thin-film layer before proceeding with grating fabrication. In this iterative approach, the thin-film parameter variations may be compensated for in the subsequent design and fabrication of the grating layer.

In this RSG application, the incident light will approach a plane wave, but each pixel size in the array must be small enough so that the entire array extent is compact. Pixel dimensions of 100–300 μm would be acceptable. We expect the peak reflectance to decrease and the spectral FWHM to increase as the RSG pixel lateral extent decreases. Our design is modeled using a fourth-order accurate finite-difference representation of the 2-D Helmholtz equation. We use absorbing and radiation boundaries along the problem boundaries. For these simulations the device parameters are $t_{\text{GRATING}} = 139 \text{ nm}$, $t_{\text{WAVEGUIDE}} = 185 \text{ nm}$, $n_{\text{SiO}_2} = 1.4525$, $n_{\text{TiO}_2} = 2.15$, and pitch = 470 nm.

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We modeled grating pixels with widths of 360 μm and 180 μm . The incident radiation is a normally incident Gaussian with a width equal to the width of the pixel. Reflectivity decreases from the idealized case of 100% to 87% and 59% respectively. The sidebands in the finite case remain low while the FWHM increases only modestly from the infinite-extent case of 1.66 nm, to 1.7 nm for the 360 μm case, and to 2.3 nm for the 180 μm -wide pixel.

Finally, we successfully fabricated and characterized large-area (1 mm) RSGs. Measurements of the peak reflectivity (87%) and concurrent minimum transmissivity (5%) confirm that large-area RSGs can be fabricated with little light loss to scatter and absorption.

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38619

Nanoelectromechanical Oscillators (NEMOs) for RF Filtering

J. P. Sullivan, C. W. Dyck, T. A. Friedmann, C. P. Tigges, W. K. Schubert, J. R. Wendt

In this project, Sandia will create high-frequency and high-quality (high- Q) nanoelectromechanical oscillators (NEMOs) for radio-frequency (RF) signal processing, and will demonstrate a solution to charge trapping in capacitively coupled RF microelectromechanical systems (MEMS) switches. NEMOs are mechanical oscillators with critical dimensions < 50 nm and GHz resonance frequencies. These devices would be valuable as simple, inexpensive passive RF filters for Sandia projects, including narrowband communications, radar, and RF signal processing. The primary obstacle to NEMOs is to maintain high Q with a high resonant frequency, F . We will address this obstacle by (1) using a new, ultrahigh modulus MEMS material, amorphous diamond (a-D) (with F twice that of silicon [Si]), (2) using a new vertical-cantilever NEMO design that should be easy to fabricate and that permits oscillator arrays, (3) using parametric amplification to increase the resonance amplitude and narrow the dispersion, and (4) performing fundamental studies of energy dissipation in nanosized structures to understand how to increase Q .

A second objective of this project is to eliminate the reliability problem in capacitively coupled RF MEMS switches due to oxide charging. We will use the dissipative dielectric, a-D, for the dielectric spacer layer and evaluate its performance. We expect this material to enable improved performance due to its charge-dissipation capability, its extreme smoothness (permits thin dielectrics), its hydrophobicity (reduces stiction), and its wear-resistance. We made fundamental measurements of internal dissipation in a-D and fabricated and tested a-D MEMS resonator structures. We evaluated the structure of a-D using solid-state nuclear magnetic resonance (NMR) on fully enriched carbon-13 (^{13}C) a-D films, and the effect of network coordination on internal dissipation and network rigidity (Young's modulus). We also fabricated and tested RF MEMS switches and evaluated the integration of a-D with these structures.

We made significant progress in two key technology areas for RF MEMS. In the area of RF switches, accomplishments include the completion of a capacitively coupled RF MEMS switch design and the fabrication of the first working switch

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prototypes. These devices use a suspended gold (Au) signal line that is electrostatically brought in contact with a dielectric spacer. Processing tests with a-D show that it has good adhesion and is compatible with the materials used in the switch (e.g., Au and gallium arsenide [GaAs]), and integration of a-D as the dielectric spacer is in progress. We expect this material to increase switch lifetime by eliminating the failure mode associated with dielectric charging. We also made progress in the development of RF NEMOs. Initial focus was on the development of a processing sequence to fabricate dense arrays of in-plane cantilevers that would be designed to have resonant frequencies from sub-MHz up to GHz. We built an experimental capability to enable testing of the internal dissipation and resonant frequency of the mechanical oscillators under high-vacuum conditions. We made the very first measurements (to our knowledge) of internal dissipation in an a-D-like carbon (C) film and found that the quality factor was ~ 2700 – 5000 . This value, which represents a lower limit because of clamping losses at the connection between the resonator and its support, is sufficiently high for use as a filter, provided it can be maintained at high frequencies. We also used the measured resonant frequency of a number of different-sized a-D mechanical oscillators to determine the material's Young's modulus. We performed annealing studies to increase the threefold to fourfold coordinated C ratio in this material and quantified the effect on Young's modulus and internal dissipation. Surprisingly, we found little softening of the modulus as the threefold to fourfold ratio was increased. This represents a significant departure from network rigidity models, which predict a power-law decrease in Young's modulus as the mean network coordination is decreased. One implication of this result is that high-frequency a-D oscillators should be possible, even for high threefold C concentrations. We performed detailed structural studies using solid-state NMR on a-D films synthesized from ^{13}C . These studies revealed that structural changes occur in a-D as a result of annealing. The most dramatic effect is a reduction in the distribution of bond lengths associated with fourfold and threefold coordinated C and a net decrease in volume of the fourfold part of the sample and a net increase in volume of the threefold part. These findings suggest a novel and unpredicted stress-relaxation mechanism in this material. To date, no major obstacles to meeting project objectives have been uncovered.

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38620

Continuous-Wave Intersubband Terahertz Sources

M. C. Wanke, G. A. Vawter, C. T. Fuller, J. L. Reno, A. V. Smith, R. J. Foltynowicz, S. Samora

There is a general lack of compact solid-state sources between 1 and 10 terahertz (THz), a challenging spectral region lying between optical devices at high frequencies and electronic devices at low frequencies. This region is of great technological importance for higher-bandwidth space-based and short-range terrestrial communications, atmospheric sensing, and near-object analysis for chem/bio sensing. While the last few years have seen much experimental work in ultrashort-pulsed terahertz sources, many important applications require continuous-wave (CW) sources, which remain in their infancy. Sandia is examining two approaches to terahertz generation based on intersubband transitions.

In the first, a quantum cascade laser simultaneously emits two mid-infrared (MIR) frequencies differing by a few terahertz. These are used to pump a nonlinear optical material to generate terahertz radiation via parametric interactions. As a specific example, we will examine difference frequency generation by three-wave mixing in a specifically engineered intersubband transition.

In the second approach, we will investigate efficient terahertz harmonic generation based on nonlinear transport and multiphoton transitions in semiconductor superlattices. The terahertz emission arises when the intersubband transition between two minibands is equal to the multiphoton resonance of the alternating current (AC) driving field.

We focused on a path toward terahertz generation, which will use a quantum cascade laser simultaneously emitting two MIR frequencies differing by a few terahertz. We use these to pump a nonlinear optical material to generate terahertz radiation via parametric interactions. The areas of quantum cascade laser development and CW solid-state terahertz source development are new to Sandia. Sandia has done extensive frequency-mixing work, but not in intersubband systems; thus this direction is also new. Success in this area has significant implications for future remote optical-based sensing capabilities.

We assembled a characterization and testing lab for terahertz and far-infrared (FIR) radiation from the ground up, enabling significant new capabilities that will be a key

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component of future work at Sandia in this spectral region for sensing and communication. We designed and tested a process for fabricating quantum cascade lasers and acquired mounting techniques capable of surviving repeated cycling to low temperatures for sample characterization. Beyond our listed milestones, we also significantly enhanced our calculation abilities for heterostructure design and analysis. We designed and grew quantum cascade structures by molecular beam epitaxy (MBE) and completed the fabrication steps. Some of these are designed to operate in the MIR as required for our initial stages to terahertz generation. We began electrical and optical characterization of these structures and have fully functioning lasers with operating wavelengths near 10 μm . Power and operating temperature are currently below design specifications, but we feel confident that these issues will be resolved soon.

Due to recent successes making terahertz quantum cascade lasers directly by others external to Sandia, we grew and fabricated a similar device. This approach is expected to be constrained by extremely low operating temperatures, but removes extra levels of complication added by the existing approach. The mixing method is expected to operate at significantly higher temperatures (above 300 K), while the direct approach may yield higher efficiency. Having both techniques will allow optimization for different needs. Measurements on this device have just begun.

We also started laying the groundwork for collaborations that will eventually take these devices out of the lab and place them in the field. While a fieldable system is still not yet in the works, early discussion of applications is influencing our design and performance metrics.

The original proposal contained a second approach toward terahertz sources by harmonic generation based on nonlinear transport and multiphoton transitions in semiconductor superlattices. We started developing the fabrication process for quasi-optical arrays.

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38621

Microsystems for Chemical Signature and Reagent Delivery

R. J. Simonson, R. P. Manginell, C. J. Brinker, D. A. Loy, S. M. Brozik, R. J. Kottenstette, H. Fan, B. G. Hance

Networked systems of low-cost, small, integratable chemical sensors will enable monitoring of nonproliferation and materials control targets and chemical weapons threats. Extension of such systems to detection of biochemical molecules could revolutionize health care by allowing in-home monitoring of drug levels and other physiological markers, as well as by enabling the use of chemical signatures for biometrics. Use of autonomous chemical monitoring in health care and other high-consequence applications will demand a high level of system surety, which Sandia is uniquely positioned to provide. A required surety component will be verification of microanalytical systems performance, which can be achieved by providing a programmable source of chemical signature(s) for autonomous calibration of analytical systems. This need for an autonomous calibration capability has proven to be a key factor in delivery and deployment of prototype chemical sensor systems for homeland defense applications. In addition, such a controlled chemical source could be used to dispense microaliquots of derivatization reagents, extending the analysis capability of chemical sensors to a wider range of targets, including biomolecules. We will continue our development of microsystems for controlled release of selected compounds, including biomolecules into the analytical stream of microsensor systems. To minimize pumping and valve requirements of microfluidic systems, and to avoid degradation issues associated with storage of dilute solutions, we are investigating candidate solid-phase reservoir materials that can be patterned onto arrays of thermally or thermopneumatically activated membrane devices. We designed these devices to release reagents when individual array elements are electronically addressed. We are currently pursuing two strategies for encapsulation of organic molecules within solid matrices. The first uses layered self-assembling silica films produced from aqueous phases at low temperature, while the second strategy uses incorporation of desired chemical moieties into decomposable organic polymers.

(1) We identified and selected candidate solid-phase reservoir materials for controlled thermal production of nitric oxide (NO), a key molecule in many biological pathways. Gas-phase quantitative monitoring of NO has potential clinical

5x2 element prototype mask.

Use of autonomous chemical monitoring in health care and other high-consequence applications will demand a high level of system surety, which Sandia is uniquely positioned to provide.

applications in health monitoring. We began evaluating the candidate source materials using bench-scale analytical methods (thermal-desorption mass spectrometry and thermal-desorption infrared spectrometry). We will use selected candidates in tests of the prototype Microcalibration Source Array (MSA) device.

(2) We demonstrated thermally controlled release of 1-octanol from solution-doped sol-gels, using single-element microhotplate devices as test-beds. We chose this compound for initial testing as a nontoxic surrogate for nerve agents on the basis of its vapor pressure. The vapor pressure of the analyte is a key parameter in the performance of our solid-phase reservoir materials, and the selection of a nerve-agent surrogate reflects our renewed emphasis on homeland defense applications of chemical detection and monitoring technology. We will use this solid-phase reservoir system for initial performance testing of our 2x5 prototype MSA.

(3) We completed mask designs and fabricated prototype 2x5 arrays of thermal elements on single die, utilizing the Sandia Compound Semiconductor Research Laboratory.

(4) We designed and fabricated a prototype package, including gas flow and electrical connections, for evaluation of the prototype 2x5 thermal MSA devices.

(5) We fabricated the required control circuits to enable addressable thermal control of individual elements on the 2x5 MSA prototype.

(6) We acquired and modified test-bed gas chromatography instrumentation required for performance evaluation of initial 2x5 prototype devices.

(7) We performed temperature sensor calibrations on the first-generation prototypes. We are now ready to begin evaluation of desorption reproducibility from the individual elements of the arrays.

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38622

Microfluidic Cellular Sample Pretreatment

P. C. Galambos, S. M. Brozik, S. S. Mani, M. Okandan, C. D. James

To counter the threat posed by biological agents, high-throughput genomic and proteomic technologies and advanced sensors are being developed to unravel biological-agent cellular mechanisms and to design countermeasure vaccines. For these technologies to be effective, dramatic improvements in the areas of biological sample preparation are required.

In this project Sandia is exploring the potential for developing a cellular sample pretreatment microsystem utilizing surface (SUMMIT™ [Sandia Ultraplanar Multilevel MEMS {microelectromechanical systems} Technology]) and bulk (reactive ion etch [RIE]) microfabrication processes. A microsystems approach has potential advantages over current methods. These include reduction in sample and reagent volumes (microliters reduced to picoliters), reduction in time required for sample pretreatment (days to minutes), and elimination of sample processing variations (automation).

We narrowed the focus of the project based on the emphasis after the anthrax attacks post-September 11 on developing portable, automated cell-handling and -lysing systems capable of processing bacterial spores. Several key decisions resulted from this focus:

(1) Our goal is to develop a rapid, highly accurate, cellular identification microsystem, so we need to get at the deoxyribonucleic acid (DNA) inside cells and spores. Thus, the microsystem developed will be a cell-/spore-lysing microsystem.

(2) The most rapid and accurate DNA identification system currently available is real-time polymerase chain reaction (PCR), so a real-time PCR system will be the downstream connection to our microsystem.

(3) The upstream input to our system will be small, aqueous liquid volumes (10 µl) such as one might get from a cotton swab swipe of a surface or a throat.

The special capability that we bring to this type of system is the potential ability to surgically lyse individual cells using MEMS or localized electrical fields; therefore, we will build the microsystem around this capability. The areas of progress are (1) mesoscale fluid-handling system development, (2) MEMS designs for cell lysing, and (3) identification and purchase of downstream sample-analysis system.

A microsystems approach has potential advantages over current methods. These include reduction in sample and reagent volumes (microliters reduced to picoliters), reduction in time required for sample pretreatment (days to minutes), and elimination of sample processing variations (automation).

- *Mesoscale fluid-handling system development.* The sample handling system filters out particles that are the wrong size, discards initial solution chemistry to clean the sample, adds a second solution chemistry to prevent destruction of cell-/spore-lysis products (specifically cellular/spore DNA and ribonucleic acid [RNA]), and splits the sample into subvolumes (up to 1000 subvolumes) before injecting the nanoliter subvolumes into parallel on-chip cell-lysis systems. The less-integrated version of this system utilizes small-volume fluid-handling components from Upchurch Scientific and a mesoscale-flow manifold to which the chip is attached. The more-integrated version incorporates all the components into a single-flow manifold.

A PDMS (polydimethylsilane) channel containing cells is integrated with polysilicon (poly-Si) electrodes in a meso-microfluidic system. We pull the cells onto the electrodes using suction. We will use this type of meso-microsystem integration to assemble the complete system. We are investigating plastic and glass as well as PDMS mesoscale-flow manifolds. We will inject the fluid sample, probably by hand using a syringe, into the mesoscale-flow manifold, route it through the microscale lysing system, and output it through a downstream mesoscale-flow manifold.

- *MEMS designs for cell lysing.* The MEMS designs will utilize Sandia's surface-micromachining (SMM) fabrication processes, specifically SUMMiT-VTM (poly-Si films) and SwIFTTM (poly-Si and silicon nitride [SiN] films). One design utilizes a horizontal drill bit or lathe driven by a torsional ratcheting actuator (TRA) into a channel through which cells flow and can be trapped. Other concepts being developed include an on-chip microsonicator for lysing individual cells in trapping chambers designed into channels, and an electroporation system built into a cell trap.

- *Identification and purchase of downstream sample-analysis system.* We purchased a real-time PCR system from Applied Biosystems that will be the downstream detector. Our microsystem will supply lysed cellular samples to this detector. We will use the real-time PCR system to evaluate the performance of any systems we develop and to determine the amount of sample cleanup that is required post-lysing.

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Emerging Threats

The Emerging Threats investment area addresses Sandia's national security mission by developing and applying high-impact technologies to counter new classes of threats (e.g., chemical and biological attacks and other forms of terrorism) that have been emerging since the end of the Cold War and most notably since recent terrorist attacks upon the United States. Focus areas for research include intelligent systems incorporating sensors, communication, processing, and data exploitation; precision defeat; modeling and simulation of real-world process and phenomena; and directed energy. This goal is accomplished primarily through partnerships to broaden the application base for Sandia's mission-driven technologies.

Current weapon technology is not adequate to destroy hard and deeply buried targets—an important national security mission. Recent studies of projectile acceleration data at high-impact velocities have failed to collect valid data. This information is becoming increasingly important to determine high-velocity penetration dynamics, multilayered target characteristics, and survivability of the fuze, explosives, and penetrator. “Micro-High-G Acceleration Recorder” will develop a suitable acceleration transducer plus the associated miniaturized

electronics to process and store the acceleration data. Important transducer attributes are small size, low power consumption, and good cross-axis signal rejection. The transducer will be evaluated both in laboratory tests and as part of a complete acceleration recorder used to instrument an earth-penetrator test.

10727

Micro-High-G Acceleration Recorder

D. A. Hoke, R. R. Lockhart, F. J. Peter, V. I. Bateman, R. G. Lundgren, R. D. Kinney, J. W. Lantz, A. Mittas, E. A. Henry

Current weapons do not hold the entire hard and deeply buried target (HDBT) set at risk. As a result, advanced penetrating-weapon designs are steadily moving toward higher impact velocities to defeat these targets. Acceleration recorders built to instrument high-velocity penetrating weapons must often survive accelerations greater than 20,000 Gs and peak transient accelerations up to several thousand Gs. Designing electronics and integrated systems to operate and survive in these high-G environments is difficult, and systems that currently exist are relatively large (approximately 24 cm³) and often record acceleration only along one axis. To support advanced penetrating-weapon design and development activities, this project seeks to develop a small, multiaxis, high-G-capable acceleration recorder.

First, Sandia completed the design of the micro-high-G acceleration recorder, implemented the design as a prototype, and completed revisions to the prototype design. The design effort included electronic circuit design, firmware design, and the mechanical design of the steel housing. We did not finish testing the design.

Second, we initiated a Cooperative Research and Development Agreement (CRADA) with Endevco to develop an accelerometer that meets our requirements for small size and low power consumption. We received the first batch of the accelerometers and integrated them into the prototype assembly.

The resulting acceleration recorder design, called a Three-Axis MilliPen, or 3-AMP, records acceleration (launch) and deceleration (impact) from three piezoresistive accelerometers during a penetrator test. The accelerometer signals are conditioned with a six-pole Butterworth filter, then digitized at a 75k samples/s rate with the results stored in nonvolatile memory. The 3 dB cutoff frequency of the filter is 15 kHz. The filtered analog signals are multiplexed into a parallel, 12-bit, analog-to-digital converter (ADC). The ADC output is directly coupled to two parallel, nonvolatile, 32k x 8-bit memory devices so that the 12-bit data word is split between two 8-bit bytes. We use four memory devices to ensure a total record time of 250 ms. A model PIC17C756A microcontroller from Microchip, Inc., operating at about 30 MHz, controls the

Mechanical model of the recorder housing and boards.

...Sandia completed the design of the micro-high-G acceleration recorder, implemented the design as a prototype, and completed revisions to the prototype design.

interaction between the nonvolatile memory and the ADC when the system is writing data to memory. The microcontroller also provides an external control interface between the user and the 3-AMP unit using a serial interface, permitting the data to be uploaded post-test, and other service functions.

10736

Dynamic Range Imaging for Terrain Mapping, Position Determination, and Obstacle Avoidance in Autonomous Navigation

C. L. Smithpeter, K. O. Wessendorf, S. K. Dunlap, J. T. Feddema, S. M. Lebien, R. O. Nellums, A. D. Niese

This project addresses the need in autonomous navigation for sensing position, generating a terrain map, and assessing/avoiding obstacles from a moving platform. The three-dimensional (3-D) image data from a conventional laser radar (LADAR) is a possible solution for this sensing need; however, current LADAR sensors are limited by cost, complexity, and sensitivity to motion. Other 3-D image data applications, such as precision munitions guidance, physical security, target surveillance, and docking of spacecraft, have similar concerns with respect to current LADAR technology.

To address the limitations of LADAR sensors, this project seeks to develop a miniature LADAR architecture that is insensitive to platform- or image-scene motion. The ultimate embodiment of this goal is to reduce the LADAR receiver to a focal-plane array, similar to a charge-coupled device (CCD) camera. In addition, Sandia seeks innovative techniques to reduce the required laser illumination power, which currently dominates system cost and power requirements.

We made significant progress in the design of the microcircuit detector array. We fabricated an 8x16 prototype array and tested it in laboratory conditions. Laboratory results indicated basic operation of the pixel circuitry. However, a design flaw in the circuit prevented an image demonstration. We fixed the flaw and initiated another run that is not yet completed. We expect to test the new device under a new project. We filed a technical disclosure early in the project and drafted a patent application.

We completed the design and fabrication of an 8x16 flash pixel array. Circuit simulation indicated that the pixel design achieved a number of design goals, including 1000-photon sensitivity, 20 MHz bandwidth, and phase stability of 2 degrees at 10 MHz. We developed a number of innovative electronic circuit concepts to combine the photosensitivity and megahertz circuit speed, which normally work against each other. We laboratory-tested the prototype to assess actual performance against the design goals. Test of the pixel amplifier confirmed gain on the order of 100 times and speed greater than 20 MHz. It was not possible to access photosensitivity because multiple pixels were connected to the input. We demonstrated pixel gain

Photo of 3-D image sensor array.

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modulation at 10 MHz. The modulation waveform is a feasibility metric in the 3-D imaging objective. However, we were unable to capture a range image, our primary testing goal, because of a misrouted circuit connection. We expect to demonstrate a 3-D image from the project design in the near future.

10752

Distributed, Reconfigurable, Homogeneous Microrobotic Systems

E. M. Hinman-Sweeney, D. A. Schoenwald, S. E. Eskridge, J. T. Feddema, G. A. Johnston

A distributed, reconfigurable microrobotic system is a collection of unlimited numbers of distributed small, homogeneous robots designed to autonomously organize and reorganize to achieve mission-specified geometric shapes and functions. Sandia investigated the design, control, and planning issues for self-configuring and self-organizing robots. In the two-dimensional (2-D) space, a system consisting of two robots was prototyped and successfully displayed automatic docking/undocking to operate dependently or independently. We constructed additional modules to display the usefulness of a self-configuring system in various situations. In three dimensions, we built a self-reconfiguring robot system of four identical modules. Each module connects to its neighbors using rotating actuators. An individual component can move in three dimensions on its neighbors. We also built a self-reconfiguring robot system consisting of a nine-module crystalline robot. Each module in this robot is actuated by expansion and contraction. The system is fully distributed, has local communication (to neighbors) capabilities, and has global sensing capabilities.

We conducted a feasibility study to help guide the initial design for a self-reconfigurable system consisting of cube-shaped modules. For this study, a constraint-based self-reconfiguration planning infrastructure was prototyped that couples the geometry, kinematics, and dynamics of the robotic system and generates the space of all possible (geometrically feasible and dynamically stable) reconfigurations.

Work in the 3-D system combined 3-D hardware systems with the configuration control algorithms to provide mission-based configuration control. In collaboration with Dartmouth University, we built a self-reconfiguring robot system of four identical modules.

- *Hardware.* We adopted the Intelligent Systems & Robotics Center's (ISRC) robotic platform, Gemini, for the 2-D space design. The original Gemini platform is a highly mobile vehicle with a passive joint between modules. It consists of two tracked robots that were passively connected at a center joint. We achieved a dramatic increase in mobility by having two separate vehicles with a joint in the middle rather than having one small robot or one large robot. The small robot could not

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get over large obstacles while the large robot lacked flexibility. Gemini turned out to be the best of both worlds.

We redesigned the passive joint by incorporating a quick-disconnect mechanism utilizing rare-earth magnets (REMs) to attach modules, an articulating joint allowing three types of joint conditions, and a release mechanism allowing Gemini bodies to intentionally disconnect and provide automatic separation in the event of power failure of a particular body. The new versions of the Gemini robots were named Castor and Pollux.

The 2-D reconfigurable vehicle extends the Gemini design by providing a latching/release mechanism and two controlled degrees of freedom (DOFs) between the two vehicles. We added the connect/disconnect feature so that both robots could work independently but could dock when posed with a problem that was better suited for a larger robot.

We developed a docking sensor subsystem that automatically guides the connection process between two vehicles.

- *Software.* We also developed a simulation of the Gemini system and used it to test a variety of cases.

The vehicles are controlled with the same embedded vehicle software used on the Sandia Swarm RATLER (Robotic All-Terrain Lunar Exploration Rover) vehicles. We extended this software to include the release mechanism and the three linear actuators. We also extended the RATLER base-station software to include latching and release buttons and the additional controlled DOFs.

- *Testing.* The robots were autonomously docked under different circumstances. We did testing both inside and outside using versions one, two, and three circuits. We ran tests with the vehicle lids both off and on and also varied distances and angles between initial start positions.

We developed a docking sensor subsystem that automatically guides the connection process between two vehicles.

10753

Robust Planning for Autonomous Navigation of Mobile Robots in Unstructured, Dynamic Environments

G. R. Eisler, P. R. Klarer, J. J. Carlson, R. R. Rosenthal, T. J. Kim, D. E. Small

Sandia's goal in this project is to develop an algorithmic-driven, multispectral approach to point-to-point navigation characterized by segmented onboard trajectory planning, self-contained operation without human support for mission duration, and the development of appropriate sensors and algorithms to navigate unattended. The project was partially successful in achieving gains in sensing, path planning, navigation, and guidance. One of three experimental platforms, the Minimalist Autonomous Test-Bed, used a repetitive sense-and-replan combination to demonstrate the majority of elements necessary for autonomous navigation. However, substantial research is still required to achieve the critical goal for overall success: developing a sensor that can distinguish obstacles to be avoided as a function of vehicle scale.

Test facilities at Sandia for analyzing the various functionalities would benefit enormously from the simulation and real-time operating options that we studied during this project. These concepts would decouple individual functionalities, thus creating a plug-and-play atmosphere that would clarify effects from and significantly lessen system impact due to upgrades, code and component changes, and tuning.

We were unable to develop a sensor that would provide a measure of "terrain penetrability" based on vehicle scale. Such a development would allow the field of mobile robotics to make a quantum leap in its quest for autonomy and significantly increase the field's penetration into the defense world.

We wrote a number of simulations in the course of this work, but models for the various functionalities, particularly vehicle mobility and obstacle sensing, were sparsely covered in the literature. Such models have little "hard" validation compared to those describing, for example, flight vehicles. More fundamental theoretical work is needed to provide computational models, which would have direct payoffs.

Sandia's goal in this project is to develop an algorithmic-driven, multispectral approach to point-to-point navigation characterized by segmented onboard trajectory planning, self-contained operation without human support for mission duration, and the development of appropriate sensors and algorithms to navigate unattended.

10772

Intense Directed-Energy Theory Initiative

J. S. Wagner, E. P. Parker, P. C. Gray, M. G. Mazarakis, M. W. Trahan

Sandia achieved national recognition for leadership in end-to-end design, modeling, and simulation of directed-energy (DE) systems, including charged-particle beams (CPBs), high-power radio frequency (RF) and high-power microwaves (HPM), and hybrid laser-assisted CPB systems. This project is advancing and leveraging these never-superseded simulation tools and techniques to enable us to tackle new national security applications. Applications under investigation include both exoatmospheric and endoatmospheric applications, as well as laboratory end-to-end accelerator designs supporting many related fusion plasma and DE applications.

We will direct future technical work toward (1) neutral-gas dynamic simulation of CPB application environments, (2) ion-beam endoatmospheric standoff weapons in collaboration with a related project, (3) globally optimal end-to-end accelerator designs for all DE applications, (4) active and passive electromagnetic (EM) signature generation, and (5) exploitation and application relevant to program-development activities.

(1) We rebuilt the Air Propagation Code (APC) and used it to guide experimental design to address unresolved issues in air chemistry models.

(2) We customized the Neutral Gas Particle (NGP) code to include a graphical user interface (GUI) and higher-fidelity physical models.

(3) We implemented genetic algorithms (GAs) that can perform global optimization and function as design tools, enabling physics-based codes to be better coupled to planned programs and experiments.

(4) We extended a 2-D PIC code to three dimensions and implemented it in C++.

(5) We interfaced the C++ particle-in-cell (PIC) module with UMBRA.

(6) We integrated the PIC code with a 6-degree-of-freedom (DOF) unmanned aerial vehicle (UAV) model. The PIC code calculates waypoints, which are used to construct the flight path(s) of swarms of unmanned combat aerial vehicles (UCAVs) pursuing enemy air assets. The PIC code also calculates the flight path of the targets of the swarm. This example provides proof-of-principle, showing that other physics-based codes could be readily integrated into a simulation environment. This would make realistic simulations

The movie shows that directed energy codes can be used in modeling and simulation, providing impetus to help save the historical capabilities (i.e., models).

Sandia achieved national recognition for leadership in end-to-end design, modeling, and simulation of directed-energy (DE) systems, ... This project is advancing and leveraging these never-superseded simulation tools and techniques to enable us to tackle new national security applications.

of weapon systems, such as particle beam weapons, available to customers such as the joint virtual battleship (JVB) and future combat systems (FCS).

26531

Air Sterilization and Decontamination

R. P. Toth, P. C. Gray, G. C. Hauser

In this project, Sandia will develop and test a new method of air sterilization based on pyrolytic decomposition. This method will be applied toward the protection of buildings and vehicles with a flow-through heating, ventilation, and air conditioning (HVAC) system.

This project will develop and test a new method of air sterilization and decontamination based on pyrolytic decomposition of all biologic agents, biologic products, and organic chemical weapon (CW) agents. The use of pyrolytic decomposition offers many advances, but the key ones are rapid destruction and its corollary ability to handle the large loads expected with an intentional chemical/biological weapon (CBW) attack.

The means to produce temperatures consistent with pyrolysis (i.e., over 1000°C) is a radio-frequency (RF)-driven, atmospheric-pressure plasma. We designed and built an RF system capable of running 10–20 such reactors in parallel. We tested the RF system to sustain an atmospheric-pressure plasma at 1200°–1500°C. The RF system includes a method of power control based on a perpendicular B-field in the drift region of the magnetron. This field alters electron trajectories to reduce the fraction that reach the anode. The electrons that do not hit the anode do not contribute to output power. In this way, the plasma temperature can be controlled over a range of 1200°–1700°C.

We designed and built a high-flow swirl-chamber reactor with sufficient dwell time to inactivate heavy loads. We designed and built a bench-top wind tunnel to test swirl-chamber designs for air flow, pressure drop, and air velocity in three dimensions. The result is a 6 in.-diameter swirl chamber in WR 975 to handle ~ 50,000 cfm air flow. We mapped air velocity with a 3-D, miniature, constant-temperature anemometer. These maps indicate a “super-coil” air flow in the swirl chamber with maximum velocity (~ 20 m/s) adjacent to the plasma channel and lowest velocity at the perimeter. Thus, the temperature-versus-time (tempxtime) profile is suitable for our purposes.

We encountered a major materials problem in the swirl reactor. Heretofore, we considered the most important parameter to be the thermal-decomposition temperature of the material. This led to the use of Al₂O₃ with a usable maximum

We designed and built an RF system capable of running 10–20 such reactors in parallel.

We tested the RF system to sustain an atmospheric-pressure plasma at 1200°–1500°C.

temperature of 1700°C. Unfortunately, we discovered that the limiting factor was not maximum temperature, but thermal-shock resistance, as the plasma temperature increased roughly 1000°C in a few seconds. The result was thermal shock, which fractured the ceramic. We returned to quartz for the swirl chamber since it has much better thermal-shock resistance, but a lower maximum temperature (1100°C). The power-control circuitry does allow some regulation of the plasma temperature, but fabrication difficulties led to other materials that could be cast. The search for shock resistance led to silicon carbide (SiC) in two forms: one fully densified, the other partially densified and suffused with excess Si (~ 20%–25%). We tested these materials in the RF system for preheating to reduce the thermal shock, and both worked quite well in that regard. However, both were sufficiently lossy that the plasma could not be sustained, even with full RF power (5 kW).

These materials problems prevented tests with microbes. We completed the means to inject and recover microbes with the swirl reactor as well as culture systems for *Bacillus cereus*, *B. thurengiensis*, and *B. subtilis*.

We will focus on overcoming the materials problem for the swirl reactor in our upcoming work.

We completed the means to inject and recover microbes with the swirl reactor as well as culture systems for Bacillus cereus, B. thurengiensis, and B. subtilis.

26532

Data Fusion and Visualization of MASINT Results for Underground Facility Characterization

M. D. Ladd, M. L. Yee, J. M. Brabson, M. E. Bukaty, R. W. Simons, A. A. Yee, J. S. Salazar

There is a need for technologies that can perform multisensor data exploitation, particularly fusion and visualization tools that provide immediate and extensive situation awareness. To characterize underground facilities (UGFs), a variety of different sensor types can be employed, resulting in two broad categories of dissimilar types of data. One category consists of map-based or image-based data, such as optical, multispectral, hyperspectral, or synthetic-aperture radar (SAR) images. The other category consists of time-sequence data, such as seismic, acoustic, or electromagnetic (EM), which is a record of measured energy over time at a given location. The dissimilar nature of these two categories of data (image versus time-sequence) makes combining these types of data challenging. The difficulties are manifest both in deriving useful new information from the fusion of these different types of data and in the visualization of the multiple types of data and the fused result for the user. In this project, Sandia is breaking new ground by employing rigorous, quantitative multisensor fusion approaches to derive useful new information from these disparate sources of data. We are also advancing the state of the art by developing new visualization tools to provide an integrated method for viewing information from these disparate sensor data. The result will be a suite of prototype algorithms that perform the feature extraction, fuse the data, and then present the results integrated with imagery for the human analyst. Results will be derived from experimental data obtained at the Nevada Test Site. The development of an integrated system of multisensor fusion and visualization tools, which is not being pursued elsewhere in the analyst community, will provide meaningful and important capabilities that do not currently exist for characterizing a UGF.

We developed a core set of queries for UGFs based on information from the UGF analyst community. We identified features from the available multisensor data for these queries. We modified existing algorithms to process these data to generate feature and classification results and generated preliminary results. We established the theoretical forms of the probability distributions of the various features and automatic

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target recognition (ATR) decisions and are verifying and modifying them with data samples. We will use these probability distributions with the fusion algorithms to be employed in upcoming work. We are using the Knowledge Generation (KG) tool for automatic analysis of the event-sequence data obtained from the various sensors and their associated processing algorithms. We developed functional models of the expected operations of the UGF for the KG tool. We implemented a relational database to store processing results, support various queries for UGF characterization, and send query results directly to the visualization tools. We developed initial visualization tools that can display processed results on an optical image of the UGF area draped over a digital elevation map (DEM), using icons to show identification and location information. The visualization tools have 3-D display capability with pan, zoom, and tilt functionality, which allows the user to visually integrate the surface contour information along with the results. We also implemented drilling down for further information (such as confidence values for event identifications, raw data, etc.) using point-and-click pop-up menus. We also developed a tool for displaying sequential event information in the form of multiple timelines displaying various event states (e.g., generator on/off).

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26533

Rapid Ultrasensitive Chemical-Fingerprint Detection of Chemical and Biochemical Warfare Agents

C. I. H. Ashby, T. J. Shepodd, R. J. Kottenstette, D. J. Muron, W. G. Yelton

Unambiguous identification of chemicals and biochemicals usable as chemical/biological weapons (CBW) is essential at nanomolar levels with short analysis times (< 5 min). Vibrational spectra can serve as chemical fingerprints for positive identification of CBW molecules. The required speed and sensitivity might be achieved with surface-enhanced Raman spectroscopy (SERS) using nanotextured metal surfaces. Although ordinary SERS produces sensitivity enhancements on the order of 10^4 versus normal Raman spectroscopy, a properly nanotextured metal surface can increase sensitivity up to 10^{14} -fold when coupled with chemical resonant enhancement and 10^{11} -fold from the metallic surface alone. Under partially optimized conditions, a single hemoglobin molecule yielded a spectrum with signal-to-noise (S/N) > 20 in 200 s, and low-noise spectra have been demonstrated for nanomolar concentrations with < 1 s data collection. However, systematic and reproducible methods for preparing metallic surfaces that maximize sensitivity have not been developed. Sandia seeks to integrate chemical-fingerprint identification of CBW molecules using SERS as the detector in the chip-scale microseparation columns developed under μ ChemLabTM. To this end, we propose to develop methods for forming high-efficiency metallic nanostructures that can be integrated with either gas- or liquid-phase chem-lab-on-a-chip separation columns to provide a highly sensitive, highly selective microanalytical system for detecting current and future chem/bio agents. We will also develop chromatographic media that permit microscale separation of proteins. The innovative aspects of this project include the separation media and the design and fabrication of metallic nanostructures that reliably provide the sensitivity for rapid nanomolar detection and identification and that can be incorporated into lab-on-a-chip architectures. In addition to speed and sensitivity, the chemical fingerprinting provided by SERS will enable rapid identification of new, nonstandard CBW agents that might be introduced to avoid detection by established sensor systems.

This year we advanced our efforts in porous polymer monoliths to an on-chip format. We continue to design improved microporous polymers for the chromatographic

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separation of proteins and peptides. We developed new polymers that show a broad range of interactions with proteins. Highly efficient chromatographic separations are possible on our more hydrophobic monoliths. Efficient separations allow the isolation of individual proteins from complex mixtures. More polar monoliths show essentially no interaction with eluting proteins—the proteins behave as they would in capillary electrophoresis without polymer present. These minimally interactive polymers are important, as they can modify the flow characteristics of the eluant without selective retention of the analytes. We also developed monoliths that will bind proteins strongly under an electric field but release them when the electric field is removed and standard pressure flow is resumed.

We now have a full suite of monolithic materials, from strongly interactive to minimally interactive to selectively interactive. We feel that we can manipulate proteins efficiently and separate mixtures for delivery to other analytical detection schemes. Our selective-interaction monoliths allow preconcentration of proteins from very dilute solutions, which increases the effective detection limits for other analytical methods used downstream.

We tested multiple approaches to forming metallized surfaces that embody the characteristics that theoretically should provide up to 10^{11} enhancement in contrast to typical enhancements of 10^3 to 10^5 , with electrochemically generated textures on gold (Au) and silver (Ag) surfaces. Achievement of an enhancement of 10^9 would produce excitation cross sections on the order of those of single-molecule fluorescence and would permit fingerprint-quality spectra to be obtained in 1 s with laser powers on the order of 1 mW. We obtained maximum enhancements on the order of 10^7 with metal-coated hemispherical arrays, as theoretically predicted in the literature. We developed procedures for forming alumina templates with pore spacings that are suitable for generating surface composed of a dense array of “metallic mushrooms” that is theoretically predicted to produce maximum enhancements and procedures for electrodepositing uniform Au and Ag nanostructures in the templates.

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Refereed

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26534

Advanced Unattended Ground-Sensor Technology

D. E. Gallegos, J. W. Giron, M. R. Heying, J. L. Zenner

During recent years, unattended ground sensors (UGS) have proven very useful for detecting, identifying, and characterizing difficult targets. However, current UGS technology places severe restrictions on real-world deployment. Specifically, their excessive bulk and their inability to covertly off-load data make them difficult to deploy in denied territories. In addition, redeveloping a distinct custom UGS for each set of varying mission requirements is often prohibitive in time and cost.

To address these challenges, Sandia is developing a novel architecture, referred to as scalable digital signal processing (SDSP), based on the incorporation of a coherent interconnect fabric that will lead to small, modular, reconfigurable sensors that can be rapidly inserted into a wide range of deployment mechanisms: microglider, projectile, robot, or hand. Our goal is to achieve a significant decrease in power consumption, thereby dramatically reducing the battery payload: the volumetric “fat” in UGS. Our architectural approach will enable the use of sophisticated power-management schemes, dynamically variable clock-rate devices, and UGS-optimized signal processing to autonomously optimize the watts-per-MIPS (million instructions per second) arrangement for a given task.

This project is designing, developing, and will demonstrate a prototype miniature ground sensor based on the novel SDSP fabric-based architecture. This architecture will be modular in nature and will provide the needed capability to rapidly respond to new data-collection needs.

We deemed the Nonarbitrated Carrier Detect Addressable Shared Multipoint Topology to best meet the requirements for the next-generation unattended ground sensors (NG-UGS). We selected two commercially available variants of the topology, the I2C-bus and the controller-area network (CAN)-bus, for implementation, comparison, and selection for development into the complete interconnection fabric (ICF).

We completed development of the CAN-bus-specific configuration firmware. We showed that the amount of custom firmware needed to implement a reasonable level of utility exceeds the capability of all low-power, field-programmable devices available today. As a result, we are able to complete only the evaluation in a piecewise-functional fashion.

Our architectural approach will enable the use of sophisticated power-management schemes, dynamically variable clock-rate devices, and UGS-optimized signal processing to autonomously optimize the watts-per-MIPS (million instructions per second) arrangement for a given task.

We completed the development of both the Texas Instruments (TI) 'C55 dual-role processor modules and the data-acquisition module using system packet interfaces (SPI). They are operational and are being used in the evaluation of the fabric-adapter variants.

We completed a copy of the tactical unattended ground sensor (TUGS) unit, to be used as the bench-top touchstone, and demonstrated it to be operational.

We completed the circuit boards for the original design of the prototype dual-configuration fabric adapters and demonstrated them to be operational. Performance of the CAN-bus variant, however, is limited to 384 Kb/s maximum due to severe physical protocol overhead on small fixed-data packets. As a result, we postponed further development of firmware and subsequent evaluation of the CAN-bus variant to accelerate the evaluation of the I2C variant.

Because of the CAN-bus firmware capacity experience, we developed a microcontroller-based adaptation of the fabric adapter for implementing the I2C variant of the ICF. At this point, we have demonstrated a simple loop-back capability using SPI interfaces on one of the 'C55 modules and a two-computer connection at 560Kb/s throughput. We expect to yield sustained 500 Kb/s with low overhead and variable-length data packets. We expect definition and development of firmware for interface handling to continue to full functionality.

We extracted the software modules, to be ported from the DSP processor, from the TUGS code library and demonstrated them to be operational on the TUGS unit. Repeatedly, we will generate a power-density spectrogram for a single-channel analog input and then transmit it over the transceiver module.

The design of the system-controller software and the DSP platform routines have begun within the context of the Real-Time Unified Modeling Language (RT UML). We completed a comprehensive use-case definition; this effort revealed that definition and development of the system-controller application are too extensive and will exceed the limited resources of this project, preventing us from completing the more pertinent task of defining and developing the device drivers and the high-level interface-handling protocol layers for the I2C variant of the fabric adapters. The software for the system-controller module will not be completed under this project. Instead, we will integrate a number of modules from other projects to expand the ICF to include a wider range of interfaces: a global positioning system (GPS)/compass module, using RS232 ports, and transceiver module, using a parallel input/output (I/O)

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interface. We will modify the intended full-up TUGS-like test and demonstration accordingly.

We incorporated the TI DSP BIOS operating system and Code Composer development environment into the RoseRT UML code generation tool to generate code for the 'C55 processor directly from the UML model.

We completed power analysis of the state-of-the-art TI 'C55 DSP module and reflected it into the power model. Evaluation of the fabric adapter variants continues.

26535

The Endowment of Simulator Agents with Humanlike Episodic Memory

J. C. Forsythe, P. G. Xavier, C. E. Lippitt, E. V. Thomas

From an engineer refurbishing a nuclear weapon for which all the original designers are no longer available, to a future combat system commander controlling hundreds to thousands of semiautonomous entities, to an intelligence analyst poring over terabits of data from disparate sources, the challenge of making intelligent national security decisions is increasing. This project advances cognitive modeling capabilities to significantly improve intelligent systems technologies. The goal is to develop adaptive tailored systems that learn and communicate, matching the needs of the humans in the loop of complex systems.

This project involves simulation of human episodic memory. This includes a capability to reason and conduct mental simulations on the basis of stories, consistent with human naturalistic decision making. One application involves technology to endow machines with humanlike episodic memory. Such a machine would store meaningful representations of experiences, recognize similarities between ongoing and past events, and reason and communicate on the basis of experience. A second application concerns synthetic humans for simulation and training. To realistically model variability in individual behavior, synthetic entities must be endowed with diverse life histories. With this capability, there is potential to simulate cultural factors and create entities endowed with life experiences of specific individuals.

Sandia developed a conceptual design for representing experience that enables recall of past experiences and mental simulation based on past or future events. Data input concerning events is interpreted relative to known schema and represented in memory as storylines, with appropriate conceptual detail. Specific incidents may be later recalled in a manner consistent with human autobiographical memory. Furthermore, ongoing events may be compared to past events for recognition of similar past episodes, again mimicking human cognitive processes.

The objective for this project was to develop a psychologically plausible computational representation of human episodic memory. This memory involves the ability to meaningfully store and retrieve past experiences through either intentional mechanisms or spontaneously in response to

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ongoing events. The resulting technical capability should have applicability to human-machine interaction, intelligent machines, and synthetic humans for simulation.

We developed a computational model that provides a psychologically plausible representation of the cognitive processes whereby humans interpret ongoing experience relative to patterns of cues within their environment. We reviewed relevant psychological and neuropsychological literature to derive specifications for the extension of the computational model to encompass human episodic memory, as well as memory processes alternately described as autobiographical memory. Consistent with this framework for modeling episodic memory, previous work focused on developing a grammar based on the schematic representation of experience and semantics based on the specific elements of experience. We developed two approaches for creating the semantics. The first utilized simulation for the derivation of schema for machine applications, e.g., mobile robots. The second approach involved identification of schema primitives for the representation of social interactions to be applied with synthetic humans.

Our attention has turned to the storage and retrieval of episodes. A synthetic entity is presented a series of stimuli consisting of various entities and behaviors. A situation-recognition process based on evidence accumulation interprets this input with regard to social interaction schema. For example, the behavior of one entity to a second entity may be interpreted as a “display of dominance.” Ongoing experience is written to episodic memory as traces containing the essential, moment-by-moment cognitive elements of experience, with an update function whereby the model exhibits properties that are consistent with human autobiographical memory, e.g., episodes are partitioned relative to time, place, causation, intentionality, and protagonists/objects.

Once populated with experiences, episodic memory may be applied in two ways. First, there is intentional recall. Episodes may be retrieved based on concepts (events involving Entity A), combinations of concepts (events involving entities A and B), schema (events involving a display of dominance), and combinations of schema and concepts (events involving Entity A and a display of dominance). Consistent with human episodic memory, when there are multiple similar episodes, e.g., multiple trips to a given restaurant, the episode(s) recalled will be that which is most salient. Similarly, recall may also be biased by ongoing events such that current cues may prime recall of episodes involving the same or similar cues.

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Second, recall may occur spontaneously. Ongoing events provide the prompts by which recall of similar past episodes are triggered. With either form of recall, once an episode has been recalled, consistent with mental simulation, the episode may be replayed with the psychological experience of events occurring in roughly the same sequence as the original experience. Depending on the application, models may or may not incorporate properties that produce behavior consistent with known biases in human recall of experience.

We collaborated with Northern Illinois University on the validation of the cognitive model through human subject studies. Validation has begun with the development of an experimental protocol that will allow a wide variety of studies to be conducted wherein subjects interpret situations based on their past experience. These studies will serve two purposes. First, the cognitive model makes a number of critical assumptions concerning human cognitive processes that must be validated. Second, the cognitive model contains a number of parameters that must be calibrated with actual human performance data.

We collaborated with Northern Illinois University on the validation of the cognitive model through human subject studies.

Refereed

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26537

An Advanced Learning Model for Agent Behavior

R. J. Pryor, D. C. Barton

The development of complex agent behavior is a critical element in agent-based applications. The state of the art today is to develop behavioral models using evolutionary algorithms. These algorithms are based on the Darwinian principal of survival of the fittest. In an evolutionary algorithm, the behaviors evolve to more fit individuals as they move from one generation to the next. This evolutionary improvement is sometimes called the learning process.

The best behavioral models have been either neural networks or genetic programs. Both are very powerful, but they do have limitations in learning complex behaviors such as war-fighting. These methods do complement each other; where one is weak, the other is strong. In previous work, Sandia proposed to develop the methodology to build a behavioral model that incorporates the benefits of both techniques. To our knowledge, this has never been done before.

To accommodate complex behaviors, we proposed using a layer learning approach. We will consider two approaches: (1) a layered planar-space of interconnected neurons and genetic programs, and (2) a layered genetic-programming approach. When an agent reaches the limit of the current layered configuration, a new layer with a limited number of unknowns is added to increase the agent's decision capabilities. Existing layers remain unchanged, thereby retaining what was previously learned.

We successfully produced a behavior for a glider unmanned airborne vehicle (UAV). We found that the best behavior was one that employed automatically defined functions (ADFs), and its fitness was very close to the theoretical maximum. A mixed neural-network and genetic-programming model could not be completed because the project was not approved for continued funding.

We also created two new simulators, one for the Macintosh and the other for the personal computer (PC). Both of these simulators can be found at: <ftp://ftp.cs.sandia.gov/pub/rjpryor>. The PC simulator allows different behaviors to be loaded and up to five UAVs to be flown at one time. We provided two behaviors that are nearly equal in fitness by taking different approaches to solving the problem.

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Other Communications

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26539

Algorithms for Improved Performance in Cryptographic Protocols

C. L. Beaver, R. C. Schroepel, D. R. Gallup, M. D. Torgerson

Public-key cryptographic algorithms provide data authentication and nonrepudiation for electronic transmissions. The mathematical nature of the algorithms, however, means that they require a significant amount of computation; furthermore, encrypted messages and digital signatures require a lot of bandwidth. Accordingly, there are many environments, e.g., wireless, ad hoc, or remote sensing network, where the requirements are too prohibitive for public-key algorithms. The use of elliptic curves (ECs) in public-key computations provided a means by which computations and bandwidth can be somewhat reduced. Sandia's purpose in this project is to further research the use of ECs and hyperelliptic curves in the hope of finding even more-efficient algorithms and making public-key cryptography available to a wider range of computing environments.

Our milestones included (1) investigation and implementation of a new point-counting algorithm, (2) development of new fast algorithms for point multiplication, (3) examination of the relationship between continued fractions and curves, (4) investigation of the use of ternary fields as opposed to binary fields for the basis of underlying computations, (5) exploration of hardware implementations, and (6) work on a draft of our final report.

We completed investigation of Satoh's point-counting algorithm and investigated its application to hyperelliptic curves. The number of points on the EC is an input parameter into every EC cryptographic algorithm. Furthermore, this number is crucial since it must have special properties to ensure that the curve is "secure," i.e., the number of points must be divisible by a very large prime. In the past, this was considered a time-consuming problem, even though it had to be done only once for each curve. Since this research began, Satoh came out with a new point-counting algorithm that is very fast and essentially solves the problem. We completed an implementation of Satoh's algorithm in both C and Mathematica. The code will be added to our cryptographic software library for wide use. We did not pursue adapting the algorithm for application to hyperelliptic curves because we found other algorithms that were better.

We completed implementations and analysis of our new point-addition algorithms. The most time-consuming part of

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any cryptographic algorithm based on ECs is the computation of a scalar multiple of a point. We hoped to find improvements by using special formulas for combining points of the form $2A+B$, $3A$, and $A+B+C$. We derived formulas using geometric constructions, e.g., realizing the sum as an intersection of curves. The only advances over usual addition algorithms were in “triplication” ($3A$), but this was not an improvement over the optimized algorithms that use point-halving. However, looking in a different direction for adding many points together, we discovered a very promising new approach that will lead to a substantial speedup in many EC applications. We filed a provisional patent and continue our investigation to extend the idea.

We completed implementations and analysis of continued fraction representations of hyperelliptic curves. It has been shown that there is a one-to-one correspondence between the order of a point on an EC (the number n such that $n \cdot P = 0$) and the periodicity of a related continued fraction. We are investigating this relationship to try to develop methods of speeding up the computation for EC key exchange. We are also looking at relationships between the continued fraction representations and a certain pairing called the *Weil pairing*. The Weil pairing can be used to map a pair of points on an EC to a number and hence can be used to translate the EC discrete log problem to the usual discrete log problem. It has also been used lately for a new identity-based signature scheme. We have postponed implementations until it is clear that these lines of research will lead to optimizations.

We began the investigation on ternary fields, $GF(3^n)$. Most efficient implementations of EC cryptosystems base their arithmetic in the field $GF(2^n)$. We have been looking for efficient implementation in ternary fields, $GF(3^n)$. We investigated various data formats and wrote some code for working with the various formats and coding schemes.

We began investigating hardware implementations of ECs. We designed a circuit for solving the quadratic equation over finite fields. This operation is one of the most expensive components of the point-halving algorithm, and the circuit design speeds up the computation in hardware considerably. We also looked at minimal circuits for many other field operations, including squaring, multiplication, reciprocal, cube root, logarithm, and exponentiation.

Other work includes research into EC-related identity-based schemes, work toward a comprehensive tutorial document, and software implementations of optimized

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algorithms for incorporation into our cryptographic software library. We have implemented EC point-halving, multiplication, and an El Gamal digital-signature scheme.

Other Communications

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26540

Low-Cost Digital Radar for Fuzing, Tags, SAR Imaging, and Targeting

D. F. Dubbert, R. E. Heintzleman, P. A. Dudley, D. Greenway, Jr., T. L. Hardin

For the past decade, wireless communication systems have reaped the benefits of digital circuit technologies to reduce cost, size, and weight, and to increase flexibility of communications devices. Digital technology has advanced sufficiently that, coupled with Sandia's innovative radar design, waveform synthesis, and digital-sampling technologies, there is the opportunity to embark on this "digital revolution." Sandia is well on the way to realizing digital receiver (DRX) and advanced waveform-synthesis hardware, which will help set the stage for our next-generation digital radars.

Sandia-developed radars for remote sensing, targeting, and fuzing demand the highest levels of performance for signal generation and processing in terms of frequency of operation, dynamic range, bandwidth, and robustness. Recent advances in high-speed digital technology have set the stage for the unique marriage of the latest high-speed digital technology and digital signal-generation and -processing techniques with Sandia's expertise in radar system design, development, and exploitation. The end product is the establishment of digital radar technology as the next-generation solution to remote-sensing and communications systems that are required to be low cost, miniaturized, lightweight, and highly flexible.

We built and bench-tested the next-generation digital intermediate-frequency (IF) receiver module and an advanced quadrature waveform synthesizer module. Both are the primary technological building blocks for the digital radar realization. In addition, we learned a great deal about the performance of track-and-hold amplifiers (THAs) catered to a high-performance synthetic-aperture radar (SAR) application.

Our accomplishments span three major efforts: the DRX, advanced waveform synthesis, and track-and-hold amplifier characterization and analysis.

We designed the DRX module as an upgrade to our current advanced radar systems (ARS) SAR experimental platform. The DRX is considered the first major hardware advance toward the realization of a next-generation digital radar. All of the board-level designs are completed, with some of the subassemblies currently undergoing bench-testing. We are bench-testing the first prototype DRX module. The DRX

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upgrade is scheduled to support the concealed target SAR (CTSAR) data collections in upcoming work.

As with the DRX, we are also progressing toward the realization of an advanced-radar waveform-synthesizer module, which employs a novel technique called *quadrature error-corrected digital-waveform synthesis* (QECDWS) developed in this project. We developed both the patentable QECDWS idea and the supporting analysis, simulation, and calibration techniques for a wideband radar exciter that employs an image-rejection QECDWS. We currently have the basic QECDWS implemented on demonstration hardware, with the final miniaturized module scheduled to begin bench-testing.

For future radar applications, the direct sampling capability afforded by the THA technology is of great potential benefit and makes the implementation of an “all-digital” radar a reality. In this project, we performed detailed measurements and data analysis of a candidate THA for application to SAR.

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digital” radar a reality.*

Other Communications

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Triggered Isomer Research*P. J. Griffin, L. C. Sanchez, J. L. Powell*

The nuclear physics community has conjectured for many years over the possibility that radionuclides could be stimulated through quantum mechanics effects to transmute or de-excite. This project focused on the forced de-excitation of nuclear isomers to ground state. There are two theoretical conjectures: (1) an atomic process can be used to initiate a nuclear physics event, and (2) direct nuclear physics coupling is used. The atomic/nuclear coupling could be accomplished by energy transfer from x-rays to outer shell electrons. Since, by quantum mechanics, the shell electrons have a finite probability of being within the nucleus, this high-energy electron would directly transfer (couple) to the nucleus. (The theoretical modeling of the atomic coupling between x-rays and the shell electrons has been previously published in the Russian literature. These models involved plasma physics theory and are too involved to be studied in detail in this project.) The electron would then change the energy level of the nucleus. This change in the nucleus energy level could also be achieved if the x-ray could be directly coupled by non-highly forbidden quantum mechanic transitions to the nucleus. For both of the conjectures, detailed hyperfine quantum mechanic models are needed to predict the excited energy level and cascade (decay branches) of the nuclear isomers of interest. Literature information by isomer co-investigators on nuclear-energy states indicates that candidate isomers for low-energy triggering are highly deformed nuclei, i.e., mid-z nuclei that have many possible energy states due to rotational and translational variations. A leading candidate is the isomer $^{178}\text{Hf}^{m2}$ (the second isomeric state of hafnium-178); another prime candidate is an isomer of tantalum. Nuclear physics theory predicts that soft x-rays (energies less than 100 keV) could trigger $^{178}\text{Hf}^{m2}$, i.e., excite its nucleus to a slightly higher energy state that is very unstable, causing it to promptly de-excite, emitting a high-energy gamma ray. Sandia investigated this phenomenon via experiments using intense low-energy x-rays (LEXR).

This project is a study on the forced de-excitation of nuclear isomers to ground state. Research in the open literature on hyperfine quantum models indicates that nuclear isomers are capable of being de-excited via coupled atomic/nuclear processes, i.e., exciting a nucleus into a higher energy state that is very unstable, causing it to promptly de-excite and release

Nuclear physics theory predicts that soft x-rays (energies less than 100 keV) could trigger $^{178}\text{Hf}^{m2}$, i.e., excite its nucleus to a slightly higher energy state that is very unstable, causing it to promptly de-excite, emitting a high-energy gamma ray. Sandia investigated this phenomenon via experiments using intense low-energy x-rays (LEXR).

energy. Our accomplishments include (1) performing intense x-ray irradiation experiments on $^{178}\text{Hf}^{\text{m}2}$ using the LEXR bremsstrahlung spectrum x-ray machine in collaboration with the Air Force Research Laboratory, (2) statistical analysis of LEXR results, (3) x-ray self-shielding calculations for x-ray targets, (4) a critical examination of theoretical models (non-highly forbidden quantum mechanic transitions for highly deformed nuclei) and experimental results obtained in collaboration with researchers from the University of Texas at Dallas and in Japan using the SPRING-8/Osaka, Japan, accelerator, and (5) a study of isomer production processes (both accelerator and nuclear-reactor production options, based on existing open literature information).

Experimental results with the LEXR were inconclusive; however, the results were valuable for identifying threshold values used in the analysis and design of future experiments. The LEXR's x-ray fluences at specific energy (trigger) levels were not large enough to provide statistically significant discrimination against background spectra due to a multitude of experimental and statistical limitations. The most significant limitations were (1) LEXR's use of a continuous wavelength, (2) LEXR's limitation of one-hour active beam-line experimental runs (due to data-acquisition system design limits, need for active cooling of beam-line target, etc.), (3) significant variation in the background measurements (24-hour background measurement data had significant variation in the x-ray regions of interest), and (4) possible experimental equipment drift (thermal effects, etc.). We performed multiple experiments and used overall findings to identify and design experiments using high-resolution mono-energetic increments (the current approach in SPRING-8 experiments).

Analytical and computational analysis and research results provided a mapping of all possible isomers, energy-storage and -release values for key isomers, and fundamental design calculations for isomeric production (using classical nuclear reactor and accelerator designs) for the leading isomeric candidate. In addition, the project report discusses the literature review of theoretical quantum models. This literature provides the foundation for the triggered isomer concept. The project report will also provide a description of the important theoretical models and their relevance to isomer de-excitation processes to outline the logical scientific explanation of the physical processes involved.

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A Scientific Basis for Robotic Ground-Vehicle Design

P. R. Klarer, M. R. Vaughn, K. M. Jensen, C. G. Hobart

Mobile robots have recently seized center stage for remote gathering of information in both the military and intelligence worlds. The difficult operational environments and mission requirements are driving systems engineers to push the performance of current unmanned ground vehicles beyond that for which they were designed. Because vehicle design is currently only loosely tied to the mission and mostly based on prior designs and experience, Sandia is developing a design methodology for mobile robots that begins with an analysis of the mission, optimizes performance requirements, and includes a modeling and simulation environment for optimizing designs and estimating probabilities of mission success. The end result of this project will be a new and unique capability to define and design mobile robotic-vehicle systems based on customers' mission requirements, providing Sandia with a differentiating capability in robotic-vehicle design.

Current accomplishments include the establishment of a virtual prototyping capability that makes use of modeling and simulation tools identified previously, as well as progress in the development of analytical, theoretical, and experimental approaches to describing and understanding vehicle mobility in terrain. Because the desired end result of this project is a capability to define vehicle-design parameters based on an analysis of mission-driven requirements, an important focus was to identify the relevant vehicle-design parameters that affect performance and their relationships to the mission-performance requirements and operational constraints imposed by the mission scenario. This project is focused primarily on the design and performance aspects of vehicle locomotion and mobility in terrain. Theoretical and analytical work to date includes a basic understanding of the kinematics and dynamics of vehicle interactions with discrete obstacles and a closed-form representation of vehicle-terrain interactions in terms of the tractive and compressive forces present at the wheel-soil interface. Results from classical analysis and parametric simulation studies indicate that there are several specific vehicle-design parameters that, when adjusted correctly, can produce optimal performance when surmounting discrete obstacles, such as a vertical step of variable height. In addition, we conducted comparisons among a variety of vehicle

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configurations, e.g., wheeled versus tracked, multichassis versus single chassis, and number of active axles, and the results indicate that there are advantages of multichassis systems over single-chassis systems strictly in terms of obstacle-climbing performance. We conducted classical treatment of the wheel-soil interaction in terms of terramechanics to produce an approach for quantifying the interactions of generic wheeled vehicles with terrain characterized by compressible soils. It has been recognized that the power consumed and traction developed as a result of the interaction of vehicles with both a shearable soil and terrain elevation changes will dominate mission scenarios and subsequent vehicle design.

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Adaptive and Mobile Ground Sensors

A. B. Maish, R. L. Williams

The goal of this project is to demonstrate the use of robotic vehicles for deploying and autonomously reconfiguring seismic and acoustic sensor arrays with centimeter-scale accuracy to obtain enhancement of the capability to locate and characterize denied targets.

Seismic and acoustic sensors configured in phased arrays are used for multiple tasks.

- Tuned to specific frequencies to create narrow beams, they are used to help in source localization (bearing).*
- Using coherent superposition of multiple sensors, they are used for increasing gain for longer-range detection and scanning for specific frequencies.*

Sandia previously determined that the optimal configuration for this project was not to have numerous robots that carried sensors, but to have one larger vehicle deploying sensor pods that communicate by radio frequency (RF) rather than by cable or fiber. By successfully achieving the goal of a reconfigurable sensor array, this project enables us additionally to enhance the foundation of our core mobile robotic-vehicle and -sensor capabilities by making dramatic progress in multiple areas that significantly enhance our responsiveness in a wide range of timely business opportunities. These areas include the following:

- Sensor-array hardware and communication. Multisensor synchronous communication of seismic-array data to a central processor has not been achieved by RF before.*
- Sensor-array processing algorithms. Real-time processing of sensor-array data and autonomous reconfiguration algorithms has not been achieved.*
- Vehicle-control code architecture. Modular robotic-vehicle control for semiautonomous operation is not currently available.*
- Precision vehicle-placement control. Autonomous precision placement of vehicles to centimeter accuracies in unstructured (outdoor) environments has not been achieved.*
- Small autonomous-vehicle mobile manipulation. We have not previously incorporated manipulation on a semiautonomous vehicle of this small scale.*

Major elements of both the vehicle and the sensor signal-processing and array-optimizing hardware and software are in place, which will lead to significant demonstrations. The

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development of the stack loader, thumper, and prototype sensor pod was delayed. We have accomplishments in the areas of the robotic vehicle and the sensor-array communication and data-analysis software and hardware.

- *Autonomous robotic-vehicle capable of deploying and retrieving sensors.*
 - Fabricated and operated a dedicated SandDragon dual-body mobile robotic vehicle.
 - Designed and mostly assembled a new sensor-deployment and -retrieval nondexterous manipulator.
 - Completed restructuring the autonomous navigation-vehicle code into a modular, multithread architecture facilitating the addition of new vehicle-control modules, such as autonavigation algorithms being developed under other projects, and payload processors, code, and hardware.
 - Developed and tested software modules for autonomous waypoint navigation using the Novatel real-time kinematic global positioning system (RTK-GPS) unit capable of centimeter-scale repeatability.
 - Began developing software modules to implement sensor deployment and retrieval.
 - Defined the software interface with the sensor digital signal-processor (DSP) control system.
- *Sensor-array software and control-system development.*
 - Developed a unified modeling language (UML) software architecture model of the DSP master module and the sensor pod code.
 - Developed signal-processing algorithms and array-optimization algorithms on a workstation (versus the target DSP) to populate the UML model.
 - Procured and evaluated vehicle-based commercial DSP processor single-board computer (TI-C6711) with a synchronous serial-communication daughter card and a commercial Transmission Control Protocol/Internet Protocol (TCP/IP)-based radio-frequency (RF) transceiver card (Sybil 802.11b wireless local-area network [LAN]) capable of simultaneous communication with 16 sensor pods.
 - Procured and evaluated the sensor processor (TI-C5500) and analog prototype boards, and the RF transceiver daughter card for the sensor pods.
 - Made progress toward a benchtop demonstration of a multisensor, synchronized, i.e., retaining original relative signal timing from the different sensors, data transfer via RF to the access transceiver unit to be mounted on the robotic vehicle.
 - Implemented high-level communication code on a workstation and wrote low-level drivers for the communication cards.

We have accomplishments in the areas of the robotic vehicle and the sensor-array communication and data-analysis software and hardware.

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Algorithm Development for Prognostic Health Monitoring and Maintenance

L. P. Swiler, J. E. Campbell

Sandia seeks to evaluate, develop, and integrate algorithms for prognostic health monitoring and maintenance (PHMM). This project will result in a decision support system (DSS) to help evaluate maintenance strategies based on risk, time, and cost. The optimal recommendations will be dynamically updated based on changing conditions and sensor monitoring. The range of applications and customers for a PHMM tool is very broad. The PHMM algorithms will be tested and validated for a real system of interest for which we can obtain extensive statistical failure data, most likely the F-16 or the Future Combat System.

Our research is divided into two major areas:

(1) For a PHMM system to be robust, it must integrate information from a variety of sources to take into account all the evidence that impacts a prognosis for system health. To integrate this information, we are developing an Evidence Engine. The Evidence Engine uses a Bayesian belief network (BBN) for fusing information at the sensor-feature and failure-mode levels. We will use additional prognostic algorithms to detect trends, abstract and identify sensor features, estimate remaining useful life, etc.

(2) We are developing algorithms to analyze the consequences of various maintenance actions. These algorithms will be included in the Consequence Engine to provide a recommended course of action based on the current system state, pending problems, and planned equipment use. The Consequence Engine will include a scenario generator that automatically creates a suite of potential maintenance actions. Consequence Engine algorithms will calculate the impact of each proposed action on system failure and present a set of high-ranking potential actions.

This research is divided into two major areas.

- The Evidence Engine integrates information from a variety of sources to take into account all the evidence that impacts a prognosis for system health. The Evidence Engine has the capability for feature extraction, trend detection, information fusion through BBNs, and estimation of remaining useful life.

- The Consequence Engine involves algorithms to analyze the consequences of various maintenance actions. The

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Consequence Engine will provide a recommended course of action based on the current system state, pending problems, and planned equipment use. Consequence Engine algorithms will calculate the impact of each proposed action on system failure and present a set of high-ranking potential actions.

Sandia will concentrate on developing and testing a robust PHMM prototype tool. In terms of general tools, we decided to focus more on the Consequence Engine and less on the Evidence Engine for two reasons: (1) the Consequence Engine utilizes Sandia's strengths in reliability analysis and simulation, and (2) we found it difficult to create a general-purpose tool for feature extraction and evidence integration, as these functions tend to be very system-specific. As a result, the Consequence Engine will continue to be developed as a general tool applicable to a wide range of PHMM applications. Further development on the Evidence Engine will focus on a specific gearbox application.

We developed working prototypes of both the Evidence Engine and the Consequence Engine. We refined our ideas about our technical approach and received validation of these ideas when we gave a presentation on prognostics at the Military Operations Research Society Conference on System Sustainment.

- *Evidence engine.* We developed an object-oriented architecture for the Evidence Engine. Algorithms in the Evidence Engine include feature extraction, trend analysis, and BBN. Objects (major classes) include a sensor class, a sensor feature class, a distribution class, a failure mode class, and a BBN class. Methods within these classes include statistical moments, Fourier transform, polynomial regression, propagation of chance nodes updating a BBN, etc. We developed an approach for peak identification/peak characterization for vibration analysis of gearboxes.

- *Consequence engine.* Algorithms in the Consequence Engine include reliability prediction, cost, and schedule models. We also wrote a spares model that is partially integrated with the Consequence Engine. A major focus was to develop a capability to allow for different operational states, e.g., partially mission-capable versus up or down. We implemented this through "success paths" in the underlying fault tree. We also developed a better method for representing a time-to-failure distribution. The Consequence Engine takes as input a maintenance-and-use schedule, spares information, and time-to-failure data on components. It then generates maintenance and failure events and evaluates performance measures, such as

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equipment availability, mission-capable rate, time-to-failure, and cost.

Refereed

Campbell, J. E., L. P. Swiler, and B. M. Thompson. 2002. Consequence analysis in predictive health monitoring systems. *Proc. PSAM 6: Probabilistic Safety Assessment and Management Conference 1* (26 June, San Juan, Puerto Rico).

26545

New Mechanism for Upset of Electronics

R. A. Salazar, L. D. Bacon, L. L. Molina

This report contains theoretical and experimental results from testing and analysis and outlines the objective, process, results, and conclusion regarding the use of nonlinear dynamics to enhance the understanding of electronic upset. This report presents comparison of theory and experimental results from the most basic of chaotic electronic circuits, the Linsay circuit, which consists of one nonlinear component (a diode), one energy-storage unit (an inductor), and one dissipative element (a resistor). These three elements are the minimum number necessary to create a condition that an electronic circuit must have to exhibit chaotic behavior. This report also presents test results obtained by inducing chaotic behavior into a phased-lock loop. Sandia shows that a continuous-wave radio-frequency (CW RF) signal induced into the phased-lock loop circuit can cause the phased-lock loop to behave chaotically.

The objective of this project is to investigate the conditions under which selected electronic circuits and systems can be driven out of stable operation through exploitation of nonlinear dynamical system behavior, and to explore the role that such behavior can play in bringing about functional upset or disablement of electronic systems through exposure to the proper high-power microwave (HPM) radiation environment.

We constructed models to simulate circuit behavior to determine conditions that may lead to chaotic behavior. We conducted experiments to validate models and simulations. The Linsay circuit is the simplest circuit that can exhibit chaotic behavior. We used this circuit as a test case for model validation. We conducted additional experiments to determine the behavior of a much more complicated circuit—a phased-lock loop. We induced both CW and pulsed RF in the phased-lock loop and recorded the circuit response to the stimulus. Simulations of the Linsay circuit agree with experimentation. We developed tools to qualitatively compare chaotic behavior between simulations and experimental results. Comparisons show close agreement between the simulations and experimentation. Both CW and pulsed RF signals induced into a phased-locked loop caused the phased-lock loop to become unstable and exhibit chaotic behavior. By understanding the normal operating characteristics of the phased-lock loop, we proposed an explanation for the nonlinear behavior of the circuit.

We developed tools to qualitatively compare chaotic behavior between simulations and experimental results. Comparisons show close agreement between the simulations and experimentation.

Through simulations and experimental validation, we studied the application of nonlinear dynamics to the understanding of electronic-circuit behavior. We developed tools to analyze circuit behavior and to determine if the circuit is in a state of operation that is either linear (normal or abnormal operation) or chaotic (abnormal operation). Simulations of the Linsay circuit successfully predicted experimental results. We now have a validated Linsay circuit model. Test results show that a proper stimulus will send a phased-lock loop into a chaotic state. Based on normal circuit operation, one can predict when the phased-locked loop may leave normal operation and operate outside of its normal regime of operation.

Nonlinear analysis enhances our understanding of circuit operation. Linear theory explains normal circuit operation (designed normal operation). When an electronic circuit operates outside of its intended range of operation, linear analysis does not fully explain the circuit's operation. Analysis and experimentation both demonstrated that the operation of an electronic circuit outside of its normal range of operation can exhibit nonlinear behavior. We conclude that nonlinear dynamics can predict circuit operations not predictable with normal linear-circuit theory. One can use this additional understanding to improve the analysis of functional upset or disablement of electronic systems.

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Flexible Robotic Maintenance Facility

W. D. Drotning, C. S. Loucks, W. J. Prentice, P. A. Watterberg

The Department of Energy's Robotics and Intelligent Machines Roadmap was the first-known study to identify classes of processes that could be automated. The Roadmap identified the technology bases that underlie noncontact, contact, and multiprocesses. The goals of this project are to develop advanced design tools for flexible robotic workcells and to apply these tools to develop a conceptual design for an automation-intensive maintenance facility for a class of complex systems.

Sandia envisions a facility that is designed for automated operations and can accommodate an entire class of complex systems, including weapon systems, so that the cost can be amortized over multiple systems and processes. The facility will have multiprocess automation equipment to reduce maintenance manning requirements. The resulting tools will be applicable to the design of robotic workcells for other complex systems. We will perform a system study of military aircraft depot maintenance to identify high-payoff automation opportunities.

We have realized elements of this vision for the aircraft painting/coating process and for nuclear weapon (NW)–component spray cleaning. In developing advanced painting/coating/cleaning systems, we discovered the need for more-advanced design tools, which we will develop in the course of this project. These will be targeted at environments requiring many changes in task or workpiece. The tools will allow rapid analysis of a workcell configuration, including both commercial and custom hardware, for operations on any component of a class of systems. The needed tools will integrate modeling and simulation, automated path planning and generation, and minimization methods to support analysis of workcell architectures. They will allow assessment of designs with variable workpiece position. The required tools will use automated methods to minimize the number of robot positions that must be specified by the operator. We will select a key process technology for analysis.

Generally, existing automation systems are utilized frequently, but as expected, are very specific and do not contain features that support flexibility. There is a common need to address the path and task planning, motion, and location of automation systems for maintenance operations. For larger

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structures, the maintenance automation system may likely be moved around the aircraft, as opposed to statically occupying a large workcell footprint. It is clear that, especially for automation operations on larger aircraft, the reachability analysis tool and tools for automated path generation and registration are needed and will benefit broad process areas such as cleaning, coating, surface preparation, finishing, decoating, sealing, fastener removal/insertion, and inspection. To optimize efficiency, a reachability analysis is essential to minimize movement of the automation system around large aircraft.

Automation of some depot processes is inhibited by the wide variety of parts to be handled in a process. If the number of part variations and types is high, and the quantity of each part is not large, the costs for automation often cannot be justified. This is clearly an opportunity for development of flexible workcells that perform automated programming of the robot system, based on inputs from sensors and models of parts and the workcell. This approach will provide automation solutions for a much broader variety of maintenance operations.

We improved and extended software tools for design analysis to encompass greater breadth for eventual application as a generalized design tool. We enhanced the design tools for automated path planning and generation to incorporate those complex robot systems with redundant joint configurations, which are likely candidate designs for a complex aircraft-maintenance facility. By employing advanced inverse kinematic-solution methods and optimization techniques, we enhanced the prior design tools for automated path generation to provide greater flexibility and generality, as well as improved performance for complex robotic systems.

We continued the development of flexible automation design-analysis tools, focusing on integrating and enhancing the automated reachability-analysis tool and the automated path-generation and optimization tools. The goal is to build these into a framework that is accessible to engineers in a more robust and generalized analysis tool and that eliminates the *ad hoc* nature of past implementations of these tools. Work is nearly complete on the task to enhance and modify these tools and to integrate them into UMBRA, a user-interface environment for advanced controls, simulation, and visualization. From prior tools, the robot-specific knowledge needed to be separated from application knowledge, so that new robot objects can be implemented rapidly without modification to the process-application or user-interface software. When completed, a demonstration of the integrated design tool will be available

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and will show the flexibility of the tool for analysis of maintenance operations. The demonstration will comprise the analysis of an automation facility containing two different aircraft (P-3 and B-2) for operation with two different processes, such as FlashJet depainting and radar-absorbing material (RAM) coating.

We selected a candidate process technology for demonstration. The process of precision surface finishing and preparation appears to be an important and broadly needed technology and one where automation has been hindered by lack of advanced technology. It is also representative of a wide variety of in-contact processes that may employ model-based position analysis, sensor-based workpiece characterization, robot motion control, and process monitoring/feedback. We continued to plan the technology development for a demonstration of this maintenance process.

Other Communications

Drotning, W. D., C. S. Loucks, W. J. Prentice, and P. A. Watterberg. 2001. Flexible automation for aircraft maintenance. *Proc. Defense Manufacturing Conference (DMC) '01 CD-ROM* (27 November, Las Vegas, Nevada): 200.

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Distributed Autonomous Navigation

G. R. Eisler, K. M. Jensen, D. D. Padilla, J. D. Bradley, C. L. Lewis T. J. Kim

This research will develop a scientific framework for distributed navigation using swarms of vehicles. This framework will allow navigation with or without the availability of the global positioning system (GPS). Our approach leverages Sandia's long-term capabilities in terrain-aided navigation (Sandia Inertial Terrain-Aided Navigation [SITAN] Program, and Inertial Terrain-Aided Guidance [ITAG] Program) and swarm robotics.

As demonstrated by the recent war on terrorism, using robotic warfighting aides will continue to grow, increasing the need for robotic navigation, command and control of distributed robotic systems, and control of robotic sensors. We envision distributed sensor grids for future battlefields in both static and mobile forms. This project addresses several of the critical navigation and control issues.

Recent efforts were in the areas of simulation and algorithm development for optimal collective trajectories, navigation tradeoff analyses for position estimation, and validation experiments of terrain-based localization models using uncorrected GPS.

We developed simulations to deploy collectives in continuous line-of-sight (LOS) communication networks over complex terrain. We used deepest-descent control to simulate vehicle deployment to ensure local LOS between nearest neighbors, thereby ensuring an end-to-end "transmission."

We carried out experiments to validate simulation results for a terrain correlation algorithm. We used our calibrated test-bed terrain, developed earlier, to provide the shared map data.

We developed a six-degree-of-freedom trajectory generator to simulate vehicle traversals on arbitrary accuracy levels of digital terrain elevation data (DTED). We mated these trajectories to a navigation error analysis simulation developed at Sandia to demonstrate component accuracy tradeoffs on position estimation. We extended a known calibration technique for missile applications, zero-velocity updating that is based on stop-and-go vehicle operation, to the land scenario. We demonstrated this technique to reduce position errors without the use of GPS.

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Other Communications

Eisler, G. R., and C. L. Lewis. 2002. Cooperative robotic map correlation from relative position and terrain slope measurements. *World Automation Congress/Advances in Robotics, Manufacturing, Automation, Control, Soft Computing, Multimedia, Biomedicine, Image Processing and Financial Engineering, Proc. 9th International Symposium on Robotics and Applications (ISORA 2002)* 3 (12 June, Orlando, Florida): 1–6.

26548

Obstacle Detection for Autonomous Navigation

D. D. Padilla, M. R. Muguira, S. E. Eskridge, D. K. Novick, J. J. Carlson, J. C. Neely, P. A. Davidson, Jr.

Since the terrorist acts of September 11, 2001, there is an ever-increasing need for autonomously navigating vehicles for counterterrorism and defense missions. The limiting factor in autonomous navigation is the ability to sense and map the environment. This project will develop a mathematical framework for obstacle detection. Sandia expects the framework to provide a basis for solutions to many complex obstacle-detection problems critical to successful autonomous navigation. One goal of this project is to characterize sensing requirements in terms of physical characteristics of obstacles, vehicles, and terrain. For example, a specific vehicle traveling at a specific velocity over a specific terrain requires a sensor with a certain range of detection, resolution, field of view (FOV), and sufficient sensitivity to specific obstacle characteristics. In some cases, combinations of sensors may be required to distinguish between different hazardous obstacles and benign terrain. In our framework, the problem will be posed as a multidimensional, multiple-hypothesis, pattern-recognition (PR) problem. We will extract features from selected sensors that allow hazardous obstacles to be distinguished from benign terrain and other types of obstacles. A weighted-nearest-neighbor (WNN) decision model will fuse feature measurements to minimize classification errors. In addition, classical estimation theory will provide the framework for estimating obstacle characteristics such as position and size. Another goal of this project is to characterize different terrain classes with respect to both positive obstacles, e.g., rocks, trees, and fences, and negative obstacles, e.g., holes, ditches, and drop-offs. The density of various hazards per square kilometer will be statistically quantified for different terrain categories, e.g., high desert, ponderosa forest, and prairie. This quantification will reflect the scale or size and mobility of different types of vehicles. The tradeoffs between obstacle-detection, position location, path-planning, and vehicle-mobility capabilities will also be characterized.

Our work focused on investigating and developing sensing technologies for obstacle detection as well as developing a simulation environment for obstacle detection.

No single sensing technology capable of fully characterizing complex, natural terrain exists. We are exploring

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innovative ways to use existing sensors. Through the evolution of various autonomous systems and missions, sensor engineers need to be able to combine multiple sensors without impacting the entire system, i.e., plug-and-play modules. We are developing a simulation environment using the modular architecture framework described in our previous work. The simulation uses various sensor attributes, e.g., spatial and range resolution, probability of detection and false alarm, FOV, and range of detection, to compute metrics of performance.

The most widely used sensor for autonomous navigation is commercial ultrasonics intended for operation in controlled environments to detect the presence of objects. These sensors output a range measurement based on the time-of-flight (TOF) of the first return to exceed a set threshold and can even detect a blade of grass. A significant amount of effort focused on the development of detection/classification algorithms using the raw echo return signal of conventional ultrasonics. Typical half-power beam-widths of these sensors are 8 degrees, resulting in poor spatial resolution. We addressed this deficiency by building an acoustic, phased-array imager providing a three-dimensional (3-D) profile of its FOV. For liquid and solid media, acoustic imaging is a highly developed tool in use in several sciences. Acoustic imaging in air is a difficult task and requires more investigation before it may be realized for autonomous vehicle navigation. We tested several transmitters and receivers in various configurations before concluding the final design. Testing shows agreement between simulation and hardware verification results.

In addition, we are evaluating the potential of using high-resolution aerial photography for mapping and obstacle detection, as well as a scanning-laser range finder.

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Laboratory-Scale Coherent Multikilovolt X-Ray Sources for Advanced Imaging Applications

A. Mar, T. R. Nelson

Sandia plans to employ a 100 fs, 248 nm terawatt laser to induce rapid multiphoton field ionization of hollow xenon clusters to create high-peak spectral-brightness (~ 4 keV) coherent x-ray sources near $2.9 \text{ \AA}$. We will confirm x-ray lasing by measuring x-ray energy yield, density/gain-length product, and spatial divergence as a function of orientation, with optimized stability and brightness. Such a revolutionary advance will have significant programmatic impact on laser-based directed-energy applications and next-generation x-ray backlighters and radiographic imaging diagnostics.

We performed single-pulse measurement of the spectral and spatial distribution of the radiation emanating from the channel using two imaging spectrometers, one located transverse to the laser channel and one positioned in the forward direction. Alignment of the transverse spectrometer will present no particular difficulty. Correct initial alignment of the forward-going spectrometer will require identification of the potential lasing transition because of the narrow rocking curve width of the spectrometer crystal for diffracting narrow collimated beams. The key hardware for this measurement is a precision mount for the forward spectrometer that can adjust the angular orientation of the spectrometer to less than the rocking curve width of the spectrometer crystal, typically better than 10 arc s .

If x-ray lasing occurs, there will be a forward-going x-ray beam with a divergence characterized by the channel length and channel diameter. Diffraction of the x-ray beam is minimal due to the wavelength. Demonstrating the presence of a forward-going beam is important. We performed this demonstration using damage patterns to titanium foil that was mounted in front of the imaging spectrometers and in front of recording film. The damage patterns indicate a beam divergence of 200 microradians .

Such a revolutionary advance will have significant programmatic impact on laser-based directed-energy applications and next-generation x-ray backlighters and radiographic imaging diagnostics.

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Microfuze

L. S. Weichman, A. D. Oliver, M. J. Retter, S. M. Harris, D. R. Koehler, A. S. Tappan, S. H. Kravitz

The primary mission of the weapon fuze is to provide system-safety enablement and subsequent control of weapon detonation events. Within this architecture, the fuze integrates inputs from various environmental sensors and, if the preset conditions for weapon function are realized, supplies the required detonator stimulus. Present fuzes found in Department of Energy (DOE) and Department of Defense (DoD) applications are based on bridge-wire or foil-detonator technologies that require a high-voltage, high-current stimulus and consequently occupy volumes from several to tens of cubic inches. Furthermore, traditional fuzing safety within these architectures is predicated on the use of insensitive explosives and the “uniqueness” offered by the electrical stimuli required to initiate the main charge detonators.

Evolving mission scenarios for future DOE and DoD weapon platforms will soon outpace the capabilities of today’s fuzing technologies. Targeting buried assets and meeting tomorrow’s battlefield engagements will require advanced fuzing architectures characterized by “intelligent” function under multiple, high-G impacts. Achieving increased fuze functionality in a size constraint implicit with high-G survivability implies development of novel system architectures, incorporating new concepts in munitions safety and the realization of miniaturized component suites based on emerging processes and technologies. Establishing a sound technical foundation and effective integration of Sandia expertise in safety enablement, microdetonics, silicon (Si) surface micromachines (SMM), microsensors, and semiconductor electronics will prove essential in achieving the required revolutionary advancement in the fuzing community.

We will direct the ultimate realization and embodiment of the proposed science and technology foundation toward accomplishing the required safety and fuzing functions on a single substrate, or “chip.” If successful, the “fuze-on-a chip” would give future system designers the tools necessary to address next-generation fuzing functions in an environment currently not obtainable by today’s technology.

We completed our preliminary application survey and subsequently sharpened the focus of our project activities on a baseline safe and arm (S&A) architecture and a corresponding

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set of enabling technologies and processes. We narrowed our focus to (1) identifying compatible safety architectures, (2) initiating process development and mechanical characterization of microelectromechanical systems (MEMS)–based S&A structures and devices, and (3) developing explosive train components and database for subsequent fuze integration.

- *Architecture/S&A device.* We established a safety architecture and identified a corresponding mechanical S&A architecture for further development. This architecture is based on an established “out-of-line” safety implementation that interrupts the energetic train, effectively isolating the “sensitive” primary explosive from the approved secondary lead or booster explosive. Building on our efforts, we fabricated a first-generation device and subsequently redesigned the S&A slider mechanism to include additional mechanical features that selectively discriminate and utilize setback shock and spin to translate the transfer charge from the safe to the arm position. We fabricated a number of key test structures (simple beams, setback cantilevers, and slider mechanisms) in silicon using the deep reactive ion etch (DRIE) process and a novel two-level mask technique. From these test structures we hope to build an initial Sandia database detailing pertinent material properties (natural frequencies, stiffness, etc.) and demonstrate survivability under high shock and operation under combined mechanical environments.

- *Igniter and explosive development.* Selection of the targeted S&A architecture aided in identifying and refining those enabling technologies and processes required for further integration of the S&A device with the required explosive components. The defining requirement for the igniter driven by our selected S&A architecture was to initiate an explosive charge located across a predefined gap. We investigated two explosive mechanisms (shock and thermal), two device types (microbridges and reactive bridges), and various explosive materials for this application. Specific accomplishments in the area of energetics and initiators include (1) development of a high-resolution photometric system for observing the breakout of extremely small bridges (10 μm), (2) characterization and successful demonstration of the explosive output and the required shock transfer from a small CL-20 lead pellet (0.040 in. x 0.040 in.) to a larger boost pellet (0.125 in. x 0.125 in.) located along the armament energetic train, and (3) design and evaluation of various reactive bridges, geometries, and materials for their electrical function and ability to initiate primary explosives. As a typical example of the ongoing igniter characterizations, we evaluated the electrical behavior and

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induced reaction zone for the titanium/boron (Ti/B) devices supplied by Auburn University. The initial device characterization suggests that the voltage threshold and reaction zone strongly depend on the bridge size and the electrical circuit used to initiate the Ti/B constituents. Testing conducted where we placed lead azide in physical contact with the reactive bridge suggests sensitivity of this igniter to particle size, purity, and containment of the primary explosive. Testing of this design with other primary explosive mixtures (lead styphnate and tetracene) continues. In a parallel manner we designed, fabricated, and evaluated first-generation Sandia igniters. These devices feature aluminum (Al) and palladium (Pd) as the reactive constituents, a zirconium (Zr) film for transferring energetic particles across the gap, and an integral barrel design to “focus” the intended Al/Pd reaction onto the primary explosive.

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Other Communications

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38623

Automated Visual Direction of Mobile Manipulation

P. C. Bennett, C. W. Wilson, T. S. Gladwell, R. J. Anderson, M. J. McDonald

Sandia will develop semiautonomous mobile manipulation technologies that enable engagement of threat devices and forces in remote environments. Most current remote technology development for national security applications focus on sensing and situational awareness. However, in close-quarter environments with ill-defined characteristics, the need for direct interaction with adversarial situations creates a unique need for new manipulation technologies. In addition, remote system technologies must be capable of adapting to and engaging widely diverse threat environments if they are to be generally useful. Example environments subject to security threats include Department of Energy (DOE) secure facilities, legacy production facilities containing hazardous-waste materials, Department of Defense (DoD) urban conflict situations, and public environments subject to terrorism acts. All of these situations require direct engagement of devices and forces in highly controlled ways to minimize collateral damage.

Explicitly, we will develop modular control technologies that enable robust operation of mobile manipulators in extremely hazardous environments. We will accomplish this by reducing dependence on high-performance sensing, facilitating plug-and-play system reconfiguration, enhancing human interfaces, and providing error and damage recovery. Such remote-system concepts have eluded successful implementation in the past due to the lack of formalisms for system integration. We will build upon past advances at Sandia to provide mathematical formalisms to support rapid integration of heterogeneous capabilities into operational systems with well-characterized performance. We will extend modular architectures developed at Sandia, to include mathematically sound integration of visual and other sensor-based control approaches. In addition, we will extend these control environments to support novel vision-based human-machine interfaces and vision-based remote-systems control approaches.

We made some modifications to the process from the original proposal because of the 11 September 2001 attacks on the U.S. to move available components more swiftly to the field. However, the task goals remain essentially identical.

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We configured and tested early versions of modular control and vision-based human-interface technologies. End-users performed remote operations, including locating buried mines, defusing antipersonnel mines, placing breaching frames on walls, cutting trip wires, chemical sampling, and others. Even with the hastily integrated early-stage technology, explosive ordnance disposal (EOD) personnel, military police, and chem/bio technicians were able to perform complex remote tasks remotely with less than one hour's training. Training at the Federal Bureau of Investigation (FBI) Hazardous Devices Training School, for example, using similar robotic devices typically requires 2+ days. We also observed approximately a 5-times speed-up in most remote operations.

EOD technicians interviewed after World Trade Center recovery operations cited needs for improved ease of use and more robust operation. In addition, the National Nuclear Security Administration's (NNSA) Office of Emergency Response has now tasked us to review nuclear EOD training and procedures based on reviewing technology under development in this project.

Technical progress is ahead of schedule, even though we elected to reevaluate user needs after 9/11. To stimulate faster technology development, the software framework UMBRA was linked to the modular robot control environment SMART. UMBRA was developed under a previous project and supports rapid integration of advanced algorithm modules without the need to rewrite software. By coupling UMBRA and SMART, we are able to more quickly and robustly integrate advanced capabilities. For example, we were able to incorporate initial components of visual servoing software into our laboratory in UMBRA very rapidly and recover initial schedule slip resulting from reevaluation of user needs. This software is being coupled to robot control through SMART. Thus we have validated the need for technology, established early metrics of performance, and have been able to remain slightly ahead of the technology development schedule originally proposed.

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38624

Miniature Fourier-Transform Ion-Mobility Spectrometer for Real-Time Detection and Identification of Explosives and Chemical Agents

E. E. Tarver, III, R. J. Bastasz, R. T. Jennings, R. Steinhaus

Ion-mobility spectrometry (IMS) is a trace analytical technique capable of sub part-per-billion (ppb) detection of either positive or negative ions formed from organic vapors. Sensitivity in IMS is a function of the duty cycle of the electronic gating grid that pulses the ions into the detector. Conventional IMS instruments pulse the grid open for 0.2 ms every 20–25 ms, or about 1% of the analytical duty cycle. As a consequence, 99% of the available ions formed are discarded. Fourier-transform ion-mobility spectrometry (FT-IMS) is an alternative mode of operation in IMS. FT-IMS utilizes dual, synchronously pulsed ion gates, which are pulsed open at increasing frequency for 50% of the duty cycle. FT-IMS instrumentation is capable of collecting 50% of the available sample ions as compared to 1% with conventional IMS. Sandia demonstrated increased sensitivity due to the higher duty cycle of the entrance gate and improved spectral resolution caused by the phasing action of the second gate. Our next goal is to combine FT-IMS with Sandia's LIGA (the German term Lithographie, Galvanoformung, und Abformung, for lithography, electroforming, and molding) microfabrication technology to develop a miniature, battery-powered detector. We will build and test the miniature LIGA ion-gating grid and drift tube for the spectrometer. We will utilize digital signal-processing chip technology and application-specific circuitry to replace current electronic hardware for data acquisition and control. We will also develop preconcentration techniques for inclusion in the same integrated package. We will optimize instrumental figures of merit and selective detection parameters through the use of variable electronic gating and controlled ion-molecule reaction chemistry. Because of the expanded control of the system possible through the use of micromachines, it is possible to operate the system in both ion-collection modes on an effective real-time basis, greatly expanding the flexibility of the device and minimizing the chance of false positives.

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- *Customization of electronics.* The Hewlett-Packard scanning square-wave generator and prototype Sandia signal commutator were replaced with programmable photonic integrated circuit (PIC) chips along with solid-state circuitry

condensed onto a custom-designed integrated circuit (IC) to perform the functions of the initial electronic hardware. We combined instrument control, data acquisition, and display electronics and software with a palm-size computer to reduce the instrument footprint.

- Refinement of LabView software.

(1) We developed software revisions to reduce acquisition/display processing time and power consumption for a battery-powered instrument.

(2) We developed a peak-recognition algorithm for compound identification using characteristic spectral identifiers, i.e., reduced ion-mobility constants, K_0 .

- Fabrication of drift tubes, ion gates, test-bed, and control electronics.

(1) We machined and assembled three stacked-ring design drift tubes and their accompanying Macor insulators (4 mm, 8 mm, and 15 mm inside diameter [ID], respectively).

(2) We fabricated Macor drift tube adaptors and stainless-steel sample inlets with Macor adaptors to secure and align each of the three drift tubes in the base of the aluminum test-bed housing.

(3) We fabricated two sets of LIGA (the German term *Lithographie, Galvanoformung, und Abformung*, for lithography, electroforming, and molding)—fabricated ion gates with 20 μm and 40 μm wire thickness with 20, 40, and 80 μm wire spacing for each drift tube ID.

(4) We developed drift/carrier-gas supply, scrubber system, and rotameters for gas-flow control.

(5) We developed Omega temperature controller, thermocouple, and (4 x 1/4 inch) heater cartridges to set and maintain constant temperature of the test-bed housing.

(6) We connected a Bertan Series 230 High-Voltage Power Supply to the Sandia voltage divider (1 M Ω resistor chain) to produce the electric field gradient for ion acceleration and separation.

(7) We connected a Faraday collector terminating the drift tube to a Keithley 428 Current Amplifier to monitor ion-current output for processing and display.

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Refereed

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38625

CONOPS Development for Automated Systems

M. E. Senglaub, P. R. Klarer, M. D. Ladd, D. L. Harris, E. M. Raybourn

The current scientific approach of assessing the capabilities of autonomous forces fails to provide a full, dynamic integration of the functions associated with autonomous forces such as multiple robotic elements, sensors, communications architecture/protocols, decision-support infrastructure, and information-fusion algorithms.

Detailed modeling and integrated representations of these entities is needed to characterize performance in combat situations. These algorithms will provide analysts with the ability to perform “what-if” decision analyses and trade studies providing a basis for the design of fully integrated systems. Employing mission-performance metrics permits us to find the optimal deployment, utilization, and design of these systems. The lack of doctrine and tactics associated with the integration of autonomous forces into a combat organization is of great concern. This limitation could translate into potential failures in combat tactics and training, in the logistics stream, and in system design and acquisition planning. The present effort (1) focuses on representing the tactics of autonomous forces, and (2) considers the issues involved in integrating the resulting algorithms into a Joint Conflict and Tactical Simulation (JCATS)-like combat simulation.

Efforts supporting countermeasure study helped identify a suite of systems-engineering analysis optimization methodologies that support needed integrated analytical infrastructure. This involves the integration of possibility theory, Taguchi analysis, evolutionary strategies, and genetic programming.

Communications system. Work focused on providing a set of first-order equations that describe the dispersion of power in a radio wave as it expands into open space. The effects of antenna aperture, gain, and transmitter power are included. A literature search for these second-order effects revealed several models that have been used to simulate radio links. We wrote a report that describes the requirements placed on a communication system by ground vehicles operating in modes of autonomous, point-and-go, and teleoperation.

Additionally, we identified an analytic approach for modeling networks that employ evolutionary-based technologies that will significantly improve computational

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performance as well as begin to address issues associated with *ad hoc* networks.

Operational terrain database. Work focused on developing a parametric composite terrain database for analysis and visualization use. We “grew” synthetic terrain to correlate to some actual digital terrain elevation data (DTED) sampled data, then overlaid operational features (foliage, soil conductivity, etc.) and vector data (road, rivers, etc.) on the generated terrain surface. To avoid the topological problems that plague purely synthetic terrain-generation systems, such as unrealistic surface drainage, we decided to try to match actual terrain by fitting a series of parametric hills using a genetic algorithm (GA) approach.

Vehicle mobility. All analysis assumed quasistatic conditions for obstacle climbing, and true dynamic equations of motion are currently under development. A simple model that accounts for two of the most important generic soil parameters for shear strength is the Mohr-Coulomb model, which is currently being investigated as a method for including soil mechanics parameters into simulations of vehicle-terrain interactions.

Interface. Research in the visualization of, and user’s ability to make sense of or interact with, the information being conveyed in simulation is under way.

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38626

Rapid Mitigation and Decontamination of Toxic Industrial Chemicals

M. D. Tucker; R. G. Betty

Recent attention has focused on responding to terrorist events involving chemical/biological warfare (CBW) agents. Our recent work on the development of a Sandia decontamination technology successfully addressed biological toxins (e.g., Ricin and botulism), biological pathogens (e.g., anthrax and plague), and CW agents that were traditionally developed for military use (e.g., Sarin, VX, and mustard). However, a more likely scenario would be for terrorists to steal readily available toxic industrial chemicals (TICs) such as anhydrous ammonia, phosgene, hydrogen cyanide, and chlorine gas for use as chemical agents. This avoids difficulties such as producing highly toxic CW agents in a safe manner, the acquisition of precursors for chemical agents that are closely monitored, and the direct handling of the agents during dissemination. In fact, the Federal Bureau of Investigation (FBI) considers the terrorist use of TICs to be more likely than the use of the traditional military-type CW agents. One objective of this research is to develop an environmentally friendly chemistry that rapidly mitigates and decontaminates TIC threats in both the liquid and the gas phases. A second objective is to develop and identify deployment options for both building and airborne plume applications suitable for use by both a first responder at the scene of a terrorist event and those responsible for restoration of a facility after an event. Development of this technology enhances Sandia's portfolio for dealing with the top six terrorist weapons of mass destruction (WMD) threats identified by the FBI. In order, these are biological toxins, TICs, biological pathogens, radionuclides, CW agents, and nuclear weapons. The technology will have broad market appeal beyond antiterrorism efforts since it could also be routinely used for nonterrorist events such as accidental HazMat spills and releases.

We emphasized the development of the appropriate chemistry for use by civilian and military first responders who may encounter TICs that are likely to be used as "chemical agents." The first step was to identify TICs that are considered to be a threat. We gathered data from Department of Justice (DOJ) and Department of Defense (DoD) sources that identify TICs that are a threat based on accessibility, production volumes, and physical and chemical properties. The DOJ, for example, identified 21 TICs at the highest threat level, 38 TICs

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at a medium threat level, and 39 TICs at a low threat level. This threat list includes irritants (e.g., sulfur dioxide [SO₂] and anhydrous ammonia), choking agents (e.g., phosgene and hydrogen cyanide), organophosphorous pesticides (e.g., malathion and parathion), and volatile organic compounds (VOCs), e.g., isocyanates. The list includes both gases and liquids.

The next accomplishment was to evaluate the reaction chemistry required for the neutralization of the TICs on the threat list. We determined that the majority of the threat list TICs can be neutralized by four reaction mechanisms and developed a reactive foam for each of these reaction mechanisms. Our focus was on developing foams, because this gives a method to rapidly deploy the reactive formulations over large areas that is especially applicable for use by the first responder.

We also began testing the reactive foams against TICs on the threat list. We successfully neutralized parathion, malathion, carbon disulfide, hydrogen cyanide, sodium cyanide, chlorine, ammonia, and benzyl isocyanate by the appropriate reactive foam.

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EM Interactions with Systems to Enhance Security

L. F. Rinehart, P. W. Cooper, G. J. Denison, L. D. Bacon

This project will explore novel electromagnetic (EM) interactions of high-frequency radio-frequency (RF) waves that will help understand the vulnerability of circuits and systems with the goal to enhance security of Department of Energy installations. One possible application is the use of RF to stop vehicles without harming their occupants. Sandia will study and select this and other applications and will study high-priority scenarios in detail. This project is a high-risk, state-of-the-art approach that may provide protection against terrorist threats in many scenarios. The research will be devoted to EM coupling calculations and experiments, acquiring systems that are relevant to security and performing tests on the systems. We will enhance security by coupling EM energy to the target systems in a nonlethal manner. Thus, this improvement could be used in many environments such as facilities in urban environments. Further, it is expected that the applications demonstrated here might also have Department of Defense applications such as in military operations in urban terrain and in the future combat system.

We modeled the scenario on a USS Cole-type attack where the attackers use conventional mining technology blasting-cap initiators (as they are known to do). Here, we assess the vulnerability of their firing circuit and blasting cap to shipboard radar radiation.

We completed the literature search with over 40 documents located and reviewed. Using blasting-cap data, we did a statistical analysis and determined probability of function versus energy deposited in the blasting cap.

We obtained “safety detonators” for testing. These are blasting caps similar to those used by terrorists, containing a bridgewire and “match,” but without their explosive output charge. We performed susceptibility experiments in a small-volume test cell (0.1 m^2) to determine which frequencies, power densities, and geometries couple the most energy to the blasting caps; we tried over 100 combinations. The effectiveness against the blasting caps varies as wavelength squared.

To enable full-scale testing, we purchased a military surplus APS-20 airborne S-band search radar and brought it up to full operational specs. The transmitter produced a maximum peak-

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power output of 2.8 MW at 2.88 GHz. Two pulse lengths are available: 1 μ s and 2.5 μ s, which may be operated at 900 or 300 pulses per second (pps), respectively. We set up the radar to operate in an anechoic chamber with ~ 7.5 m of range available between the antenna and the test-object location. We measured the antenna E-plane and H-plane patterns so test objects could be located for optimum exposure. With the radar in its short-pulse mode, we measured 406 kW/m² peak and 406 W/m² average power density on boresight.

We measured the antenna E-plane and H-plane patterns so test objects could be located for optimum exposure. The large-volume exposure may couple more energy to the blasting caps, even though the power density is lower.

We then investigated alternate methods to attack the detonators. Since the effects vary as wavelength squared, we decided to operate at lower frequency. Toward that end, we purchased high-frequency band (2–30 MHz) shipboard communications equipment capable of 1 kW continuous output and are making it operational. Coupling to the blasting-cap wires should be orders-of-magnitude better at these frequencies. We used the rack-mounted transmitter and three-element Yagi beam antenna with an operational 100 W transmitter on top of the rack. High-frequency testing against blasting caps has begun.

Additionally, we are performing wire-scramble coupling experiments using an instrumented blasting cap to determine the boundaries of the coupling problem. Resulting data should point us to the optimum frequency.

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38628

Adaptive Awareness for Personal and Small-Group Decision Making

C. M. Pancerella, S. Tucker, R. D. Kyker, R. J. Malins, H. H. Hirano, K. J. Perano, E. P. Parker, A. B. Doser

A number of military and civilian applications can benefit greatly from intelligent agents that can process sensor data, reason about a situation, enhance both personal and situational awareness, warn humans about situations, and act as decision-making aids. Existing environmental sensors (chemical and biological), location sensors, and health sensors provide an interesting collection of sensors that can be used by intelligent agents to recognize cues from sensor data and previous experience, warn humans of possible scenarios, and advise humans during a stressful situation. By coupling sensors, secure wireless communications, and intelligent agents, Sandia seeks to prototype an adaptive awareness, warning, and decision-making tool for use by individuals and teams in stressful situations.

To realize this tool, we will develop a sensor-independent architecture for integrating self-awareness information across a distributed team, and the design approaches, concepts, and software agents for a tool that supports squad-level decision making. Distributed agents coordinate to deliver both personal awareness and situational awareness. Agents reason across sensor and simulation data and communicate with other agents. Underlying the agent reasoning will be the Recognition Primed Decision (RPD) model, which describes human decision making in real, stressful situations. The RPD model describes how human decision makers integrate information, develop cues, and learn to recognize situations based on relevant cues. The products of recognition are an understanding of goals, expectations, cues, and courses of action.

Over time, agents learn. Hence, the tool's capability will improve as information from previous attacks and expert models is used to prime the recognition capability of the chemical monitor system. Agents will create situational story lines, another adaptation of the RPD model, and will also use data gathered by the team.

(1) We collaborated with the U.S. Army Research Institute of Environmental Medicine (USARIEM), which agreed to share its data and to collaborate on algorithms for interpreting and real-time processing of physiological monitoring data.

(2) We began experimentation and data collection on the Body Media sensing device.

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(3) We demonstrated Bluetooth as a wireless Personal-Area Network with two sensors.

(4) We completed the design of the ERI sensor component.

(5) We designed agent architecture and reasoning algorithms.

(6) We did the preliminary research and development on self-organizing map (SOM) technologies.

(7) We currently are developing (implementing) agent architecture.

(8) We implemented a scheme incorporating a SOM in MATLAB to aid in decision making. We developed a new clustering algorithm *in situ* to process the information produced by the SOM. The clustering scheme is a cross between supervised and unsupervised learning.

(9) We tested the SOM using actual physiological sensor data taken from multiple persons with the Body Media sensor and showed it to successfully differentiate between seemingly difficult cases, such as sleeping versus reclining on the couch while watching television.

(10) We procured Zaurus processors and ported sensor framework to this platform.

We tested the SOM using actual physiological sensor data taken from multiple persons with the Body Media sensor and showed it to successfully differentiate between seemingly difficult cases, such as sleeping versus reclining on the couch while watching television.

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38629

Use of Seismic and Acoustic Responses to Assess Bomb Damage to Underground Facilities

L. C. Bartel, H. D. Garbin, J. G. Arguello, Jr., N. P. Symons, M. D. Ladd, G. J. Elbring, D. F. Aldridge, G. E. Sleaf, J. F. Holland

The precise location of the weapon explosion and resulting pressures within the target facility are critical for both bomb damage assessment (BDA) and battlefield planning. Simultaneous observations of seismic and acoustic waves coupled with state-of-the-art modeling offer the opportunity to determine detailed blast location and predict pressure regimes within buried facilities. Weapon detonation in rock produces significantly different seismic and acoustic-energy partitioning from detonation in the void of the facility. Interior detonations produce additional variations arising from possible blast venting through facility openings. Understanding and modeling of the amount of energy generated in both seismic and acoustic modes can provide critical information to determine where the blast occurred and estimate the resulting pressures within the facility. Preliminary numerical simulations utilizing an existing three-dimensional (3-D) seismic-acoustic algorithm demonstrated the capability to model these differing seismic and acoustic signatures. Sandia will develop a methodology to quantify BDA through seismic and acoustic numerical simulations and by analyzing data, both preexisting and new data, collected in community experiments. Critical aspects include the inelastic behavior of the blast, its coupling into elastic and acoustic-wave propagation models, and the acoustic-seismic coupling in the facility and at the air-earth interface. The end result will be a validated numerical capability to predict pressures within underground facilities (UGFs) for various bomb-drop scenarios. In addition, we will have a methodology to characterize the explosive source signature.

For a bomb blast in earth materials, there will be a nonlinear-linear elastic boundary. One of the key technical issues is to define this boundary and use the time-dependent particle velocities on this boundary as input to a 3-D wave-propagation code. Our initial focus was on defining this boundary and modifying our existing 3-D acoustic-/seismic-wave propagation code to accept the time-dependent source function provided by the nonlinear deformation modeling. We are using the state-of-the-art Sandia code PRESTO for the nonlinear calculations. We calculated the particle displacement

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and velocities histories using PRESTO out to a radial distance of 5 m. We used material properties appropriate for Solenhofen limestone in the elastic regime, combined with the Drucker-Prager failure criteria to determine when plastic failure occurs. We modeled the explosive source using the Jones-Wilkins-Lee (JWL) equation-of-state where the JWL material generates a time-dependent internal pressure. We placed the bomb-cavity radius in a whole space and 10 m below an air-earth interface. In both cases, the plastic zone extended out to a radius of approximately 3.2 m into the rock. At a radius of 5 m from the source, the calculated particle displacement and velocity are well within the elastic regime. We successfully utilized the output from PRESTO at the nonlinear-linear elastic boundary as a time-dependent source function for our existing 3-D seismic-/acoustic-wave propagation code. However, ongoing research into PRESTO indicates that some nonphysical periodic behavior is present in nonlinear explosive modeling that the PRESTO code developers need to address.

Another key issue is the acoustic-seismic coupling at the air-earth interface. Understanding the coupling and being able to model the coupling are critical in the determination of the pressure in a facility following a bomb blast. Depending on the earth material at the air-earth interface, a poroelastic approach may not be necessary as indicated from the comparison to some actual field data. However, we need to understand when the poroelastic approach is necessary. We are investigating possible modifications to the existing acoustic-/seismic-wave propagation code to simulate the poroelastic behavior at the air-earth interface, if necessary, for a better representation of the acoustic-seismic coupling than presently used in the code. It is beyond the scope of this project to develop the full-blown code for poroelasticity. The approach that we are investigating is to take the approach of Rice and Cleary (1976) and let a single Lagrangian variable specify the material behavior at a point, whether it is a porous solid or air. Using the single-variable approach, we applied two different constraints to the fluid flow: (1) the fluid and the solid move in unison, and (2) fluid flow obeys Darcy Law flow where the driving pressure is supplied by the seismic-wave propagation. Accommodation of constraint (1) does not require a modification of the existing seismic-wave propagation code, only a change in the input data. Utilizing constraint (2) introduces attenuation to the propagated seismic wave through a convolution kernel. We are investigating the inclusion of constraint (3) into the framework of an existing code.

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We investigated analytic solutions to guide and validate our numerical algorithm development. Using an analytical model (Aldridge, 2002), we successfully inverted velocity and pressure traces generated by a spherical source in a linear-elastic whole space. The source signature is accurately recovered. This successful inversion of analytically calculated results gives promise to a successful determination of the pressure in the facility using actual field data.

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38655

Free-Space Electrooptic Sampling and Remote Mapping of Electromagnetic Fields from Emitting Structures Using Femtosecond Terahertz Transceivers

S. M. Cameron, T. S. Luk, F. J. Zutavern

New optoelectronic-sensor technologies are required to remotely measure spatial and temporal distributions of free-space pulsed radiation and to probe localized electric-field and space-charge distributions in circuit and emitter structures at range. The ability to measure high-frequency field transients and the associated short-pulse-duration electromagnetic power (EMP) spectrum is a critical diagnostic tool for assessing susceptibility of directed-energy (DE) weapons threats against electromechanical structures, ultrawideband (UWB) (optical/radio frequency [RF]) signature discrimination, and nonresonant (direct current [DC]-terahertz) impulse ranging of EM scattering signatures. Femtosecond terahertz transceivers based on the reciprocal behavior of optical rectification (difference mixing) and the Pockels effect in a nonlinear crystal can be used to alternatively transmit an EM interrogation waveform and to electrooptically sample a perturbed return signal from a targeted component on an optical carrier. By introducing a linearly chirped optical probe pulse for mixing with the microwave field, it is possible to encode (wavelength-division multiplex [WDM]) the temporal modulation onto the baseband optical frequency spectrum and subsequently decode (demultiplex) the waveform signature (frequency, time, space) in a single-shot measurement using spectral dispersion. Interaction kinematics will modify the broadcast pulse, and we can use the resulting analysis to externally probe internal operation of an integrated circuit (IC), spatially map radiated-field patterns, or interrogate carrier dynamics of an illuminated semiconductor interface. Because the EM pulse is rectified from the intensity derivative of the optical pulse, we can use adaptive pulse-shaping techniques to produce arbitrary modulation formats to exploit coupling or enhance signatures with application to communications, tomographic imaging, and remote sensing.

The main goals of the project were to (1) construct a femtosecond terahertz generation and detection apparatus for imaging and remote-sensing applications, and (2) perform experiments to demonstrate electrooptic sampling of electric-field modulations in an emitter structure. We constructed a terahertz transceiver employing optical rectification in gallium

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arsenide (GaAs) for the generation of UWB microwave pulses and electrooptic sampling using the transient bias produced by the Pockels effect in zinc tellurium (ZnTe) for time-gated coherent detection of a photonic mixed signal. We calibrated measurement sensitivity to terahertz signal with an Austin antenna and bolometer. We currently are using this system to understand plasma emission and gas-phase remote sensing. We utilized phase-sensitive detection using polarization and interferometry to remotely measure electric-field oscillations across a calibrated GaAs photoconductive switch. We detected both phase and amplitude contributions to the modulation spectrum in a reflected optical carrier as a function of applied electric field without external frequency synchronization. These preliminary results suggest future remote-sensing strategies that integrate signature attributes in different portions of the EM spectrum.

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38658

Kinematics-Based Video Compression Using a Foveated-Imaging Sensor for Remote Telepresence Applications

J. J. Carlson, D. V. Wick, D. R. Hayward

The use of remote video sensors is severely restricted by bandwidth limitations of non-line-of-sight (LOS) radio-frequency (RF) communications links. This has inhibited applications such as remote video surveillance and remote operation of robot vehicles. To overcome these limitations, Sandia is developing an innovative, foveated-imaging sensor coupled with complementary image-compression algorithms based on kinematics. The sensor and algorithms are specifically optimized for remote telepresence applications. The imaging sensor uses state-of-the-art liquid-crystal spatial-light modulators to correct off-axis aberrations of a very simple, wide-field-of-view (FOV) optical system. Foveated imaging is a key characteristic of the sensor. The sensor naturally mimics the physiology of the human visual system and lends itself to data compression by creating a variable-resolution image over a wide FOV. Maintaining high resolution only in a spatially restricted area in the focal plane, the sensor is expected to provide significant advantages in terms of reducing data-transmission-bandwidth requirements. A key feature is the ability to rapidly alter the position of the high-resolution region of interest. We will use kinematics information and operator input to intelligently select and control this position. Kinematics information can come from motion detection in surveillance applications or vehicle parameters (speed, heading, orientation) in the remote operation of mobile robots. We will also use kinematics information to intelligently sample and compress the video signal. We expect the combination of the proposed sensor and algorithms to dramatically expand the capability of systems that use remote video telepresence.

Research thrusts focused on demonstrating the feasibility of both kinematic-based video-compression concepts and variable-resolution, wide-FOV, foveated imaging. We made several technical strides in our first year. In collaboration with New Mexico State University (NMSU), we developed kinematic-based compression algorithms and met our milestones for compression algorithm development. We demonstrated the feasibility of the foveated-imaging sensor concept in collaboration with the Air Force Research Laboratory (AFRL). Besides research, we also assessed

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customer interest in the proposed technical developments. Following the events of 9/11, we received extremely positive feedback on the application and ever-increasing need for this technology from several customers, including the intelligence, DOE, and DoD communities.

Refereed

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38659

Information Assurance for Wireless Ad Hoc Networks

B. P. Van Leeuwen, M. D. Torgerson, F. J. Oppel, III, H. Y. Chen, E. L. Witzke, D. Kilman

Wireless networks are critical to many national security systems. Commercial industry is focusing their wireless research and development on efficient routing, bandwidth efficiency, and cost-effective implementation with little emphasis on security and information assurance (IA). This research will bridge the gap between commercial efforts and government IA requirements for wireless communication networks. The Department of Energy (DOE) and other federal agencies (OFA) have critical network-centric distributed systems that depend on successful, timely, and secure wireless communications. Currently, no effective solution exists for wireless IA, resulting in severe network vulnerabilities and survivability issues, as demonstrated by the recent vulnerabilities discovered in the 802.11 wireless local-area network (LAN) standard.

This research will leverage wireless ad hoc network-routing methods characterized in previous Sandia research. Subject to the networks' control-plane data requirements, we will select the most appropriate architectures to balance control-plane security with a typical scenario, i.e., distributed autonomous robotic effort, and develop and apply cryptographic and non-cryptographic approaches for system IA. We will use modeling and simulation to determine the effectiveness and scalability of the approach under the influences of wireless channel interference, impairments, and adversarial stressors. This research will build Sandia's modeling and simulation capability by integrating the OPNET (operating network) and UMBRA simulation environments with the high-level architecture (HLA). We will develop higher-fidelity network models to represent wireless networks for national security systems in difficult environments such as urban terrain.

An effective solution for the security and survivability vulnerabilities of wireless ad hoc networks will provide Sandia with an advantage in developing the network security and IA for network-centric systems being considered by DOE and OFA. In addition, the research will build upon our ability to assess and improve the security lifecycle of wireless systems and to predict performance of the developed approaches with an advanced simulation capability.

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The research team selected several scenarios that focus on the autonomous operation of robotic vehicles. We grouped the robotic vehicles to form network-centric systems that depend on timely and assured command and control information exchange among group members. In some scenarios the network-centric system comprises different types of assets and forms a heterogeneous multilayer network. System operation depends heavily on wireless networks, and thus the availability of the network becomes critical. To examine the impacts of selected network IA methods, we created a baseline model of the robotic system in the UMBRA system simulator. Using HLA, we integrated the network-modeling capability of OPNET Modeler with UMBRA to include the effects of the communication protocols. The overall system-simulation capability allows us to examine the system operation with the impacts of the IA methods, wireless network protocols, and wireless channel. The HLA interoperability consisted of developing a preliminary HLA interface using the Run-Time Infrastructure software environment. The interface consists of “interface objects” that allow the interchange of simulation attributes between the UMBRA and OPNET simulators.

In our selected scenario, any node may compromise the network operation by disrupting the network-control data. Thus, nodes must reject any fabricated, compromised, or replayed control data. Our work identified a cryptographic method based on message-authentication codes that supports our objective of secure-control message exchange. For authentication services in the network-centric scenario, we selected an adaptive security approach that combines a centralized security server for its efficiency that can transition to a decentralized approach if the security server is destroyed. We are examining this security framework in our selected scenario to determine its operational performance. An example of this framework uses a network with an unmanned aerial vehicle (UAV) operating as a central security server.

To examine the impacts of selected network IA methods, we created a baseline model of the robotic system in the UMBRA system simulator. Using HLA, we integrated the network-modeling capability of OPNET Modeler with UMBRA to include the effects of the communication protocols. The overall system-simulation capability allows us to examine the system operation with the impacts of the IA methods, wireless network protocols, and wireless channel.

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38661

Low-Toxicity Hypergolic Propellant System Using H₂O₂ Oxidizer

W. R. Escapule, M. S. Krein, M. C. Grubelich, B. M. Melof, B. V. Ingram

Less-toxic, storable, hypergolic propellants are desired to replace nitrogen tetroxide and hydrazine in certain applications. Hydrogen peroxide is a very attractive replacement oxidizer, but finding acceptable replacement fuels is more challenging. Sandia's focus in this investigation is to find fuels that have short ignition delays, high specific impulse, and desirable storage properties. The resulting hypergolic fuel/oxidizer combination would be highly desirable for virtually any high-energy-density applications such as small but powerful gas-generating systems, attitude control motors, or main propulsion. These systems would be implemented on platforms ranging from guided bombs to manned space vehicles.

- We conducted an extensive library search to identify potential fuel candidates and to aid experimental design and testing.
- We developed a simple laboratory test to screen potential rocket fuels. In these "drop" tests, we placed a 0.1 mL portion of candidate fuel into a 5 mL disposable polyethylene beaker. We added approximately 0.4 mL of 90% hydrogen peroxide to the fuel using an automatic pipette. We slipped a 1" length of silicone rubber tubing over the tip of the glass pipette and replaced it after each test to prevent contamination and to allow reuse of the pipette. Visual observation determined if ignition occurred and the relative rate and intensity of reaction.
- We carried out computer calculations using the New Propellant Evaluation Program (NEWPEP) to evaluate potential performance and relative ranking of candidate fuels with hydrogen peroxide. We also used NEWPEP to quantify performance when using hydrogen peroxide at a variety of dilutions, as well as 100% purity. We carried out a total of 2550 separate fuel/oxidizer system calculations for 17 candidate fuels, 5 peroxide concentrations, and 30 fuel/oxidizer ratios.
- We developed prototype thin-film catalyst beds for decomposing hydrogen peroxide for bipropellant engines.
- We designed and built a high-pressure cell to test with potential catalyst solubility and liquid ammonia fuel.
- We conducted a preliminary investigation of a possible hypergolic-hybrid rocket motor.
- We began design and development of a laboratory rocket motor to test final fuel/hydrogen peroxide combinations.

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46687

Exploiting Polarimetric Information in Synthetic-Aperture Radar Images for Automatic Target Recognition

J. A. Richards, W. J. Bow

Synthetic-aperture radar (SAR) is a mature remote-sensing technology with numerous military applications. One important SAR application is the detection and identification of targets of interest. Recognition of targets by a human image analyst is a difficult task, especially with the increasingly high data rates and coverage areas of modern SAR sensors. The development of automatic target recognition (ATR) systems for use with SAR imagery is thus an active research topic. Sandia developed a real-time ATR with operationally significant performance. The Sandia ATR, like most ATRs, operates on single-polarization SAR imagery. There are indications, however, that incorporating additional polarization channels could benefit ATR performance. This research investigates the use of additional SAR polarization channels in ATR and suggests a method for incorporating additional polarization channels into the Sandia ATR framework. This method is tested using dual-polarization SAR imagery. The results of this testing demonstrate a clear and significant benefit to ATR performance.

This research provides a clear indication that multiple-polarization data have significant benefit to SAR ATR. In particular, the incorporation of horizontally transmit and vertically receive (HV)-polarization data into the operational Sandia horizontally transmit and receive (HH)-polarization ATRs identification stage enables improved target detection, improved clutter rejection, improved target identification, and improved robustness to nonsystem targets. The gains achieved in each of these areas are significant and nontrivial. The proposed method for utilizing multiple-polarization data requires very little modification to the existing Sandia HH-polarization ATR and can be accomplished in a computationally efficient manner.

Our research provides a strong indication that multiple-polarization SAR imagery has the potential to provide significant gains in ATR performance over that seen in single-polarization systems. We hope that the next generation of SAR and ATR systems developed at Sandia will exploit this potential. This research represents a first step in developing a fielded SAR ATR system that utilizes multiple-polarization data.

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46688

Moving-Target Identification Using Ultrahigh-Range Resolution Data

J. S. Salazar, D. W. Harmony

The use of high-range resolution (HRR) radar for automatic target recognition (ATR) is an emerging field and is one of a few technologies being considered to assist in tracking and identifying moving targets. The importance of this technology was emphasized by recent military conflicts where it showed that battlefield vehicles are typically moving and that stationary battlefield vehicles are very rarely in the open.

Sandia carried out significant research on two-dimensional (2-D) ATR approaches for sensor technologies such as electrooptical (EO) and synthetic-aperture radar (SAR). However, these approaches have significant limitations with regard to moving targets. For example, EO ATR systems are effective only in daylight, and they are severely impacted by adverse weather conditions including clouds. Also, the EO sensor resolution degrades with increased altitude (range from the target). Although radar can be used day or night and is not affected by range or weather, SAR imaging is ineffective against moving vehicles. This gap in conventional approaches opens the way for ATR using HRR target signature data.

HRR target signatures (profiles) can be formed when a vehicle is moving and in a fraction of the time needed to produce a SAR image. However, HRR profiles pose new and formidable challenges for use in target identification. For example, HRR profiles constitute 1-D target signature information and provide a fraction of the information provided by SAR imagery at the same resolution. The limited informational content represented in HRR profiles combined with the relative instability of the target signature information further complicates the inherent difficulties in ATR.

This research investigates the utility of HRR data for template-based ATR. It also investigates the use of ultrahigh-range-resolution (UHRR) profiles derived by simulated means. This research has as its primary goal to develop metrics for the extraction of stable features from HRR and UHRR data that can be exploited in 1-D ATR algorithms.

This research provides some extremely valuable insights into the potential for HRR radar ATR. The results derived from this research show that features useful for ATR can be extracted from HRR data and also extend well to simulated UHRR data. As shown with low-resolution HRR data (both actual and

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simulated), the extracted features suggest that targets should be identifiable and distinguishable from each other. It is clear that multiple “looks” (i.e., multiple HRR profiles) collected along a moving target’s path will be necessary to establish a target identification hypothesis. However, the strength of these features improves as the resolution of the data improves, as in the case of UHRR data. Thus, if UHRR data are attainable, fewer “looks” along a moving target’s path may be necessary to identify it at these resolutions, as indicated by simulated data.

It should be noted that we found real and simulated HRR and simulated UHRR target signatures to be relatively less stable than SAR target signatures. However, and more importantly, we found that HRR/UHRR template ranges could be commensurate with SAR template-based ATR systems. Template ranges for template-based SAR ATR are larger than what might be expected to be useful for HRR data because HRR target signatures tend to change more rapidly, compared to SAR images, given the same change in viewing aspect and depression. This characteristic is important since fewer templates than expected should be necessary to characterize target variations due to aspect and depression. However, increasing the number of templates by restricting the range and interval remains a possible avenue for further template fine-tuning.

We made the following specific accomplishments:

(1) Adapted and implemented two distinct 2-D template-based metrics proven in SAR ATR applications for use as 1-D HRR ATR algorithms. These include the Multinomial Pattern Matching (MPM) and Mean Squared Error (MSE) match metrics. The goodness-of-fit (GOF) measures, resulting from the application of the MPM and MSE metrics, constitute the features that can be used in a follow-on fusion approach. The significant software/algorithmic functions required by these implementations include:

- (a) HRR profile alignment
- (b) HRR training (template generation)
- (c) HRR testing

(2) As a baseline and as an initial source of data, acquired and formed HRR profiles collected with Veridian Corporation’s Data Collection System (DCS).

(3) Applied the alignment, training, and testing algorithms to DCS data.

(4) Generated performance characteristics on DCS data.

(5) As a precursor and in possible absence of actual UHRR data, simulated UHRR and HRR data from very high resolution Ka-band SAR data.

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(6) Applied the alignment, training, and testing algorithms to the simulated UHRR and HRR data.

(7) Generated performance characteristics for simulated UHRR and HRR data.

(8) Compared and quantified performance between simulated UHRR and HRR data.

(9) Compared and quantified performance between simulated UHRR and HRR data and DCS HRR data.

The successes of these results represent new and important steps in HHR ATR research. Although the results of this research are necessary, they are not sufficient for a complete HRR ATR solution. This preliminary work establishes a firm foundation for further advances that need to occur in this area to solve the moving-target ATR problem using HRR data.

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49771

155-mm Munitions Reutilization Study

J. M. Macha, D. E. Salguero, R. D. Tucker, T. M. Jordan-Culler, T. H. Summers

In this project, Sandia seeks to make an initial assessment of the technical and economic feasibility of adapting the existing abundant supply of 155-mm munitions to alternative delivery concepts that overcome these limitations. Baseline requirements for the conceptualized systems are (1) the employment of existing 155-mm unitary and submunitions rounds, (2) target points within the range of 5 to 20 km, and (3) accuracy at least equal to current systems. Additionally, the concepts will strive to incorporate one or more desirable features: deployable in inaccessible/denied areas, amenable to predeployment ahead of the maneuver force and remote/semiautonomous operation, and changes minimized to existing fuzes.

This work draws broadly on Sandia's expertise in rocket systems, navigation, guidance and control, weapons fuzing, and systems engineering/integration. The potential payoffs ultimately derived from this initial study are a low-cost, timely, enhanced capability of maneuver forces and the reutilization of the large supply of 155-mm munitions that are likely destined for costly disposal.

The concept deemed most promising is an adaptation of the standard 155-mm projectile as a rocket-boosted guided weapon. The nominally 30 in.-long unitary or submunition-dispensing round is made controllable in flight by the addition of a tail extension with four cruciform fins operated by electromechanical actuators. Navigation and guidance functions are performed by an electronics package consisting of a microprocessor, tactical-grade inertial measurement unit (IMU), and global positioning system (GPS) receiver. Fuzing options are similar to those for current gun-fired projectiles—point detonation, variable time, or proximity. Actual fuze design would be modified since the safe/arm functions are currently initiated by the high-acceleration and high-spin rate attendant to a gun-fired round. Maximum acceleration of the rocket-boosted projectile is approximately 50 G compared to ~ 10,000 G for a gun-fired round. The lower acceleration translates into a lower-cost, more-reliable electronics package than would be required for proposed gun-fired projectiles (e.g., the Army's XM982 Excalibur projectile or the Navy's Mk171 extended-range guided munitions). Preliminary analysis indicates that the GPS-aided IMU navigation system would

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meet the accuracy goal for circular error probability (CEP) independent of range. Prior to launch, the GPS coordinates of the launch and target locations are uploaded to the projectile's microprocessor. During flight, the GPS receiver provides position updates to the IMU to correct for bias and drift errors. The projectile with its control-section extension is boosted by a short-burning solid-rocket motor. Launch is from a near-vertical orientation, and the burn-time is less than 2 s. At burnout, the motor is separated from the projectile/control section to decrease drag and minimize booster size. A minimum impulse of about 15,000 lb-s will achieve the 20 km range. Maximum velocity at motor burnout is about 2,000 ft/s. The control section is activated after separation and guides the projectile to the designated target point. Trajectory apogees are about 6–8 km for the minimum impulse motor, and time-of-flight to 20 km is about 90 s. Preliminary aerodynamic simulations indicate reasonable size for the control fins (planar area of $\sim 20 \text{ in.}^2$ each) and reasonable fin deflection and projectile angle of attack (< 15 degrees and < 12 degrees, respectively.) Maximum fin hinge moment is $< 15 \text{ ft-lb}$.

The navigation, guidance, and control requirements are met with proven, available electronic components. These components include a Sandia-designed microprocessor flight computer, commercial IMU and GPS receiver, a Sandia-designed conformal GPS antenna, and commercial rotary DC motors. The preliminary estimate of power consumption is on the order of 50 W-hr, which can be provided by thermal batteries. All of these components are accommodated in the cylindrical control section with a 155-mm diameter and length of 18 in. or less. With current solid-fuel rocket technology, the required 15,000 lb-s impulse can be provided by a 155-mm diameter, 45–60 in.-long motor. The overall system would be 90–105 in. tall in the launch configuration. The length can be reduced by increasing the diameter of the motor, with little penalty from increased drag since the motor is separated at fewer than 2 s into the flight.

We envision several of the rockets (perhaps 12 to 20) packaged in an integrated storage/transportation/launch container that is easily transportable by cargo aircraft, helicopter, or land vehicle. The container would be emplaced on the ground or made mobile by installation on a wheeled or tracked vehicle. Additional electronic components would be installed on the container, including (1) a general-purpose computer to make missile and fuzing selections and transfer container location, target location, GPS ephemeris, meteorology data, etc., to the projectile's computer, (2) a GPS

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receiver for autolocation of the container, (3) a precision IMU to shorten time required for autoalignment of the projectile IMU, (4) firesets for igniting the thermal battery and rocket motor, and (5) communications equipment to link the container with FA command and control.

49915

Critical Technology Development for Hard Target Defeat High-G Tolerant Fuze and High Explosives

C. L. Smithpeter, T. C. Togami, S. M. Harris, F. H. Anderson, R. S. McEntire

It is widely recognized that many of our nation's adversaries are using hardened underground facilities to safeguard essential operations such as command and control, weapons production, and personnel sanctuary. The recently completed Department of Energy (DOE)/Department of Defense (DoD) Science and Technology Plan for Hard Target Defeat included the following technology needs on the list of critical items required to hold more of these hard targets at risk: (1) intelligent high-gravity (high-G) fuzing, and (2) high-G tolerant energetic materials.

Not only do these technologies have direct application to needs in the conventional weapons community, but they are also important technology areas for future DOE weapons. The urgency and importance of progress in this area were made even more apparent by recent events in Afghanistan.

Sandia will conduct a series of concurrent design, fabrication, and testing of fuzing technologies guided by modeling and simulation in high-G environments. We will focus on the maximum collection of relevant data and support advanced development of high-G survivable technologies.

We focused on four areas: the preliminary design of the SIPE-2 (Sandia Intelligent Penetrator) fuze, the evaluation of high-voltage components for performance and survivability, an interaction with the DoD safety board to understand the safety requirements constraints on design, and the integration of the fuze, explosive train, and penetrator.

The preliminary design of the SIPE-2 fuze is complete. We selected the main microcontroller and are learning to understand the associated code for the controller, communications protocol with weapon systems, and the use of diagnostic code for fuze performance analysis at various stages of fabrication and test. Software is estimated at 20% complete.

Several high-voltage components are under evaluation for performance and survivability during high-G shocks applied by drop tables. We are addressing several issues: capacitor voltage variations induced by piezoelectric effects created by impact shocks of the system, rapid voltage variation sensitivity of our high-voltage switches, electrical noise generated by test cables,

It is widely recognized that many of our nation's adversaries are using hardened underground facilities to safeguard essential operations such as command and control, weapons production, and personnel sanctuary. ... Sandia will conduct a series of concurrent design, fabrication, and testing of fuzing technologies guided by modeling and simulation in high-G environments. We will focus on the maximum collection of relevant data and support advanced development of high-G survivable technologies.

and optimization of packaging of components in fuze architectures for high-G survivability. We completed a series of tests; follow-on evaluations are under way with significant progress being made. We made improvements in minimizing electrical noise and component survivability.

The team recently completed its first safety review. Preliminary feedback indicates that our design concept is acceptable with modifications. We incorporated the requested modifications and plan follow-on discussions with two fuze board members.

We developed conceptual layouts for fuze, explosive train, and penetrator integration. We completed detailed circuit schematics for the first variation of SIPE-2 and a preliminary mechanical layout of the fuze.

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50001

Unmanned and Unattended Response Capability for Homeland Defense

P. C. Bennett, T. S. Gladwell, R. J. Anderson

Sandia will conduct an analysis of the potential for unmanned and unattended robotic technologies for forward-based, immediate-response capabilities that enable such access and control. We will research and define high-impact response scenarios in conjunction with homeland security organizations, such as the National Nuclear Security Administration (NNSA) Office of Emergency Response (OER), the Federal Bureau of Investigation (FBI), the National Guard, and the Army Technical Escort Unit, to cover a range of radiological, chemical, and biological threats.

We analyzed the potential for unmanned and unattended robotic technologies for forward-based, immediate response capabilities that enable such access and control. We investigated the evolving needs of homeland security organizations, such as the NNSA OER, the FBI, the National Guard, and the Army Technical Escort Unit, to cover a range of radiological, chemical, and biological threats. We then developed a conceptual high-impact solution to issues common between the organizations. This solution included pre-positioning robotic and remote-sensing capabilities stationed close enough to multiple potential domestic target sites to enable immediate, ground-deployed action.

We established the following requirements:

- Response assets should be based on current threat and located to respond rapidly to major population centers.
- Search and identification must be pushed forward to the maximum extent possible.
- Search needs to be conducted and/or coordinated by the Radiological Assistance Program (RAP)/National Guard Civil Support Team(s) (CST)/local responders, depending on the type of threat and team proximity.
- An explosive ordnance disposal (EOD) reach-back for weapons of mass destruction (WMD) needs to be developed for police bomb squads, CST, FBI, and other federal assets.

To meet the needs identified in this analysis, we can use forward-based, remote, unmanned robotic technologies. One concept for consideration is to enable the existing fleet of EOD robots currently deployed around the U.S. to execute more advanced operations more easily and quickly than currently possible. Armed with new tools and sensors, predeployed

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robots in the population centers of the U.S. would be able to quickly remotely access buildings and vehicles, find the target object, and stabilize the situation or render the device safe. They would be used for routine civilian law enforcement and hazardous materials (HAZMAT) situations and have the ability to be “federalized” with additional sensors and communications.

Communications will have to be enhanced to provide visual and sensory data uplinked to federal support assets. We conducted an experiment of this nature to show how an EOD robot can send data from the scene through satellite communications to other locations, where subject-matter experts (SMEs) can analyze the data in real time and provide recommendations directly to the technicians onsite. This experiment indicated the need to research maximizing the effect of data transmitted on narrow bandwidths, the need to coordinate the feedback from multiple analysts, and the possibility of the SME to temporarily “take over” the field asset, either for analytical purposes or to recover from dangerous situations.

Approximately 200 EOD remote-controlled vehicles (RCV) are currently deployed in civilian law enforcement agencies in population centers, with another 200 in military hands in U.S. and abroad. Further, Sandia demonstrated through this and other activities that the control systems of 80% of these vehicles can be upgraded with commercial off-the-shelf equipment and specialty software to provide simultaneous improvement in sensing, mobility, manipulation, and ease of use.

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50066

Application of Nonlethal Weapons to Counterterrorism

G. M. Loubriel, L. E. Larsen, S. M. Cameron, B. N. Turman, K. T. Stalker

This project studied how nonlethal weapons and concepts can be applied in the War on Terrorism (WoT). Sandia generated and evaluated several ideas to determine which of them are more likely to impact the WoT and to determine development time. The areas that we investigated include the following:

- (1) Optically enabled radio-frequency (RF) tags,*
- (2) Acoustic disruption of postural reflexes for temporary incapacitation,*
- (3) Stealth deployment of sensor nets,*
- (4) Brain disruption with various deleterious effects,*
- (5) Robotic high-power microwaves (HPM) delivery,*
- (6) Secure chaotic communications,*
- (7) Three-dimensional baggage inspection with backscattered x-ray and T-rays using automatic target recognition (ATR) techniques,*
- (8) Remote sensing,*
- (9) Detonation of explosives,*
- (10) Vehicle stopper at extended ranges, and*
- (11) The use of high frequencies for crowd control and other applications.*

The conclusion was that items 2 and 11 are worthy of further investigation.

Our main accomplishment was the evolution of ideas on the use of acoustics and high-frequency microwaves to affect the WoT. These ideas will apply in different areas: (1) for peacekeeping (crowd control, to identify and isolate troublemakers in crowds and to reduce martyr creation), (2) in self-defense and hostage situations (to create keep-out zones around high-value assets, for hostage rescue, to stop a hijacked vehicle), and (3) warfighting (when there are noncombatants in military operations in urban terrain [MOUT], for prisoner taking, to create confusion, to allow covert/deniable operations).

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51536

Concept Definition for an Integrated Biodefense System

T. H. West

When designing a system of dedicated environmental detectors, it is critical to first understand the tradeoffs between the sensitivity and deployment density of the detectors to be used. These parameters will play a significant role in determining the cost and complexity of the detection architecture as well as its ability to recognize a given attack. In this project, Sandia explored how this density depends on a range of factors, including the type and sensitivity of the detectors and meteorological and release conditions. We also derived an order-of-magnitude estimate of the detector density required for high-confidence detection of attacks resulting in a range of casualty levels.

To address the above issues, we used the Hazard Prediction and Assessment Capability (HPAC) modeling program. We modeled both point and line releases of anthrax and plague bacteria for a range of atmospheric conditions (wind speed 2–15 m/s, Pasquill-Gifford-Turner stability class B to G). To make our analysis broadly applicable, we did not incorporate terrain or building-scale data. This generic approach, together with a range of other uncertainties, means that the results presented in this report should be considered “ballpark” estimates of actual outcomes. Future analysis will focus on a defined region of a specific city and will incorporate the appropriate building-scale, terrain, and other local effects.

- For similar numbers of initial infections, anthrax point releases are more difficult to detect than anthrax line or plague releases. Thus, a system that is designed to detect anthrax point releases should be sufficient to detect the other release types.

- The density of detectors required to detect an attack resulting in a fixed number of infections is relatively insensitive to meteorological conditions.

- Current and near-term concentration-based detectors do not appear suitable for broad-area environmental monitoring as 100,000s would be required (for typical cities) to provide high-confidence detection of attacks resulting in 10,000 initial infections.

- Even concentration-based detectors with sensitivities as low as one agent-carrying particle per liter of air (ACPLA)—the “holy grail” for such devices—would have to be deployed at densities of several per kilometer squared (i.e., several thousand to cover a typical city) to detect 10,000 infection attacks.

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- Current and near-term collection-based devices appear much more suitable, with $\sim 1,000$ to 10^6 required to provide high-confidence detection of attacks resulting in $10,000$ initial infections.

51708

A Maneuvering, Hypersonic Pathfinder/Test-Bed

J. M. Macha, D. W. Kuntz, M. A. McWherter-Payne, W. H. Rutledge, K. T. Stalker, T. S. Prevender, J. D. Bradley, S. K. Showalter, A. C. Watts, M. R. Ackermann, D. J. Rigali

This is a classified project.

52395

Feasibility of Using Pulsed Intense Ion Beams to Improve Wear Behavior of Metals and Plastics

T. J. Renk, C. M. Wehlburg, R. P. Goehner, D. F. Susan, R. L. Clough

Pulsed intense ion beams have been shown to improve the wear durability of metal surfaces. Cyclic heating and cooling from such beams (at $1e9$ K/s rates) promote grain refinement, dispersal of second-phase particles, and formation of metastable phases, all of which can lead to wear improvements. In some applications, such as in hip or knee implants, where counterfaces exist between metals and polymers, it is desired to reduce wear of both the polymer and metal surfaces, either by hardening the surfaces, reducing the friction between the counterface surfaces, or both. Previous experiments with ion beams also demonstrated improved wear performance of polymer surfaces, mainly by promoting cross-linking of the polymer.

Sandia formed a working group to study the technical issues connected with improvements to metal/polymer contact surfaces. The group consists of Sandia, Anderson Orthopedic Research Institute, a leading medical practitioner group, and DePuy, a leading hardware manufacturer. The materials of interest include both metal (Ti [titanium] and Co-Cr-Mo [cobalt-chromium-molybdenum] alloy) and ultrahigh-molecular-weight polyethylene (UHMWPE). The objectives include improvement of the abrasion resistance of UHMWPE, the demonstration of analytical methodologies for monitoring degradation of the UHMWPE, and reduction of friction wear of the contact surface between UHMWPE and the metals listed. The analysis could be applied to the study of aging and wear behavior of a wide variety of different polymers (and metal surfaces) currently being used in the nuclear stockpile.

Pulsed intense ion beams improve the wear durability of metal surfaces, and cyclic heating and cooling from such beams (at $1e9$ K/s rates) promote grain refinement, dispersal of second-phase particles, and formation of metastable phases, all of which can lead to wear improvements. In some applications, such as in hip or knee implants, where counterfaces exist between metals and polymers, we desire to reduce wear of both the polymer and metal surfaces by either hardening the surfaces, reducing the friction between the counterface surfaces, or both. Previous experiments with ion beams also demonstrated improved wear performance of polymer surfaces, mainly by promoting cross-linking of the polymer. This work

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led to the following conclusions. Pulsed ion-beam treatments can modify the surface properties of either or both the polyethylene, and the Co-Cr-Mo and Ti metals. We investigated the feasibility and potential application interests in this technique. The next step in the work is to evaluate improvements in wear durability by hardening the plastic, or reducing the friction between the plastic and metal, or both. We established materials and components for such tests.

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Mo and Ti metals.*

Energy and Critical Infrastructures

The Energy and Critical Infrastructures investment area seeks to enhance the surety (safety, security, and reliability) of our nation's energy and other critical infrastructures and to provide security against malevolent attacks. Surety is defined as confidence that a system will perform in acceptable ways in both intended and unintended circumstances. The Energy and Critical Infrastructures area invests in research with the potential to impact national security applications through the development of clean and efficient energy sources, unique and effective nuclear technology, infrastructure security, and water safety and sustainability.

The focus of “A Micro-GC–Based Controller for Energy-Intensive Processes” is to develop a viable solution for science-based, real-time control of chemical and petroleum processes to increase efficiency and to decrease energy consumption. Intelligent sensors are not widely used to control processes in the chemical and petroleum industry. A reluctance to implement new energy-saving technologies can be attributed to a lack of proven sensors that can adapt to a variety

of complex processes. Advancements made in this project will impact other μ ChemLab™ projects and have applications to further sources of funding in the national security and industrial processing arenas. Two patent applications have been filed.

10718

A Novel Microcombustor for Sensor and Thermal-Energy Management Applications in Microsystems

R. P. Manginell, R. J. Kottenstette, S. B. Margolis, D. L. Mowery-Evans, C. W. Colburn, M. W. Moorman, L. F. Anderson, P. G. Clem, T. J. Gardner

The development of a small and stable on-chip flame/combustor (μ Combustor) would permit the adaptation and translation of several very useful macroscopic devices into the microsystem domain: on-chip flame ionization detectors (μ FIDs), microreactors, micropropulsion, energy conversion, and, importantly, heating and thermal management. The argument for the use of on-chip combustive heating is compelling. The energy density of butane, including storage cylinder mass, is 50 times that of the best high-output batteries (LiMnO_2 non-rechargeable). Thus, a tiny fuel tank could replace several bulky batteries in hand-held microanalytical systems like the μ ChemLabTM and would supply a μ Combustor for efficient heating of essential components.

Sandia plans to develop a μ Combustor as a basis for thermal-energy management in microsystems as well as in the development of new μ FID devices for use in intelligent process control of energy-intensive processes (e.g., reactors, distillation columns, and dryers in the petrochemical industry). Stable flames are difficult to achieve on a small scale due to enhanced heat loss arising from large surface-to-volume ratios. Catalytic materials provide a natural surface-based method for flame ignition and/or stabilization of the reaction zone. Further stabilization can be achieved by the use of a thermally isolating membrane as a support for microfabricated fuel injectors. One key enabling technology for the μ Combustor will be the development of active and stable (deactivation-resistant) catalyst materials (likely supported precious-metal catalysts) for the combustion of different feedstocks, ranging from hydrocarbons (HCs) (e.g., butane or propane) to hydrogen (H). Deposition of these catalysts in a high-surface-area form on relevant platforms (i.e., resistively heated filaments) to facilitate rapid combustion may also be required for device fabrication.

Critical advances in supported catalysts, as well as improvements in fixturing, data acquisition, and data analysis, allowed us to satisfy almost all of our project goals. We previously used thin-film platinum (Pt) or drop-coated commercially available catalysts to initiate and sustain

Combustion of CH_4 on platinum on the microcombustor.

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combustion on the μ Combustor. At combustion temperatures, the thin-film catalyst routinely failed due to delamination, hotspots, and metal agglomeration induced by metal migration. The commercially available catalysts were difficult to obtain, and methods for controlling their deposition were lacking. We took two steps to address these problems. First, we prepared alumina-supported automotive catalysts. Thus far, we have tested 1 wt.% Pt and palladium (Pd). We then prepared these materials for micropenning. Humectants minimized cracking of the thin catalysts. Importantly, these techniques permitted precise depositions of catalysts on the μ Combustor; control of the catalyst boundaries is $\sim 25\text{--}50\text{ }\mu\text{m}$, and catalyst thickness can be applied in $10\text{ }\mu\text{m}$ steps down to $20\text{ }\mu\text{m}$ total thickness.

We abandoned the polyetheretherketone (PEEK) fixture described in previous reports because of volume restrictions and temperature incompatibility. We designed and built another fixture with slightly larger volume and made from Al. This fixture allowed for visual inspection, thermocouple inputs, and the ability to control the inlet height and internal volume, and it had exit ports adequate for water vapor egress.

The new fixture, improved catalysts, and new automated data-acquisition and -analysis systems permitted an experimental combustion matrix. We heated the μ Combustor to initiate and sustain combustion using an in-house constant-temperature circuit implemented this year on a circuitboard. We evaluated the combustion of H₂, methane, ethane, propane, and natural gas (NG) in air with flowrates from 5–40 ml/min and concentrations from 2.5%–40%. For all gases studied, we extended limits of flammability (LOFs) via MicroPenned catalysts relative to conventional flames. For example, we obtained an unoptimized NG LOF of 1%–32%, whereas conventionally we observed 4%–16%. Although originally we planned to use butane for μ Combustor heating, we used only the abovementioned fuels. Nonetheless, we observed unoptimized heating of 38 mW/mm^2 for NG, a fuel source as common as butane, though not as energy-intensive. This work shows the viability of using common fuels in μ Combustor heating of microsystems.

To independently verify catalyst performance and understand catalyst activation and deactivation, we used a conventional u-tube reactor. This year, we performed tests on MicroPenned Pt/alumina to study light-off and methane conversion and demonstrated behavior similar to bulk catalysts.

We undertook modeling and simulation of the μ Combustor to understand ignition and extinction behavior and failure modes. Fundamental studies of ignition and extinction

We designed and built another fixture with slightly larger volume and made from Al. This fixture allowed for visual inspection, thermocouple inputs, and the ability to control the inlet height and internal volume, and it had exit ports adequate for water vapor egress.

explained catalytic extension of LOF despite enhanced microdomain heat losses; these studies also showed the possibility of multiple operating points. Simulation in AURORA, a continuously stirred reaction model, predicted average temperature increases and helped explain premature failure of the μ Combustor under certain operating conditions.

Finally, we demonstrated FID on the microscale. We used original dual in-line packaging (DIP) to take advantage of previously machined flow lids with integrated electrodes. Because this demonstration took place prior to micropenning, we used commercially available catalysts. Essential to this demonstration was the development of an electrometer capable of detecting the expected picoammeter signal. We modeled, breadboarded, and tested this circuit and implemented a circuitboard version. We found that 100 pA gave 2 V output; 10 pA steps were discernible, and we observed a noise floor of about 1–2 pA. To demonstrate the FID, we established 20 V between the electrode in the lid and a counter electrode on the microcombustor. We established an oxyhydrogen flame and introduced propane; the gases reaching the μ Combustor were premixed, atypical for FID, but easy to achieve with our existing apparatus. Nonetheless, flame ionization did occur, and concentrations of 1%–4% of propane were easily detected. This is the first-ever demonstration of FID on the microscale using catalytically stabilized combustion using premixed fuel/air/analyte.

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Refereed

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10725

A Micro-GC–Based Controller for Energy-Intensive Processes

W. Einfeld, D. A. Loy, R. J. Kottenstette, R. P. Manginell, G. R. Dulleck, Jr., F. Gelbard, D. Cruz, S. K. Showalter

Intelligent sensors are not widely used to control drying and distillation processes in U.S. chemical and petroleum sectors. A reluctance to implement new energy-saving technologies can be attributed to a lack of proven sensors that can adapt to a variety of complex processes and detect a wide variety of compounds within a single process. Currently, pilot-scale processes are empirically scaled to full-scale processes with safety factors added to meet quality-control standards. Quantitative analytical testing is time-consuming and not currently possible in real time. Drying and distillation in the U.S. chemical and petroleum sectors consume about 12 Quads of energy annually. A need exists for intelligent, real-time control based on robust, configurable sensors with a wide dynamic range to implement a science-based solution that can improve the process efficiency and decrease energy consumption. Research and development are required to meet this goal.

Sandia's focus in this effort is to develop a viable industry solution for science-based, real-time control of chemical and petroleum processes to increase process efficiency and decrease energy consumption. Sensor development, on-line calibration, data fusion, and system-integration architectures require research and development. Current research efforts on the μ ChemLab™ sensors will provide the fundamental platform for the microsensor-based system. Key sensor research elements will focus on identifying new absorbing materials and methods for coating the microgas-chromatograph (micro-GC) column, on-line delivery of reference samples, investigating and implementing new front ends (such as valve matrices), identifying and implementing carrier-gas options and detectors, and developing a quantitative rather than qualitative output.

We will integrate these elements into a workable prototype that can be used for intelligent real-time process control. We will use existing industry ties to ensure the viability of the directions taken during this project.

- *Thermal conductivity detector (TCD).* Following our success with the feasibility test of a TCD using our current personal computer (PC), we initiated a plan to develop an engineered TCD detector. We generated designs based on microelectromechanical (MEM) fabrication methods, modeled

Light hydrocarbon analysis is performed on μ packed GC columns.

Sandia's focus in this effort is to develop a viable industry solution for science-based, real-time control of chemical and petroleum processes to increase process efficiency and decrease energy consumption.

them for thermal sensitivity, then fabricated and tested them. Three design morphologies resulted in the fabrication of 19 unique devices involving a filament suspended on a 1 μm -thick silicon nitride (SiN) membrane over an etched well in Si. We based the fabricated devices on modeling results and attempts to quantify the models. The morphologies were parallel (assumed laminar flow directed over the surface of a filament), perpendicular (impact flow on the membrane to facilitate mixing), and dual (same flow as perpendicular system, but with two filaments on the same membrane). The size of the membrane and channels through it resulted in the large number of devices. These measurements varied from 100 μm to 500 μm . We tested a sampling of the devices based on a design of experiments (DOE) model. We tested the devices using various gases in a helium (He) carrier gas stream. The results indicate that the perpendicular flow devices are the most sensitive.

- *Preconcentration.* Since the TCD is not as sensitive as our current surface acoustic-wave (SAW) detector, we recognized early on that the typical PC would not have sufficient capacity to capture the analytes of interest. Calculations indicate that a collection of volatile organic compounds (VOCs) on a suitable adsorbent support could be achieved with multiple PCs being pulsed by an electronic firing control. The material can be thermally driven off of the surface of the PC into the next PC, where another aliquot of material is added until the carrier gas is saturated. Timing and analyte band broadening concerns narrowed the focus to a linear array of three PCs. Initial tests showed this method to be feasible, but at some loss of sharply defined chromatography peaks.

- *Interconnections.* Previous methods of interconnection involved the use of polyetheretherketone (PEEK) plastic and glass capillary tubing epoxied into various unique fittings and parts needing to be physically broken apart to remove or replace components. We discovered newly developed Nano-Port connectors as a viable option for pressurized leak-tight connections. UpChurch Scientific produces these state-of-the-art fittings from the plastic PEEK. These are swage-type fittings that create screw-in leak-tight seals on tubing and can be very easily modified to fit our parts. Modifications required included boring out the nuts and receivers to properly swage onto our flexible polytetrafluoroethylene (PTFE) tubing, as well as milling down surface-mounted input/output ports to fit on the MEMS devices. Fixtures were also manufactured from PEEK to hold the valves, PCs, and TCD detector while allowing the use of these fittings. This resulted in less time spent ensuring

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that the system was leak proof, as well as the ability to quickly switch components in and out as needed for testing.

- *Calibration.* We incorporated work from previous years into the system in the form of a calibration source. The source is composed of a toluene diffusion source, a PC (and associated fixtures) to inject the material into the analysis stream, and a valve to control connection with the fluidic system.

- *Packable columns.* We developed packable microfabricated GC columns for this project as well as a number of other needs within our programs. They offer the ability to use supports either that are not available as a liquid coating or that can not be easily modified to adhere to a Si/SiOH interior wall. Unfortunately, the small size of the columns limits the use of commercial off-the-shelf packings; therefore, we synthesized carbonaceous beads circa 100–150 μm in diameter to act as supports. Expectations were that large-surface-area carbon beads could be produced with high porosity and the ability to separate and retain volatile organics. The beads produced were of low surface area. This proved to be advantageous in using them as a support for other commercial liquid coatings.

...we synthesized carbonaceous beads circa 100–150 μm in diameter to act as supports. Expectations were that large-surface-area carbon beads could be produced with high porosity and the ability to separate and retain volatile organics. The beads produced were of low surface area. This proved to be advantageous in using them as a support for other commercial liquid coatings.

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10748

Nanostructured Silicon Surfaces for Cost-Effective Photovoltaic Efficiency Improvements

D. S. Ruby, S. Zaidi, S. A. Kemme, R. J. Buss

Sandia's goal in this work is to evaluate a new regime of plasma surface texturing by using silicon (Si) solar cells as an experimental vehicle. We will develop plasma models to explain, predict, and guide the plasma texturization process. These models will then be useful in future applications whenever surface texture evolution needs to be better understood and utilized. We will also develop optical modeling to optimize the surface texture required for maximum performance. The optical models developed here should be extremely useful in many of the nanoscale optoelectronic applications currently under development. Additionally, the development of textured surfaces on low-cost multicrystalline silicon (mc-Si) solar cells could significantly advance the photovoltaic (PV) industry and potentially enable new thin-film crystalline-silicon (c-Si) approaches that may produce high-power, lightweight, mobile power supplies.

This interdisciplinary project utilizes Sandia's expertise in PV, plasma processing, sensor-based controls, and process modeling to develop environmentally benign processes that can reduce costs and improve product performance. We will use large-area (130 cm²) commercial mc-Si solar cells as the test vehicle in this project so that improvements in performance can be immediately adopted into mass production. Successful completion of this project will also provide validated process models that can be used in a variety of applications for surface texturing, such as to promote adhesion for neutron generator assembly and to optimize new optoelectronic devices.

- *Optical modeling task.* The goal of this task was to develop numerical modeling procedures that would allow us to determine the precise height, width, spacing, and shape of the textured features to produce the optimum solar-cell performance. We would accomplish this by minimizing incident light reflectance and maximizing diffracted light absorption within the bulk of the solar-cell material. This morphological information was then to be used in conjunction with the texture evolution model to obtain the plasma chamber parameters needed to reproducibly obtain textured surfaces with the desired properties.

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We performed numerical modeling of surface-relief, single-spatial frequency Si gratings using rigorous coupled-wave analysis to determine if experimental measurements of one-dimensional (1-D) gratings on Si can be verified. We measured reflected light using a hemispherical reflectance system with well-known incident-light polarization. However, nonuniformities in plasma-texturing resulted in variations of the spacing and depth of the gratings across the surface of the wafer, resulting in measured data obtained from an average of grating depths and spacings. Because one set of grating parameters did not match the experimental data, we developed an averaging method.

From scanning electron microscopy (SEM) photographs, we estimated the grating depth and pitch. We used these estimates as midpoints for a range of values for modeling parameters. We chose a range for the depth and duty cycle such that the feature shapes of the averaged calculated reflectivity closely resembled those of the measured data. In all cases, we obtained good agreement between the experimental and calculated curves.

Calculated reflectivities of 1-D gratings with a single pitch and depth result in reflectivity values that resemble those measured, but with finer features. Small variations in these dimensions change, sometimes significantly, the placement and amplitude of these fine features. Moreover, the fabrication process cannot reproduce a single pitch or depth; consequently, the measured grating response is an integrated result over several pitches and depths. Therefore, while we can confirm measured grating responses by averaging a set of calculated grating responses, this method would not be an appropriate predictor of reflectance until the fabrication process results in a more uniform grating.

- *Solar-cell fabrication task.* The quality of low-cost mc-Si has increased to the point that its cell performance is close to that of single-crystal (c-Si) cells, with the major difference resulting from the inability to texture mc-Si affordably. We expect a low-cost, large-area, random, maskless texturing scheme independent of crystal orientation to significantly impact the cost and performance of mc-Si PV technology.

Tricrystalline Si wafers could produce cells with 5% higher yields than mono-Si due to their increased strength, but their use would require a replacement of the low-cost anisotropic wet texturing that works well only on single-crystalline Si. The use of stronger wafers with improved light-trapping properties could allow thinner cells to be fabricated, thereby increasing the

From scanning electron microscopy (SEM) photographs, we estimated the grating depth and pitch. We used these estimates as midpoints for a range of values for modeling parameters. We chose a range for the depth and duty cycle such that the feature shapes of the averaged calculated reflectivity closely resembled those of the measured data. In all cases, we obtained good agreement between the experimental and calculated curves.

number of wafers produced per ingot by 60% and markedly reducing cell costs.

Previous work showed that up to a 7% relative improvement in cell efficiency was obtained when we applied two different reactive-ion etching (RIE)-textured processes to groups of mc-Si wafers from BP Solar and compared them with cells using planar control wafers. Recently, we applied these same two RIE-textured processes to groups of tricrystalline wafers from Shell Solar. We processed these groups identically with two other groups of control wafers: One received their standard alkaline, wet-texture process; one remained planar. Then we processed all wafers through their industrial cell production line using standard process schedules.

The RIE-textured tricrystalline Si cells performed better than the standard untextured cells. We eliminated plasma damage while minimizing front reflectance. We obtained internal quantum efficiencies higher than those of planar and wet-textured cells, boosting textured-cell currents and efficiencies by up to 6%.

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Refereed

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10763

Control Strategies for Homogeneous Charge-Compression Ignition (HCCI) Engines

J. H. Chen, J. C. Oefelein, A. R. Kerstein, T. Echehki, C. A. Kennedy, J. C. Hewson, J. E. Dec

Sandia proposes to implement novel computational and modeling tools to develop active control strategies for in-cylinder fuel/air/residual mixture composition and temperature in homogeneous charge-compression ignition (HCCI) engines. HCCI engines are an attractive alternative to diesel engines, offering the potential for high, diesel-like efficiencies ($> 50\%$), while concurrently producing extremely low emissions (super-ultralow-emission vehicle [SULEV] standards) without expensive aftertreatment. An HCCI engine operates on the principle of compressing a dilute premixed charge until it autoignites and burns volumetrically. This is a relatively new realm of combustion, wherein the mixture is often sufficiently dilute so as to prevent flame propagation; hence, combustion occurs volumetrically. For appropriate mixture and fuel type, engines have been successfully operated in an HCCI mode. However, achieving appropriate combustion across the load-speed map of the engine and slowing the combustion to achieve a smooth heat-release time history—so as to prevent engine damage and noise—remains a formidable challenge. Recent zero-dimensional computational studies show that it is difficult to achieve a smooth heat-release history with a fully homogeneous mixture. A key technical challenge, then, is how to actively control the intake protocol and in-cylinder fluid motion to obtain the needed heat-release time profile across the operating conditions of the engine.

We completed the development of computational tools (i.e., one-dimensional turbulence [ODT], direct numerical simulation [DNS], and large-eddy simulation [LES]) to simulate HCCI engine conditions. We used these tools to develop and evaluate a reduced description of HCCI ignition, to understand a fundamental issue regarding the existence of flame propagation under HCCI conditions, and to characterize the cold mixing field in an engine cylinder.

(1) Using a simulation tool based on the ODT approach developed in previous work, we developed and evaluated a reduced description of HCCI ignition that has a sound theoretical basis and is convenient for conceptual design evaluation. The reduced description involves an extension of a previously developed ignitability metric that was based on one-

We completed the development of computational tools (i.e., one-dimensional turbulence [ODT], direct numerical simulation [DNS], and large-eddy simulation [LES]) to simulate HCCI engine conditions. We used these tools to develop and evaluate a reduced description of HCCI ignition, to understand a fundamental issue regarding the existence of flame propagation under HCCI conditions, and to characterize the cold mixing field in an engine cylinder.

step Arrhenius chemistry. The extension involves the interpretation of multistep ignition chemistry as an equivalent one-step mechanism with chemical-kinetic parameters determined from homogeneous compression-ignition computations. The ignitability metric is based on high-activation-energy asymptotic analysis of near-top-dead-center compression-ignition conditions with a parameterization of mixture inhomogeneity. Based on chemical-kinetic parameters inferred from the homogeneous computations, we found that the ignitability metric correlates well with ignition times obtained from inhomogeneous turbulent-mixing computations using the ODT-based simulation tool. This comparison was based on hydrogen (H) fuel. We performed analogous simulations for n-heptane fuel and are near completion of the ignitability analysis for this fuel.

(2) An outstanding question regarding HCCI is under what conditions flame propagation coexists with volumetric autoignition. Preliminary DNS autoignition studies of H-air mixtures with initial spatial variations in equivalence ratio and constant initial temperature have been studied at 10 atmospheres. Results show that some mixtures ignite and form sustained premixed flame fronts while other mixtures tend to ignite “volumetrically,” i.e., nearly uniformly and without flame fronts. We found the “mode” of autoignition and the propagation of any subsequent premixed flames to depend strongly on the mean and amplitude of the variations in the mixture equivalence ratio, the length scale of the mixture variations, and the initial temperature. We found similar ignition modes for the autoignition of uniform mixtures with spatial variations in the initial temperature. Detailed parameter studies are currently under way to “map out” the various ignition modes with respect to the initial conditions for H-air mixtures under various pressures. We will conduct similar mapping studies using higher hydrocarbon fuels, such as propane and n-heptane, which are more relevant to HCCI engines. These fuels have disparate reaction rates, and hence, we developed and implemented a new additive Runge-Kutta method to address this source of numerical stiffness. With this new capability, these one-dimensional (1-D) parameter studies will also be used to determine relevant initial conditions for 2-D DNS autoignition studies for a range of hydrocarbon fuels.

(3) LES are focused on model synchronization over full engine cycles. The calculations performed to date are limited to H-air systems. We conducted the simulations using a time-varying grid system composed of an idealized port-valve cylinder configuration and a moving piston that matches the

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geometric and operating conditions associated with the metal and optically accessible HCCI engines currently under experimental investigation at the Combustion Research Facility (CRF). We performed case studies to synchronize the model bases used for the LES and DNS codes and to complete tasks related to the validation of thermal-ignition, compression-heating, and compression-ignition processes. These studies led to a fully synchronized model base between the LES and DNS codes. We are in the process of performing initial LES calculations to characterize the full multidimensional turbulence and scalar mixing processes that occur inside the idealized port-valve cylinder configuration over full engine cycles. These simulations will provide a unique glimpse of the complex interactions between key geometric features and the subsequently induced turbulence. We will also attempt to investigate the merits of LES as a tool to provide locally accurate, time-varying initial and boundary conditions inside the cylinder for use with DNS.

Other Communications

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10771

Silicon/Carbon Nanocomposites for Rechargeable Battery Applications

D. Ingersoll, K. J. Gross, M. A. Rodriguez

The need for small, lightweight electronic devices not only for consumer electronics products but also for national security needs, as well (e.g., in support of the war on terrorism and counterproliferation activities), continues to spur the drive toward development of small, lightweight power sources for autonomous micro- and mesoapplications. Furthermore, the performance characteristics of energy-storage devices, including their ultimate size and weight, are dictated by the intrinsic characteristics of the materials making up the device. Consequently, by improving the performance characteristics of these materials, we can improve the overall system device performance. Toward this end, Sandia initiated development of new nanocomposite materials for use as the anode in reversible energy-storage systems in the hope of significantly increasing their energy and power densities as well as their specific energy and power, thereby allowing a reduction in both the size and weight of the overall system. Our work focused on the preparation of nanomaterials that form alloys with lithium (Li), as well as on carbon (C) nanocomposites of these same materials. The materials of principal interest include silicon (Si), aluminum (Al), tin (Sn), antimony (Sb)/Sn, etc., with the primary focus being on Si. In this project, we successfully developed an inexpensive method for preparing C/Si composites that exhibit high reversible capacity in excess of 800 mAh/g. This is more than twice the reversible capacity of the currently used materials. In addition, these materials exhibit stable reversible capacity over the limited cycling regime that has been used for evaluation.

We initiated development of new nanocomposite materials having higher energy/power densities and higher specific energy/power than currently used materials. Successful attainment of this goal will allow for a reduction in both the size and weight of the overall system. The material currently in use is graphite, and it exhibits a theoretical capacity of 370 mAh/g. By way of contrast, Si has a theoretical capacity an order of magnitude higher than that of C, on the order of 4200 mAh/g when fully loaded. However, Si will undergo large volumetric changes during Li insertion and removal, leading to irreversible structural damage that limits cycle life. Furthermore, solid-state diffusion of Li during the insertion/extraction process limits the practical rate capability of the material. Through formation of

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Si/C nanocomposites, we developed novel materials exhibiting high storage capacity and improved cycle life in comparison to the currently used and pure materials. While the main emphasis of this activity focused on Si/C nanocomposites, other inexpensive metals should perform similarly, including Al and Sn.

The three major tasks in this project are (1) acquisition of the nanomaterial, (2) structural characterization of the nanomaterials, and (3) electrochemical characterization of the nanomaterials.

We used several approaches to obtain the nanomaterials. These included purchase from commercial sources, chemical synthesis from simple precursors, and mechanical formation. Nanomaterials are an emerging area of research and science, and as such, they are not readily available. In fact, we could not obtain C nanocomposites of any kind commercially, but we were able to acquire several samples of single metal and alloy nanomaterials from a number of sources, including universities and start-up companies. However, characterization of these materials revealed that many of these samples were in fact macroscopic-sized materials, and not nanosized. Of the nanosized samples, it was possible to attain very high capacities, sometimes in excess of 1000 mAh/g. However, they did not cycle well, and the capacity dropped precipitously after very few cycles. We also synthesized several nanosized Si samples (again, not composites) and attempted an electrochemical evaluation. However, oftentimes there was not enough material available to attempt the characterization, or when there was sufficient material, a passive layer, presumably a surface-oxide layer, prevented and/or inhibited the charge-transfer reactions.

The remainder of this summary describes the mechanical approach used for formation of the nanocomposites, which did allow for preparation of nanocomposite materials having the desired performance characteristics, namely, high capacity and good cycling behavior.

The mechanical approach is relatively straightforward and consists merely of grinding the materials. However, when a brute-force approach is utilized—that is, prolonged grinding of the material until nanosized materials are obtained—the resulting materials perform poorly. While we found higher capacities in some cases, they did not cycle well. Furthermore, in several instances, a compound like silicon carbide (SiC) was formed instead of a composite. Instead, a more subtle grinding approach was required for preparing materials that performed well. We evaluated the effect of many of the processing

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parameters on performance, including relative ratios of Si-to-C, grinding durations, grinding order, etc. Through these studies we prepared composite materials with high capacities in excess of 800 mAh/g while retaining good cycle life. In fact, in some cases we observed an increase in capacity upon repeated cycling.

Once we determined the appropriate processing parameters, the mechanical approach to preparation of high-capacity nanocomposites was relatively straightforward. Furthermore, since the starting compounds are relatively inexpensive, as is the processing step itself, the likelihood of commercialization of these materials is significantly increased.

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Other Communications

Roberts, G., C. Gross, D. Ingersoll, and J. Wang. 2002. *In situ and ex situ* XRD characterization of silicon/carbon nanocomposites anode materials. Paper to be presented at the 2003 Spring Meeting of the Electrochemical Society.

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1999/1

Use of Apatite and Substituted Apatites for *In Situ* Barriers for Radionuclide Containment and Waste Stabilization and Arsenic Removal from Potable Water

R. C. Moore

This work describes a new in situ technique for placement of apatite, $\text{Ca}_{10}(\text{PO}_4)_6(\text{X})_2$, where X is monovalent anion such as OH-, Cl- or F-. It is well documented that apatite is a strong sorbent for radionuclides and heavy metals. The new placement process is based on injecting a solution of calcium citrate and sodium phosphate into soil. As the citrate is biodegraded, calcium (Ca) is gradually released and immediately reacts with the phosphate to form insoluble calcium phosphates that transform into apatite. In this work, Sandia formed apatite in soil by adding a solution containing sodium citrate, calcium chloride, sodium phosphate, ammonium nitrate, and sodium fluoride at a pH of 8. We analyzed the apatite precipitated on the soil particle surfaces by x-ray diffraction (XRD); it closely matched the pattern of hydroxyapatite, $\text{Ca}_{10}(\text{PO}_4)_6(\text{OH})_2$. Batch sorption studies using soil in which apatite was formed indicated that strontium (Sr) and uranium (U) are irreversibly sorbed to the apatite. Column studies are under way. We adapted the process for irreversible sorption of technetium (Tc). We will investigate redox reagents for use with Tc. This work also investigated the use of bovine apatite to sequester arsenic (As). Initial experiments indicated that As was quickly removed by contact with bovine apatite. We identified the material responsible for As sorption and completed sorption experiments. A pilot plant study on using the material in a new process is under way. The process is based on using magnesium oxide (MgO) to sorb As and remove the MgO by centrifugal methods.

This project is divided into two parts: sorption of As from drinking water and formation of apatite for containment of radionuclides. A new sorbent based on zirconium (Zr) has been developed for As sorption. Zr is an environmentally benign material found in many common products such as toothpaste. It is currently used in water treatment and is very inexpensive. In this project, Sandia bonded Zr to activated carbon (C), zeolites, and sand. Because of its high charge in ionic form (+6), Zr is a strong sorbent for many anions, including As. In equilibrium experiments, we reduced As concentrations in water from 200 parts per billion (ppb) to less than 1 ppb in 1 minute of contact time. We developed a new *in situ* technique for constructing a

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permeable, reactive barrier composed of apatitic material for sequestering actinides, Sr, and heavy metals in soil and groundwater. We make the barrier by injecting an aqueous solution of calcium citrate, sodium phosphate, and microbial nutrients into the path of contaminated groundwater flow. As microbial activity degrades the citrate, Ca is released and calcium phosphate minerals form and crystallize. Under the proper conditions of reagent concentration and pH, apatitic materials form in the soil. By passing the calcium citrate and sodium phosphate solution through a column packed with the soil, a white precipitate was visible in 1–2 weeks. We identified the material as apatite by using transmission electron microscopy (TEM), electron dispersive spectroscopy (EDS), XRD, and Fourier-transform infrared (FT-IR) spectrometry. We then performed batch experiments to determine the effectiveness of the *in situ*-formed apatitic material to sorb uranium (U). The results indicated that the treated soil strongly sorbs U. Furthermore, 72-hour reversibility experiments indicated that only trace amounts of U were released from the treated soil, while untreated soil released approximately one third of the sorbed U. Experiments with Tc indicate that apatite will strongly sorb Tc in the presence of tin chloride (SnCl_2), and Tc will not desorb, even in oxidizing conditions.

This work resulted in two patent applications: the use of Zr-doped materials for removing As from drinking water, and the use of magnesium oxide (MgO) in a process for treating drinking water.

We are advertising for information on the use of MgO for preconcentration of As for quantification. Results from this work on sorption of neptunium (Np) by hydroxyapatite are being published in *Radiochemica Acta* and formation of apatite for containment of radionuclides in *Environmental Science and Technology*. The development of Zr-based sorbent for As will be presented at the New Mexico Environmental Health Conference.

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Refereed

Moore, R. C., K. Holt, and C. Sanchez. 2002. *In situ* formation of apatite for containment of radionuclides. *Environmental Science and Technology*, accepted.

Moore, R. C., K. Holt, and C. Sanchez. 2002. Sorption of neptunium by hydroxyapatite. *Radiochemica Acta*, accepted.

21559

Regional Dynamic Simulation Modeling and Analysis of Integrated Nuclear Futures

A. B. Baker, W. E. Beyeler, S. H. Conrad, D. L. Harris, P. E. Rexroth, N. E. Bixler

Sandia will produce an integrated framework and a dynamic simulation model of key aspects of nuclear energy, nuclear-materials storage and disposition, global nuclear materials management (GNMM), defense nuclear materials, and nuclear-proliferation risk, and will link nuclear energy dynamically to global energy and greenhouse-gas emissions. Specifically, this framework will “reduced-form” model the “back end” of the nuclear-fuel cycle (waste storage and disposition), the “front end” of the nuclear-fuel cycle (nuclear-power generation), and the defense materials system (nuclear materials from weapons).

To provide for integrated energy and environmental systems integration, this project also will “reduced-form” model global energy demand by sector (industrial, residential/commercial, transportation, and electricity), by fuel (oil, natural gas, coal, nuclear, renewables), and for global carbon emissions. The Defense Materials Module will “reduced-form” model the nuclear materials flow from weapons to the “back end” of the fuel cycle and will be benchmarked to credible sources as far as possible. Research will proceed in parallel for these main modules and for dynamic characterization of both proliferation risk and environment. Thus, this project will produce an integrated model of nuclear energy, energy-based carbon emissions, and GNMM of defense- and civilian-generated waste streams that will permit strategic assessment of integrated research needs and provide a tool for complex policy analysis.

The proposed model enhancements will facilitate critical decision making to support regional and global assurance of the safety and security of nuclear materials and environmentally acceptable, reliable, and cost-effective energy production.

The model consists of six modules that together provide a picture of the consequences of alternative energy choices. The modules are as follows:

- *Fuel-cycle back-end module*
- *Energy module*
- *Fuel-cycle front-end module*
- *Defense nuclear materials module*
- *Nuclear-proliferation environmental module*
- *Environmental module*

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The use of a dynamic simulation model to illuminate issues concerning the use of carbon (C)-based and nuclear fuels has been a success. The model generated much debate about the issues of C, spent nuclear fuel, nuclear fuel recycling, and proliferation. Due to the interactive nature of the model, policymakers can try to mitigate both expected and unforeseen consequences of the status quo and other policies.

The primary goal of recent work was to validate the model both at Sandia and externally. We completed the internal validation of the GNMM. This validation crossed many departments and subject areas, including nuclear engineering, nuclear policy, nuclear weapons, nuclear nonproliferation, and environmental restoration. We also completed an external validation of the model at the Texas A&M University (TAMU) Department of Nuclear Engineering and with the Distinguished Advisory Panel, which is composed of members of academia, nongovernmental organizations, and government officials. The TAMU group included the nuclear engineering and economics departments. We completed numerous demonstrations (DOE, universities, government officials) of the model, accepted feedback, and made changes when possible. We are now leveraging the model to future projects and incorporating portions of it into other simulation activities.

Refereed

Bixler, N. E., A. B. Baker, W. E. Beyeler, S. H. Conrad, D. L. Harris, L. A. Malczynski, and P. E. Rexroth. 2002. The global nuclear futures model—a dynamic tool for energy strategies. *Proc. ICONE10* (April): 1–7.

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26549

Very High Temperature Gas-Cooled Reactor

R. J. Lipinski, S. A. Wright, D. R. Anderson, G. E. Rochau, E. J. Parma, Jr., P. S. Pickard, R. O. Gauntt

Sandia's goal in this project is to develop and analyze concepts for next-generation power reactors. High temperatures are needed to allow for higher electrical generating efficiency and to enable high-temperature process heat applications, such as thermochemical hydrogen production. Ideally, the next-generation power-reactor system would be cost-effective as compared to current power-generating plants, passively safe, and proliferation-resistant. To achieve these goals would require the use of high-temperature advanced fuels, fuel elements, coolants, and materials. Initially, the study focused on advanced high-temperature fuel options, fuel element configurations to minimize temperature differentials, criticality, and burnup.

From the preliminary assessments, we proposed three reactor concepts and studied them further.

- Advanced high-temperature reactor (AHTR): a low-pressure, molten-salt-cooled reactor using prismatic graphite fuel elements with current-technology coated-particle fuel; process heat applications, exit coolant temperature of 1000°C*
- Very high temperature gas-cooled reactor (VHTGR): a high-pressure helium-cooled reactor using prismatic graphite fuel elements with advanced coated-particle fuel; electrical-power generation with ~ 57% thermal efficiency at 1100°C*
- Ultrahigh-temperature gas-cooled reactor (UHTGR): a high-pressure helium-cooled reactor using fuel pebbles with highly advanced coated-particle fuel; electrical-power generation with greater than 60% thermal efficiency at 1200°C or higher.*

Sandia analyzed peak operating temperatures, passive-safety decay-heat removal, criticality, burnup, reactivity coefficients, and material issues to determine technical feasibility of each concept.

The AHTR concept can achieve an exit coolant temperature of 1000°C and relies on existing technology, current particle fuel design, and low pressures. Disadvantages include corrosive coolant and material compatibility. The VHTGR achieves temperatures of ~ 1100°C and is evolutionary in nature, building on the current technology with some advances in fuel technology. The UHTGR would allow for extremely high exit coolant temperatures greater than 1200°C. However, to achieve this goal, significant advances in fuel design and material research and development would be required.

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High-temperature coolant outlet conditions for advanced reactor concepts are limited by the fuel and fuel-element design. The maximum operating temperature of the fuel is limited by the type of fuel and its performance characteristics. The temperature differential from the fuel to the coolant is limited by the conductivity of the fuel, the proximity of the coolant to the fuel, and the fuel-element geometry. These factors play important roles in determining the maximum outlet coolant temperature conditions.

We studied high-temperature fuels to determine the current state-of-the-art technology and assess potential future advancements. The next-generation high-temperature reactor will most likely use coated-particle fuel similar to that developed by General Atomics in the 1960s and 1970s. Particle fuel embedded in a graphite matrix has been used for helium (He)-cooled power reactors in both the U.S. and Germany. The tri-isotopic (TRISO) particle fuel is the current state-of-the-art fuel for high-temperature applications. The TRISO particle fuel uses a UO_2 kernel coated with multilayers of silicon carbide (SiC) and graphite. We selected this approach since no metallic clad was identified that could maintain a fission product barrier at these temperatures. The TRISO fuel can operate at 1250°C indefinitely and to 1600°C for short off-normal periods. To achieve temperatures above 1250°C , we considered higher-temperature coatings. Zirconium carbide (ZrC) is currently being studied in Japan and is the most likely option. To achieve fuel temperatures greater than 1400°C , additional technological developments would be required for the fuel. Additional refractory carbide coatings, such as niobium carbide (NbC) or others, could be used to mitigate the diffusion of selective fission products. Advanced fuel kernels would also be required, using carbides, oxycarbides, or mixed carbides. These advanced fuel forms have as yet only been proposed, with little or no experimental research and validation.

To maximize the coolant outlet temperature and minimize the peak fuel temperature, the fuel element must be designed for a temperature drop from the coolant to the peak that is as low as possible. For pebble bed reactor designs, this is achieved by flowing gas directly over the surface of the pebbles. For prismatic configurations, the temperature drop can be minimized by maintaining the coolant channel in close proximity to the fuel and adjusting the fuel and coolant channel dimensions. We analyzed several fuel-element configurations for power densities of 5 W/cc and greater. At 5 W/cc for a prismatic element and molten-salt coolant, the temperature drop between the fuel and coolant is calculated to be 190°C for a 1

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cm radius flow channel and 10% coolant volume. The pumping power was very small, $\sim 0.0002\%$ of the total core power. For He coolant at 1000 psi, the temperature drop under similar conditions is 160°C . The pumping power for He is $\sim 0.5\%$ of the total core power. At 5 W/cc for a 3 cm-radius pebble, the temperature drop is calculated to be 65°C and the pumping power for the He is $\sim 0.01\%$. Lower temperature differentials can be achieved by maintaining smaller coolant channels for the prismatic element, and smaller fuel pebbles for the pebble bed design. The penalty is a larger pumping-power requirement for the He-cooled designs.

Passive-safety decay-heat removal, high-burnup efficiency, and proliferation resistance are all design characteristics that are possible for the design concepts.

The AHTR and VHTGR concepts, with coolant outlet temperatures of 1000°C or higher, meet most of the current high-temperature requirements, i.e., thermal efficiency greater than 55% and high-temperature process heat. These concepts can be developed and built using new engineering design approaches and evolutionary technological advances. These concepts represent the logical next step for high-temperature nuclear systems. The UHTGR, with coolant temperatures exceeding 1200°C , represents a more revolutionary design requiring major advancements in fuels and materials and requiring a major development effort. The benefit of the UHTGR design, thermal efficiency of $\sim 60\%$, is not commensurate with the technological difficulty in developing the system.

Passive-safety decay-heat removal, high-burnup efficiency, and proliferation resistance are all design characteristics that are possible for the design concepts.

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26550

Solid-State Ballistic Chemical Sensors*A. H. McDaniel, R. J. Bastasz, W. K. Schubert, J. A. Whaley, J. W. Medlin, D. J. Morrison*

Sandia proposed to develop a new type of solid-state detector, sensitive only to hydrogen (H) and H-containing moieties, that is derived from a metal-insulator-semiconductor (MIS) capacitor. We fabricated an array of palladium (Pd)- and nickel (Ni)-based MIS capacitors via lithographic methods in complementary metallic-oxide semiconductor (CMOS) architecture. These devices are known to be extremely sensitive and selective to H; however, they suffer in mixed-gas environments due to undesirable catalytic reactions on the sensor surface. The technical advance pursued in this work was to investigate the possibility of bypassing surface-mediated events by implanting charged particles directly into the sensing junction. In effect, this would eliminate interference from surface-catalyzed reactions and impart sensitivity to a larger class of H-containing molecules.

The original hypothesis proved true: Coated MIS sensors can selectively detect charged particles derived from H-containing gases. However, our recent accomplishments reflect a modification of the project objectives. Instead of pursuing a prototype sensor with integrated ionizer and ion optics, the research effort focused on characterizing MIS sensing structures and investigating the interaction of charged particles with the device. In so doing, sensor manufacture migrated to full CMOS processing. In addition to Au overcoat, we attempted Si₃N₄ deposition, but failed. The team also investigated Ni-based MIS capacitors with native oxide as the filter layer. We fabricated and characterized second- and third-generation MIS capacitors, with and without overlayers, for (1) nascent capacitance-voltage (C-V) response, (2) sensitivity to neutral H, oxygen, C₁ to C₄ hydrocarbon (HC), C₄F₈, and carbon monoxide (CO), (3) sensitivity to ionized argon, and (4) sensitivity to ionized H, C₁ to C₄ HC, and C₄F₈.

We successfully fabricated second- and third-generation sensing elements of Pd, Au-coated Pd, and Ni in CMOS via lithography, metal deposition, and liftoff. Differences between generations were significant, e.g., Au-coating of second-generation devices was discontinuous, creating leak paths through the protective layer. For application as a ballistic sensor, the permeable overcoat was ineffective at screening molecular H. However, the pore size and depth of the leak paths

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were such that the coated Pd-MIS sensors exhibited desirable CO sensitivity in H₂ ambient. In addition to a porous overcoat, the gate oxide thickness of second-generation sensors was less than targeted, resulting in poor process yields and sensor-to-sensor variability in nascent C-V characteristics. We incorporated lessons learned into third-generation devices, improving yield, stability, and reduced variability in device response.

To investigate application of alternative filter-layer materials, we experimented to survey methods of sputtering thin, pin-hole-free layers of Si₃N₄. Unfortunately, these efforts did not meet with success. The experiments consisted of varying the amount of N₂ backpressure present during sputtering of a pure silicon (Si) target in the presence of partially processed wafers having only gate oxide and Pd. We deposited thin Si₃N₄ films atop the Pd/gate oxide wafer; however, coating failed pin-hole test in potassium hydroxide (KOH) etchant, which indicated that stoichiometry favored Si and not SiN. We abandoned further attempts to sputter-coat using a Si₃N₄ target due to a combination of personnel turnover and equipment failure. As a result, we characterized only bare Pd, Au-Pd, bare Ni, and oxide-coated Ni-sensing elements.

The aforementioned group of sensing elements were subject to an extensive array of experimental conditions that included exposure to various gas mixtures from near-atmospheric pressure to high vacuum, irradiation by ionized species in pulsed and CW modes, discrete and continuously variable ion energies from 0.2 to 3.0 keV, and device temperatures ranging from 323 K to 473 K. The experimental results verify the hypothesis that ballistically implanted protons derived from H and H-containing molecules (such as hydrocarbons) can be detected by both Pd- and Ni-based MIS capacitors. Additionally, the Au overcoat acts as a high-pass energetic-particle filter.

Perhaps the most interesting observations that challenge our understanding of these structures are (1) the sensor recovery mode, and (2) the inability of the energetic particles to penetrate a thin oxide coating over Ni. Initially, we anticipated that it would be difficult for implanted H to escape from the device because the “sensing” interface is encapsulated by a dense metal overcoat on top and silicon dioxide (SiO₂) on the sides and bottom. The coated Pd-MIS sensors exhibited recovery modes that clearly indicate that H is able to leak out of the device with little difficulty. We also observed that oxide-coated Ni sensors did not respond to either molecular H or implanted

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protons, whereas oxide-free samples were sensitive to both. The wealth of information collected has proven concepts necessary to develop advanced ballistic-sensing elements.

26551

Novel Catalytic Systems for Energy-Efficient Feedstock Hydrocarbon Separations

T. M. Nenoff, S. M. Thornberg, I. C. Abraham, Q. G. Buelna

This project combines Sandia's expertise in catalyst/zeolite synthesis, nanoscale reaction kinetic testing, and catalytic testing to produce a novel selective catalytic system that is highly energy efficient and to develop analytical tools for rapidly assessing the nanoscale performance of catalysts. Current processes for manufacturing the commodity feedstock cumene (isopropylbenzene) involve a two-step process of heating reactants with acid catalysts (300°C), and in some cases cooling for transport (25°C), followed by an energy-intensive distillation product separation (130°C). Reaction and separation in a one-pot reactor, noncorrosive zeolite catalysts, and the elimination of the cooling and transport steps will combine to produce a more-efficient process with a potentially tremendous payback in energy savings.

In this project, synthesized catalysts will be reacted with benzene and propylene reactants to produce the feedstock cumene. We will determine optimized catalyst choice through development and application of nanoscale kinetic tools obtained with Fourier-transform ion cyclotron resonance mass spectroscopy (FT-ICR/MS), a uniquely suited analytic tool. With FT-ICR/MS, the zeolite catalyst is fragmented by laser ablation and then allowed to interact with the hydrocarbon (HC) molecules. This gives binding energies, reaction mechanisms and kinetics, gas-phase reactivity, and selectivity of the catalyst per HC system. Results from the nanoscale studies will guide which catalysts are tested in bulk scale in a unique one-pot combined catalytic reaction/distillation cumene synthesis process (130°–200°C).

We are highly qualified to undertake this novel research due to our expertise in catalyst synthesis and testing and nanoscale kinetic studies. Our labs are equipped for full reactants and product characterization, including in-house reactors, FT-ICR/MS, and gas chromatograph/mass spectrometry (GC/MS) product characterization.

This project comprises two major areas: catalysis research and nanoscale research. To provide a test-bed for correlation of nanoscale results with bulk experiments, we tested various reactor configurations. Reactors tested to date are the Parr reactor, a tee reactor, and a continuous-flow reactor.

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We performed a test matrix of variables that influence cumene production/yield, including zeolite type (beta, novel Sandia zeolite catalyst SOMS [Sandia octahedral molecular sieves], a protonated niobate molecular sieve), reactor type, catalyst acidity, temperature, and concentration. We performed and analyzed more than 100 bulk-scale studies and correlated them to literature values as well as previous Sandia experiments. These data show that the best results were obtained in the continuous-flow reactor using protonated beta zeolite (12:1 silicon:aluminum) at 200°C with a benzene:propylene dilution of 7:1. In comparison studies with H-beta zeolite 12 (7:1), the Parr reactor had good yield (75%) and good selectivity (77%), but the continuous-flow reactor had better yield (95%) and selectivity (95%). Consequently, we used the continuous-flow reactor in the remainder of the experiments. MCM-22 catalysts are showing similar results and are being studied further.

We used a low-resolution MS (residual-gas analyzer [RGA]) to monitor catalytic reactions in real time. We monitored unique signals from each reactant, as well as each product, as a function of time so that the reaction progress could be determined. We connected the Parr reactor to the MS via a heated line and monitored characteristic peaks for each compound. From these data, we determined that the optimal reaction time is ~ 1 hour to get the best production of cumene and very little byproduct formation.

In the nanoscale research, we accomplished the first-known laser ablation of a heterogeneous catalyst and monitoring of HC attachment to zeolite fragments. While the real-time RGA data give information on the bulk scale, *in situ* FT-ICR data give information on the nanoscale. The nanoscale tool hardware (FT-ICR/MS and laser ablation) is operational, experimental procedures are established, and testing of heterogeneous catalysts is under way. For these experiments, we chose protonated beta zeolite as a test case for several reasons, e.g., its ability to form cumene, the extensive literature about its use in cumene production, and our experience with it. We fragmented beta zeolite reproducibly in the FT-ICR and tentatively identified the resulting fragmentation series (a “series” is a pattern of evenly spaced peaks resulting from fragmentation of large molecules, e.g., $[\text{SiO}_2]_n\text{AlO}_2$). Recent successful attachment of propylene to beta zeolite fragments yielded new series, i.e., HC attached to zeolite fragments, and is a major accomplishment in the nanoscale-tool development. This is important because the attachment of propylene to the zeolite is noted in the literature as the first step in cumene production, given an Eley-Rideal mechanism. Testing with isotopically labeled HCs (^{13}C , ^2H) is under way to aid in the identification of fragment series. Isotopically labeled samples cause a series

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of peaks containing the labeled HC to be shifted by the mass increase in the HC. For example, if propylene (C_3H_6) attached to a fragment series and another experiment was run using deuterated propylene (C_3D_6), the deuterated propylene series would be shifted six daltons higher than normal propylene and thus be clearly identified. We developed software tools to decipher very complex FT-ICR mass spectral data to aid in understanding the molecular reactions. A typical mass spectrum will have hundreds of peaks of varying heights, so extraction of the meaningful data is greatly simplified through the use of pattern-recognition algorithms identifying common groups of peaks (wavelets).

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26552

A Model of Infrastructure Interdependency Using Communication Agents

D. C. Barton, R. J. Pryor, D. A. Schoenwald, E. D. Eidson, K. L. Stamber

U.S. infrastructure has always been vulnerable to malevolent acts and natural disasters. Today, however, the most serious threat comes from the increasing complexity of the system and its growing interconnectedness. The communication infrastructure is the link that allows interconnection between all other infrastructure networks and enables the transfer of goods, services, and information. Communication literally constitutes both the foundation and an upper limit to the economic functioning of a society.

Several research institutions, including Sandia, are developing agent-based models to simulate infrastructure systems. These models treat communication infrastructure simply as message passing between agents. A limitation of current agent-based infrastructure models is that communication is treated simply as always-successful message passing between agents. In other words, the communication infrastructure is not specifically represented. None of these models simulates the differences in communicating over telephone, computer, wireless, or other networks, and thus can determine neither the impact of specific failures in communication on the whole system, nor the impact of other infrastructure failures on communication infrastructure. A more useful agent model of infrastructure interdependency is one that would interpret communication as a separate agent system capable of creating, transforming, sending, receiving, and storing information and messages over time and across distance.

This project is developing an agent-based model of infrastructure systems that explicitly simulates the dependence of infrastructure transactions on communication infrastructure. While Sandia is already considered a leader in infrastructure interdependency analysis, specific handling of communication systems in our agent-based models will clearly differentiate Sandia's capabilities in agent-based infrastructure simulations. Success in this project will provide a unique capability for developing financial threat assessments, i.e., business case models, to better understand the economic impact of critical infrastructure failures and the potential impact that financial failures might have on national security.

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The goal of this effort was to design business models and behaviors for telecommunication and other infrastructure agents into CommAspen, Sandia's agent-based model of infrastructure interdependency. We completed a working version of CommAspen. CommAspen incorporates business models into the agent design that allow simulation of market reliance on supporting infrastructure networks like telecommunication and power, as well as the reliance of production operations and infrastructure reliability on the availability of commodity supplies, such as durable or commercial goods.

- Develop business models; determine how changes in communications industry structures affect pricing and reliability.

- We developed business models for agent production using input/output (I/O) functions and for consumption using distribution functions.

- Production of any commodity is defined by an I/O table. The purpose of I/O analysis is to provide the formulas for the inputs that an agent needs to produce its output(s). The data are obtained from the Bureau of Economic Analysis for different industries in the U.S. This provides a recipe that shows how much of every other agent's outputs that a particular agent needs to produce its own output.

- As with most economic decision problems, agents need to be able to rank-order the relative value of its alternative consumption choices. A common mathematical method for rank-ordering preferences is to create a utility function that assigns weights to each type of consumption. We developed three specific distributions for use in creating agent properties: uniform, normal, and lognormal.

- Develop methods to represent the use of a variety of communications mediums to transfer messages between agents.

- Communications mediums, such as mail, paging, and phone, are represented either as markets for a single infrastructure supplier or as two distinct infrastructure networks. For a single supplier, there can be multiple communication markets, e.g., residential and commercial, but all calls are funneled into the same infrastructure. A separate infrastructure is used to represent the difference between cellular and telephone communication. Thus, failure in one system does not necessarily affect the other. Some fraction of the lines subscribed to by the agent may become busy, and there could be an outage due to call volume. Use of alternative communication infrastructure would be allowed.

- Incorporate additional telecommunications agent classes into the model.

The goal of this effort was to design business models and behaviors for telecommunication and other infrastructure agents into CommAspen, Sandia's agent-based model of infrastructure interdependency. We completed a working version of CommAspen.

— We developed three agent classes that represent all telecommunications interactions in the model. Individual peculiarities are handled by overwriting individual methods that would be unique to a particular agent. These three high-level classes include:

- *TelcoBuyer*: defines the infrastructure need for telecommunications; all agents that use the telecommunications infrastructure use this class to access telecommunications services.

- *TelcoSeller*: defines agents that provide communications infrastructure services. Each medium is represented as a separate infrastructure.

- *TelcoProduction*: defines the infrastructure and commodities required to produce telecommunications services. I/O tables are used to define production requirements like power, labor, etc.

In other accomplishments, work is in progress that will allow our agent-based simulation to interact with other agent models in different locations. CommAspen was connected over the Web to Argonne National Laboratories' agent-based simulation of power and fuel markets.

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26554

Investigation of Potential Applications of Self-Assembled Nanostructured Materials in Nuclear-Waste Management

Y. Wang, P. I. Pohl, C. R. Bryan, C. J. Brinker, K. Yu, H. Gao

Successful nuclear-waste and environmental management requires the development of novel functional materials that can be used for effective waste treatment, containment, and monitoring. Traditional approaches for material development are no longer able to meet increasing waste-management needs. Fortunately, with the emergence of nanotechnology, Sandia is now able to manipulate material structures at nanoscales, thus opening up unlimited possibilities for new functional material development. This project investigates the potential applications of mesoporous nanostructured materials (NsMs) in waste management. Mesoporous NsMs possess nanopore structures and are synthesized using self-assembled supramolecular templating processes. Due to very large surface area, controllable pore size, and overlapped electrical double layer, NsMs can potentially be good ion getters, separation membranes, catalysts, and sensing materials with high-sorption capacity and chemical selectivity. Specifically, we will (1) study the sorption capability of mesoporous NsMs versus non-NSMS, (2) use surfactant-templating processes to synthesize mesoporous anionic clays and test their sorption capacity for arsenate and other anions, (3) modify the pore-surface chemistry of mesoporous silica with functional molecules for developing high-performance ion getters and sensing materials for volatile organic compound (VOC) detection, and (4) investigate the photocatalytic effect and pore-size control of mesoporous titanium dioxide (TiO_2) films on the oxidation of organic chelators. This work will demonstrate a wide range of applications of NsMs in nuclear-waste management and establish the theoretical foundation and engineering approaches for such applications. One of the final products of this project will be a set of functional materials with demonstrated capabilities that potentially can be used as high-performance ion getters, catalysts, and sensing materials. The success of the project will create a synergistic effect across Sandia's nuclear-waste/environmental management, advanced materials development, and chemical-sensor development organizations, and can potentially attract investments from various customers.

We made significant progress in understanding the effect of nanoscale confinement on ion sorption by mesoporous

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materials. We demonstrated that the nanoscale confinement has a significant effect, most likely via the overlap of the electric double layer (EDL), on ion sorption onto mesoporous materials. We performed a molecular simulation using a density-functional theory (DFT) to calculate ion-adsorption coefficients as a function of pore size. The calculation shows that as the pore size is reduced to nanoscales (< 10 nm), the adsorption coefficients of ions can vary by 1–2 orders of magnitude relative to those for unconfined interfaces, which is confirmed by sorption experiments. We gained a great deal of experience in the purposeful control of morphologies and structures, e.g., interlayer spacing, of layered double hydroxides (LDH) using surfactants. The engineered LDH materials showed useful chemical and physical properties. Based on our knowledge obtained from synthetic materials, we developed a technique to form a continuous layer of metal-oxide nanocrystallites on granular bauxite materials for large-scale applications. We initiated the experiments on the pore surface modification of mesoporous silica. We developed techniques for the formation of a thin layer of activated carbon or amorphous TiO_2 on the pore surface of mesoporous silica. Our efforts have generated sufficient candidate materials for further engineering application studies.

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26555

Development of Detection Techniques and Diagnostics for Airborne Carbon Nanoparticles

H. A. Michelsen, P. O. Witze, T. B. Settersten

Newer-generation compression-ignition direct-injection (CIDI) diesel engines, which have been designed for low particulate-matter mass emissions, emit no visible soot, but they may generate far greater numbers of small particles than older diesel engines. Hybrid cars incorporating CIDI engines are expected to be commercially available in the U.S. by 2004. New evidence strongly suggests that gasoline engines also emit large numbers of small particles under some operating conditions. These small (submicron) particulates are classified as a toxic emission in California, may pose a greater health risk than larger soot particles, and are expected to have a significant impact on the Earth's climate. Small particulate emissions are thus of emerging concern.

Sandia is developing the capability to determine size and mass distributions of submicron soot particles for future studies of their formation in flames and in diesel and gasoline engines and their evolution when cooled and diluted. Our goal is to study nanoparticle formation and evolution using noninvasive optical techniques, particularly laser-induced incandescence (LII) for measuring particle mass concentrations and laser elastic scattering (LES) for determining particle size.

We performed experiments in an ethylene-diffusion flame to refine quantitative aspects of these detection techniques. We modeled these results and, combining model and experimental results, identified physical mechanisms that have a strong influence on the LII signal. Several mechanisms included in the model are speculative or highly uncertain and require further investigation. We are currently building an experiment that will allow us to investigate these processes on shorter (subnanosecond) time scales. We also constructed and characterized a particulate-matter simulator, which allows us to dilute and cool the particles before detection. Some of this work facilitated construction of a mobile LII demonstration instrument that will be used at the General Motors research and development facility for particulate-matter measurements in engine exhaust.

LII involves heating the soot particles by laser irradiation to temperatures (2500–4500 K) at which they incandesce, i.e., emit observable blackbody radiation, and detecting the emitted light. In our experiments, we heated soot particles with pulses

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of ~ 7 ns duration (10 Hz) at 532 nm from an injection-seeded Nd:YAG laser. Because LII is extremely nonlinear with laser fluence, a homogeneous laser-beam spatial profile is critical for interpreting the results. Our newest results include an aperture placed in the laser beam and imaged into the flame to provide a homogeneous spatial profile, which we characterized using a charge-coupled device (CCD) camera. Using this arrangement, we collected data from an atmospheric ethylene coflow diffusion flame to fluences as high as 1 J/cm^2 with a temporal resolution of 0.3 ns. We imaged the signal onto a fast silicon (Si) photodiode and collected it over the wavelength range 570–1100 nm. We varied the fuel, burner dimensions, and flowrates to test the sensitivity of the technique to different conditions.

We used these data to guide the development of an LII model that accounts for particle heating by laser absorption, and oxidation and cooling by sublimation, conduction, and radiation. We refined the model treatment of oxidative heating and annealing and added mechanisms for convective heat and mass transfer, melting, and nonthermal photodesorption of carbon (C) clusters. These changes allowed the model to reproduce features of the temporal behavior for which there were significant discrepancies in previous models. The new model is capable of reproducing the magnitude of the signal as a function of fluence, the fast decay at high fluences, and the slow decay at low fluences; these features were not reproduced by earlier models. In addition, comparisons of this model with the experimental temporal profiles provided valuable insight into the sensitivity of LII signals to measurement conditions and highlighted uncertainties in the model that result from a lack of understanding of the microphysical mechanisms involved in the LII process.

Cooling and mass loss by sublimation and photodissociation are the predominant mechanisms for determining the temporal behavior and magnitude of the LII signal at fluences $> 0.2 \text{ J/cm}^2$. This part of the model is the most complex and uncertain. Although previous studies suggested that laser photodesorption of C clusters from graphite can proceed by a nonthermal mechanism, the nature of this mechanism is not known. Our model includes such a mechanism with a cross section and enthalpy approximated by comparing the results with the data. Including this term allows the model to reproduce the lack of fluence dependence of the peak signal at high fluences.

Soot particles anneal into multishell C anions at temperatures above $\sim 2500 \text{ K}$ or during laser heating, and

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graphite surfaces have been shown to melt at atmospheric pressure when heated rapidly with a laser. Changes in the phase of soot primary particles are likely to influence heating and cooling rates because of differences in physical properties, such as the index of refraction, enthalpies and entropies of formation of C clusters, and thermal accommodation coefficients. Soot annealing rates have not been measured under the conditions encountered during laser heating on subsecond timescales; we infer these rates from annealing rates measured on graphite at lower temperatures on longer timescales.

Parameters to which the model is sensitive include the initial soot temperature, the ambient temperature, and the partial pressure of oxygen. To reduce uncertainties in the model associated with experimental conditions, such as ambient and initial particle temperature, we built a soot source in which we can control the ambient environment. Soot is generated by a coflow laminar diffusion flame, which is intercepted by a cross flow of N₂ to extract, dilute, and cool the soot. This source is equipped with a scanning mobility particle sizer (SMPS) for characterization of the aggregates.

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26556

Photonic Crystals for Enhancing Thermophotovoltaic Energy Conversion

S. Y. Lin, J. B. Moreno, J. G. Fleming

Thermophotovoltaics (TPV) converts the radiant energy of a thermal source into electrical energy using PV cells. TPV has a number of attractive features, such as fuel versatility (nuclear, fossil, solar, etc.), quiet operation, low maintenance, low emissions, light weight, high-power density, modularity, and possibility for cogeneration of heat and electricity. Some of these features are highly attractive for military applications. TPV could also be used for distributed power and automotive applications wherever fuel cells, microturbines, or cogeneration are presently being considered, if the efficiencies could be raised to around 30%.

This project will primarily examine approaches to improving the radiative efficiency. Optimizing a combustion chamber for maximum thermal efficiency is a well-known art, and the PV component is already under development and is at a high degree of sophistication.

Sandia will examine photonic crystals (PhC) and advanced optical structures to substantially improve the radiative efficiency in TPV. Photonic lattices use a periodic modulation of the refractive index to alter the photonic density-of-states spectrum. Photonic lattices can alter the radiative spectrum and angular distribution of a radiator; or it can be used as an optical filter with a potentially 180-degree acceptance angle for a three-dimensional (3-D) photonic lattice ("photonic crystal"). Control of the angular distribution is important for minimizing the radiative losses in the TPV cavity.

First, we realized a 3-D metallic PhC and measured its absorption measured at infrared (IR) wavelengths. We found the metallic absorption rate to be suppressed in the photonic bandgap (PBG) regime ($\sim 8\text{--}20\ \mu\text{m}$) and strongly enhanced at the photonic band edge ($6\ \mu\text{m}$). We showed that the peak absorption originates from the intrinsic tungsten (W) material absorption and is enhanced by the photonic band-edge effect. The enhancement is caused by a longer photon-matter interaction length as compared to the metallic skin depth and the slower group velocity of light at the photonic band edge.

Second, we successfully fabricated two new W 3-D PhC structures, operating at $4\ \mu\text{m}$ as well as $2.5\ \mu\text{m}$ wavelengths regime, and tested their optical properties. The transmission reflection absorption data indicate that these structures function

3-D tungsten photonic crystal.

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as expected. There exist large IR PBG, sharp band edge, and a selectively enhanced absorption at the band edge.

Finally, preliminary emission data taken from the 4 μm PhC thin-film samples at $T=400\text{--}600$ K show a selective emission also at the band edge. From the temperature dependence of emission amplitude, we found that the emission is an equilibrium emission. We also tested the emission measurement for the 2.5 μm W PhC sample. Consistent with the absorption, transmission, and reflection results, we observed a strong emission at 2.5 μm . We optimized the structure for ease of handling and ease of electrical contact. The sample structure is to be reduced by another 15%, so that the emission can be at the desirable 2 μm wavelength.

Refereed

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We also tested the emission measurement for the 2.5 μm W PhC sample. Consistent with the absorption, transmission, and reflection results, we observed a strong emission at 2.5 μm . We optimized the structure for ease of handling and ease of electrical contact. The sample structure is to be reduced by another 15%, so that the emission can be at the desirable 2 μm wavelength.

26557

Specific Anion Nanoengineered Sorbents for Water Purification

D. M. Teter, J. L. Krumhansl, P. V. Brady

The objective of this project was to identify new means for decreasing dissolved arsenic (As) levels below 10 parts per billion (ppb). Originally, research focused on identifying, designing, and synthesizing solids possessing high-anion-exchange capacities. More recent efforts resulted in determination of new methods for enhancing As uptake during standard coagulation and lime-softening. Additionally, Sandia identified a means for boosting As uptake in situ in As-contaminated aquifers.

We submitted three patent applications, collaborated with researchers at the University of New Mexico (UNM) and elsewhere, and developed a better understanding of optimal synthesis conditions of the original specific anion nanoengineered solvents (specific anion nanoengineered sorbents [SANS]) filtration material.

- *Coagulation patent.* We demonstrated that the addition of surface adjunct molecules to precoagulating liqueurs resulted in enhanced As uptake upon coagulation.

- *Lime-softening patent.* We demonstrated that the addition of surface adjunct molecules to lime-softening solution resulted in enhanced As uptake upon lime-softening.

- *In situ patent.* We demonstrated that the addition of surface adjuncts to Fe(III) (iron)-containing sediments substantially enhanced the uptake of As from adjacent solutions and from input solutions containing high levels of As.

- We performed a number of tests to better identify the chemical and physical synthesis controls over optimal SANS material production.

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Refereed

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32807

Low-Work-Function Material Development for the Microminiature Thermionic Converter

D. B. King, K. R. Zavadil, D. R. Jennison, C. C. Battaile

Microminiature thermionic converters (MTCs) provide a unique approach to developing power sources. Possible applications range from micron- to large-scale and include microrobotics and sensors, space-based power, mobile and remote electrical-power sources, and commercial-power production. MTCs can be scaled from the microwatt range to kilowatts. Sandia made significant progress in developing small-scale MTCs; however, the electrode materials are not well understood, and thermionic properties are highly sensitive to the electrode-chemical content, bulk and surface structure, and manufacturing processes. Advanced theoretical and modeling capabilities are required to achieve the desired thermionic emission from the electrode materials, aid in the electrode-fabrication process, and enhance the performance of MTC diodes. Sandia's advanced thermionic theory and detailed modeling of properties that influence thermionic-electron-emission performance will greatly enhance understanding of thermionic diodes. Using only an experimental approach is costly; a better theoretical understanding is needed to guide the expensive fabrication process.

We produced microscale electron-emissive films that possess the thermionic properties of macroscale dispenser cathodes. We deposited these films, which were based on a modulated structure of tungsten (W) and ternary barium oxide (BaO) layers, using sputter deposition. We demonstrated that an alloy surface layer of W and iridium (Ir) can be retained at the surface at operational temperatures of 1200 K. These films exhibited a uniform work function of 1.9 to 2.2 eV and an emission coefficient of 2 to 26 $\text{A}\cdot\text{cm}^{-2}\cdot\text{K}^{-2}$. Characterization of the film with operation showed that gradual W coalescence and pore formation provide an effective route for transport of Ba and O produced in the bulk of the film to the film surface. The presence of surface Ba and O lowers the work function and allows more-efficient electron emission. We demonstrated electron emission at zero applied fields using these films in vacuum diodes. Emission tests using commercial dispenser macrocathodes demonstrate that these films exhibit improved low-temperature characteristics.

Microstructure modeling work focused primarily on the structural evolution of layered films. The goal was to

Simulations of coarsening in layered two-phase microstructures, showing (a) the initiation of layer breakup at $t=9,000$ mcs and (b) the coarsened microstructure at $t=173,000$ mcs. (c) Annealed specimen shown for comparison.

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understand the behavior of a layered two-phase microstructure as it is annealed. To accomplish this, we started with a simple kinetic Monte Carlo model of two-phase coarsening (essentially Ostwald ripening). The model qualitatively reproduces the microstructural features observed in the experiment, although it does not address the voiding nor the strong vertical inhomogeneity in the structure. The latter is possibly due to diffusion and surfaction of titanium. The former is a result of reactions between W and oxide that form Ba and calcium (Ca) tungstates. To address this phenomenon, we extended the coarsening model to allow reaction and void formation.

We used density-functional theory (DFT) calculations to study probable structures and work functions for Ba and BaO-containing surface complexes at various coverages and when mixed with other likely materials such as scandium (Sc), yttrium (Y), and lanthanum (La). The base metal slab upon which the Ba, O, Sc, Y, and La materials were layered was composed of seven layers of W atoms, and we investigated both the (100) and (110) surfaces. The layer of BaO on either W surface was quite stable, with the (100) having a lower work function. We found that a very stable structure exists if the top layer is BaO, the second layer is ScO, and the third layer is W(100), with the first two layers forming a rocksalt-structured ionic film. However, this structure produced a work function above that of pure Ba or BaO monolayers on W(100), or that of ideal Ba-Sc cathodes. We then did calculations on BaO/YO/W(100) and BaO/LaO/W(100). We found the first to have a work function similar to BaO, but the latter had a lower work function by a significant amount. These theoretical results suggest that BaO/LaO/W(100) should be investigated for two reasons: (1) it may produce a useful low work function, and (2) the rocksalt ionic structure in the oxide film may produce unusual stability under real operating conditions.

The patch model developed previously was successfully benchmarked against thermionic emission of test cathodes (thin-film microdispenser cathodes and Ba-Ca-strontium (Sr) oxide films). Both cathode types exhibited non-Schottky-type current emission in the high-field Schottky regime of operation (emission was higher than expected). We developed a model to predict this anomalous emission based on field incursion into the cathode film material. Studies showed that a high field applied to the surface of a semiconductor oxide may reduce the work function beyond that predicted by Schottky. The analysis assumes that part of the metal-capping layer of the microdispenser loses intimate electrical and physical contact with the oxide below it after thermal annealing for some

Microstructures of annealed layered films at various annealing times from simulations of ripening, reaction, and voiding. Red and green represent the two original phases (e.g., W and oxide), blue is the reaction product, and black is voided.

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fraction of the surface. This feature would allow field incursion into the lower layers.

Other Communications

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32809

Autonomous Microexplosive Subsurface Tracing System

N. R. Warpinski, M. C. Grubelich, S. H. Kravitz, B. P. Engler, B. V. Ingram, B. M. Melof, J. J. Nogan

The objective of this project is to image the location and geometry of hydraulically induced or naturally occurring fractures in subsurface petroleum or waste-disposal reservoirs. The basic concept is to use existing fracturing technology (pump trucks, fluid systems, etc.) to insert autonomous microenergetic packages throughout the hydraulic fracture, have those packages function (i.e., trigger and explode) under appropriate conditions, detect the induced seismic energy with available seismic receiver arrays, and use conventional processing techniques to determine the source location, thereby marking the fracture. The packages are to be designed and built so that they function at appropriate times or under appropriate environmental conditions (e.g., timer, pressure switch, reaction with fluid), have sufficient energy and risetime to produce detectable seismic waves, and have external packaging capable of surviving in the harsh environment (high pressure, somewhat elevated temperature, highly abrasive, aqueous conditions). To fit in the fracture, the microenergetic devices would need to be quite small, but they could have a shaped design with a small cross-sectional area. To realize this technology, the following key research problems need to be addressed:

- Determine the minimum detectable size of a microenergetic device using seismic monitoring.*
- Construct trigger mechanisms to function at appropriate times and conditions.*
- Produce a device with energy-release rates appropriate for seismic monitoring.*
- Pack sufficient energy into a package small enough to fit in subsurface fractures.*

A combination of modeling, laboratory experiments, and field tests is required to achieve the objectives. We envision that the successful development of autonomous microenergetic devices could then be used for other applications involving both critical infrastructures (pipelines, dams) and military (underground structures) application.

Our focus of development has been on characterizing a pyrotechnic initiation mixture that may be activated by fracture fluid. There exists a variety of possibilities for the ignition composition, which includes silver nitrate with magnesium

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(Mg), silver nitrate with magnalium, and ceric ammonium nitrate with Mg.

We eliminated the ceric ammonium nitrate mixture based on the low decomposition temperature of the ceric ammonium nitrate and the hygroscopic nature of that oxidizer. The silver nitrate with magnalium mixture held promise for possible handling advantages of an aluminum (Al)/Mg alloy over pure Mg. The differential scanning calorimetry (DSC) data, however, point to the silver nitrate with Mg as the logical choice since it ignites in the region of 170°C, and its reaction is nearly complete at this point.

Work is ongoing to finish characterization of the ignition mixture, as well as possible output charges. We are using accelerating rate calorimetry (ARC), an adiabatic calorimetry used for reactor and pilot-plant safety analysis, to determine time, temperature, and pressure relationships for these exothermic reactions. To understand the effects of heat-soak, high-temperature storage, and, in particular, aging, we are conducting isothermal long-term aging tests to observe any adverse effects that aging will have on the mixture/components.

The compatibility of BNCP (bis[5 nitrotetrazolato]-pentaaminecobalt{III} perchlorate), lead azide, and THKP (titanium subhydride potassium perchlorate) with the ignition composition has to be addressed, and we will conduct tests to observe effects of these combinations. For the purpose of these tests, we constructed a Henkin-McGill apparatus. The Henkin test apparatus gives time-to-explosion for these mixtures as a function of temperature.

The triggering process work took place along two separate approaches. The simple approach was to design a case with a corrodible plug. We designed the corrosion plug so that it has an appropriate “safe time,” based on fracturing conditions and other parameters (typically a couple of hours).

The more-sophisticated triggering process involves the use of a microsemiconductor bridge (micro-SCB). In this design, some power source (battery or capacitor) would power a timer to fire the SCB. Work on the SCB proceeded along three lines with some success. Previous work on tungsten (W) devices has some issues (particularly bridge resistance), so we first attempted to try some new metal stack configurations using silicon/platinum/gold (Si/Pt/Au), silicon/palladium/gold (Si/Pd/Au), and Pd/Si/Au. Although we were able to fabricate and test these devices, voltage requirements were too high, and these were discarded.

Efforts shifted back to the tungsten (Si/W/Au) devices, and we made numerous improvements. These included adding a

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silicon-dioxide (SiO_2) preclean prior to titanium (Ti)/Si evaporation, controlled exposure of the Si film to airborne contaminants before W sputter deposition, extensive preconditioning and testing of Ti and W targets before product runs, very aggressive ion mill of the Si prior to Ti/W sputter deposition, controlled exposure of W film to O_2 and airborne contaminants before Ti/Au E-beam evaporation, and very aggressive ion mill of the W prior to Ti/Au E-beam evaporation. We tested initial devices and will soon complete and test refined devices.

The third area of work was on reactive bridge designs, including Ti/boron and Al/Pd bridges. Both of these are designed and fabricated and are being tested to determine if their characteristics are superior to standard SCBs for this application.

We performed seismic modeling to characterize the amount of energy coupled into the rock from the fluid-filled fracture and the type of waveforms generated (e.g., are they analyzable). Results show that a significant amount of energy is coupled directly into the rock and that the amount of energy and the shape of the waveforms are somewhat dependent on the crack width and source pulse shape.

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32815

Security Models of Agent-Based Coalitions

S. Y. Goldsmith, C. L. Beaver, S. V. Spires, H. E. Link, L. R. Phillips, W. F. Young

Most analyses of threshold cryptographic protocols are prefaced by assumptions about the capabilities of the adversary. A specific threat scenario is developed in terms of the number of agents that the adversary can corrupt in a fixed period of time. A static adversary chooses a fixed subset of the coalition prior to the initiation of the protocol. A mobile adversary can choose different subsets between successive executions of the protocol. An adaptive adversary chooses agents to corrupt during the execution of the protocol. Each threat model entails hidden assumptions about the computing environment and the institution's security policy. Little work has been done to examine the implications of these assumptions in light of security policies that seek to ensure confidentiality, integrity, and availability in the coalition. To gain the credibility in an organization necessary for deployment, threshold-based coalitions must have a well-understood relationship to well-known security policies (e.g., Clark-Wilson).

Sandia focused on three objectives: (1) understanding security models and policies of an autonomous agent group tasked with distributed network defense and intrusion detection, (2) implementation and validation of the threshold protocols developed previously, and (3) development and implementation of a reputation mechanism for ranking the level of trust among agents.

We focused on coalitions of agents assigned to provide network security functions. This narrowing of the scope of the research allowed us delve deeper into the issues of security policy for an agent group with threshold cohesion by giving us an application scenario that was sufficiently detailed to define a security model. We chose the security monitoring application because of its relevance to national issues regarding cybersecurity and because the security of monitoring systems has been largely ignored by the intrusion-detection community. The major results follow:

(1) Analyzed the security policy requirements for coalitions of agents performing network intrusion detection (NID). We developed a life-cycle analysis of the agent group's operations from deployment through retirement.

(2) Performed comprehensive security-code walkthrough and redesign for the group protocols.

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(3) Investigated models of reputation mechanisms for agents in a closed coalition and their use for detecting malicious insiders. We implemented a simple model in the agent test-bed and tested it with various forms of malicious insiders.

(4) Further investigated population dynamics models for coalitions of network security agents. This was a minor effort to finish up previous tasks.

We performed a comprehensive security analysis and code walk-through for the group protocols. This involved a deep analysis of the implementation of the protocols on the part of Sandia cryptographers and the code designers. The analysis uncovered some important gaps between the theory and practice of threshold protocols.

We accomplished the following: (1) validated and repaired vulnerabilities in the implementation of the threshold protocols, and (2) discovered some general gaps between theoretical aspects and implementations of threshold protocols.

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32816

Vulnerability Assessment of National Power Grid

D. G. Robinson, R. E. Carlson, A. E. Lutz

This project concentrates on the identification of critical nodes within the national bulk power system and the use of distributed generation as a means of diminishing the impact of the disruption of those nodes. There are over 11,000 generation facilities, in excess of 200,000 miles of very high voltage transmission line, and thousands of substations that constitute one of the largest machines ever constructed in the U.S.—the national power grid. Between 1980 and 1989 there were 5000 worldwide attacks against power transmission lines and towers; 386 of these were documented attacks against U.S. energy assets. The cost of a power disruption has been estimated to be approximately \$1–\$5 per kilowatt-hour, including both direct and indirect costs. An outage in August 1996 cost the state of California in the neighborhood of \$1–\$3 billion dollars. In addition to the obvious costs to consumers and the direct impact on the U.S. economy, there are obvious national security implications. As noted in a special U.S. Senate report, the destruction of bulk energy systems would not only affect the ability of the U.S. to mobilize its forces, but also would obviously impact the ability to support the war effort of a North Atlantic Treaty Organization (NATO) member. Through the identification of critical elements and the quantification of the consequences of their failure, site-specific vulnerability analyses can be focused at those locations where additional security measures could be effectively implemented. In particular, with appropriate sizing and placement within the grid, distributed generation in the form of regional power parks may reduce or even prevent the impact of widespread network power outages. Even without additional security measures, increased awareness of sensitive nodes can provide a basis for more-effective national, state, and local emergency planning.

The critical node area of research initially focused on developing appropriate performance measures to characterize criticality and the investigation of different approaches to identifying critical nodes. Researchers at New Mexico State University continued developing a power-flow program to calculate these performance measures when integrated with the vulnerability-analysis software. In support of 9/11, all nuclear power plants were investigated to determine the impact of failure on the national power grid. Finally, they identified three

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different families of methods to identify critical nodes: small-world theory (graph theory), polyhedral dynamics (systems theory), and particle swarm optimization (artificial intelligence). Each of the methods was coded and tested using the Institute of Electrical and Electronic Engineers (IEEE) 300 bus Reliability Test System. Critical nodes on small power networks were identified using the associated BUZZARD software.

The objective of modeling a supervisory control and data-acquisition (SCADA) system and integrating that into a “system of systems models” representing an infrastructure is to more accurately represent the combined interaction of the command and control system with the physical system, especially under stress created by an adversary. We made significant progress that will lead to a unique capability. Accomplishments associated with the SCADA modeling effort began with the development of a preliminary model of SCADA system elements. This SCADA model was then represented in universal modeling language (UML) in the Rational Rose-RT development environment for real-time systems. In the process, we can show leveraging of the interface requirements for the power-flow model and now utilize the same datasets for SCADA. The resulting capability allows a preliminary capability to change the power system state from the SCADA and observe the resulting influence on the bulk power system.

The power-park modeling activity resulted in the development of a model of a typical distributed-energy system using a library of Simulink modules. The system generates H_2 by means of a steam-methane reformer (SMR) that runs at steady state. The H_2 is fed a fuel-cell stack to follow a local load over a daily use cycle, or compressed and stored in a high-pressure vessel for later use. When connected to a model of the grid, the stored H_2 could be used by the fuel cell to supply power to the grid. The model evaluates the combined efficiency of the power system.

The tools are now in place to identify the optimum set of targets within the national power grid, which, if attacked by a terrorist group or disabled through a natural series of events, would cause the most disruption to the delivery of electric power in the continental U.S. Validation and verification will continue in upcoming work, leading up to the integration of physical and SCADA models and culminating with a series of virtual Red Team attacks on the national power grid.

We made significant progress that will lead to a unique capability. ...The resulting capability allows a preliminary capability to change the power system state from the SCADA and observe the resulting influence on the bulk power system.

Refereed

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38662

Natural-Gas Production Problems: Solutions, Methodologies, and Modeling

J. C. Lorenz, W. A. Olsson, J. G. Arguello, Jr., S. P. Cooper

Natural gas is a clean fuel that will be the most important domestic energy resource of the twenty-first century. Ensuring a stable supply is essential for our national energy security. Sandia proposed research that will maximize the extractable volume of gas while minimizing the environmental impact of surface disturbances associated with drilling and production. We are developing a system for comprehensive evaluation and modeling of the total gas system within a basin focusing on problematic horizontal fluid-flow variability. We will accomplish this through extensive use of geophysical, core (rock sample), and outcrop data to interpret and predict directional flow and production trends. Side benefits will include a first-order approximation of probable carbon dioxide (CO₂) flow patterns during sequestration (injection and storage) of this greenhouse gas, and reduce environmental impact of drilling due to the reduced number of required wells for resource extraction.

Our work focused on creating a broad-based team and developing an initial geological framework of the Raton Basin fracture system. This framework is based on three datasets: core descriptions, well logs, and field data. Over 6500 ft of core has been logged in detail. The logs describe extension, conjugate, and compaction fractures predominately within finer-grained rock units. Review of new, state-of-the-art geophysical logs shows that open fractures are oriented east-west (E-W), and the current stress state of the basin is oriented north-south (N-S) nearly 90 degrees off from early predictions. This information influences the predicted direction of fluid flow to a well and the direction that hydraulic fractures (used to stimulate production) propagate. Fieldwork details vertical extension fractures oriented roughly E-W and vertical conjugate shear fractures. It has become apparent that all three data sources are required to completely describe the system. Using any of these data sources separately produces an inaccurate model of the fracture system. An initial, two-dimensional (2-D) mechanical model is in the developmental stage using the Sandia-developed, large-deformation, nonlinear finite-element (FE) code JAS3D.

In summary, members of the Raton Basin team pursued the characterization of natural fractures and stresses in outcrops, cores, and downhole logs, in addition to beginning the modeling effort based on the data acquired from the physical

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characterization studies. Progress on these studies has been recognized within DOE and the petroleum industry, with members of our team being invited to present results at several conferences and meetings.

Refereed

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38664

High-Efficiency Turbine Blade Coatings

*D. L. Youchison, J. M. McDonald, T. J. Tanaka, T. J. Lutz, F. J. Bauer,
G. A. Hebner, R. E. Nygren, M. A. Gallis*

Although gas-fired industrial gas turbines (IGTs) have increased in popularity among electric utilities, the recent shortage in natural-gas supplies makes it likely that new high-temperature gas reactor (HTGR) power plants will be built soon. Yet, turbine designers still struggle with achieving higher operating temperatures to improve efficiency in the Brayton thermal cycle and take full advantage of the HTGR fuel cycle. Now, it may be possible to deposit thermal barrier coatings (TBCs) of yttria-stabilized zirconia (YSZ) using plasma-assisted electron beam physical vapor deposition (EB-PVD) that possess thermal conductivities 50% to 70% lower (near $1 \text{ W/m}\cdot\text{K}$) than conventional TBCs. This would allow the turbine blades to operate at higher temperatures and have a significant impact on increasing the efficiency of IGTs by 4% to 6%, while at the same time minimizing hydrocarbon emissions. Sandia seeks to produce this revolutionary new class of TBCs. In an innovative approach, instead of thermally growing the aluminum-oxide (Al_2O_3) scale, a functionally graded layer of alumina and YSZ is evaporated with simultaneous argon ion bombardment using a biased, dual-ingot evaporation technique recently developed at Sandia. The momentum transfer causes a complete amorphous-to-alpha-phase transformation in the Al_2O_3 necessary for good adhesion to the MCrAlY bondcoat. The graded layer is then transitioned into a YSZ coating. When coupled with alternating the substrate bias, the ion bombardment also reduces the grain size and increases the intercolumnar porosity in the YSZ microstructure in a layered fashion. This drastically lowers the thermal conductivity of the coating, but retains the desired high-strain compliance.

We used ion-beam-assisted deposition (IBAD) and substrate pivoting to control submicron layering of YSZ and, using 30-degree substrate pivoting at 90 s intervals, produced scanning-electron microscopy micrographs of a layered YSZ structure made by the EB-1200. We demonstrated that we can control layering at the micron level. We also verified that we could reduce the background O_2 pressure by over an order of magnitude and reduce background temperature in the thermal cage by 200°C and still produce fully stoichiometric YSZ coatings by using IBAD. This is an extremely significant discovery, since it opens up a much wider processing window

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for TBCs. We identified Kaufman gun parameters that produce distinct layering; because the layering results were favorable, we decided to move to graded layers.

On the modeling front, we completed a two-dimensional (2-D) direct-simulation Monte Carlo (DSMC) model of the thermal cage and ingot. We also completed parametric studies of the oxygen (O) injection, excitation states, chemistry, and thermal management. Although sensitivities studies reveal the importance of various parameters, lack of fundamental physiochemical data remains a challenge. We first investigated the sticking probability of $\text{ZrO}/\text{Y}_2\text{O}_3$ to the walls. Experimental observations indicated nonzero-sticking coefficients due to the significant buildup on the walls of the chamber. Similar buildup on the backside of the substrate paddle signified incomplete sticking of ZrO to the walls. Qualitative comparisons indicated that an average sticking coefficient of 70% was adequate to describe the problem.

We also addressed the influence of the internal mode excitation of the molecules (Al_2O_3 , ZrO_2 , Y_2O_3). The internal modes of these species can store significant amounts of energy leading to a reduction in the deposition rate. We modeled the process assuming full and frozen vibrational/rotational excitation (two extreme cases). The results indicated that the effect was small as long as the background pressure was low. It should be noted that most of the plume expansion takes place in the near free-molecular regime with reduced collisions and less probability of energy exchange. The gas-phase chemistry does not play an important role in this regime. It also means that most of the chemical reactions that do take place must occur on the surface of the paddle. Industrial experience shows that a small addition of O improves the quality of the deposited film. O release rates from 6 to 120 sccm were simulated and produced negligible differences. It is our finding that the release of O compensates only for the faster diffusion of O into the vacuum pumps.

The final part of this investigation was the addition of Al_2O_3 to the plume. We learned that at temperatures greater than 2300 K, all the molecular species are partially or totally dissociated and must recombine at the substrate. Al_2O_3 dissociates almost completely, providing most of the free O required to achieve stoichiometry at the substrate. The ingot E-beam sharing times are influenced by two parameters: (1) the need to achieve a particular temperature at the ingot to ensure dissociation of the molecular species, and (2) the ratio of the deposition rates is directly related to that of the evaporation rates. This means that any control of the graded layers must be independent of temperature. Upcoming work will investigate this.

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Time-Domain Reflectometry for Remote, Real-Time Water-Quantity/-Quality Monitoring of Ephemeral Streams

V. C. Tidwell, L. M. Desonier, J. R. Brainard, R. A. Jepsen, D. S. Ruby

Thousands of acre-feet of water go unutilized in New Mexico every year because of inadequate stream gauging, costing the state millions in lost economic development. Sandia proposes time-domain reflectometry (TDR) as a remote, real-time method for monitoring the quantity and quality of perennial and ephemeral stream flows. TDR operates by propagating an electromagnetic pulse (EMP) down a transmission line while monitoring the returned signal. The pulse is susceptible to reflection by dielectric discontinuities (i.e., air-water and water-sediment interfaces) and attenuation by the dielectric properties (dielectric of water, sediment, and air is 80, 25, and 1, respectively) and conductivity (i.e., salinity) of the sensed medium. Thus, with one method we can measure simultaneously the depth of water, depth of scour, sediment load, and salinity at numerous locations across the channel.

Development of this monitoring system began in the laboratory where we test, calibrate, and optimize the TDR sensor for this application. We controlled experiments under static conditions using sand tanks and under simulated stream conditions using the Sediment Erosion Flume at Sandia-Carlsbad. Concurrently, we are designing, testing, and optimizing a remote-monitoring package, including photovoltaic (PV)/battery power, telemetry, Web-based data-management/-visualization, and analysis software. Later in the project we will investigate ways to miniaturize and minimize the cost of the monitoring system. In cooperation with the United States Geological Survey (USGS), we are conducting field-testing of the full TDR monitoring package on local perennial/ephemeral streams.

Water managers in New Mexico agree that stream gauging is one of the highest-priority issues in the state. Relative to current technology, the TDR system offers the advantage of real-time monitoring, concurrent water-quality/-quantity monitoring, and improved precision by way of multiprobe sampling, all at a reduced cost. As such, we believe that this monitoring technique has significant market potential, here and abroad, once fully developed.

We focused on acquiring sound, quantitative evidence demonstrating the ability of TDR to measure stream depth, depth of scour, sediment concentration, and salinity. We used a

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variety of field and laboratory experiments to meet this goal. Concurrent with this activity were efforts to begin designing the remote-monitoring package for the TDR.

- *Laboratory tank experiments.* We performed the first series of tests to characterize the base-line TDR system. This included measuring the input signal from the cable tester, the dielectric properties of the coaxial cable, and the dielectric mismatch between the cable and probe. We also checked the dielectric properties of key media, including deionized water, tap water, air, and saturated sand. We need data from these tests to model the TDR traces.

We then performed tests under static water conditions in small tanks in which the TDR probe was secured to the bottom. Experiments involved the sequential variation in depth of water around the probe, depth of sand (with the probe submerged in water), and concurrent variations in the depth of sand and water. We conducted tests using both deionized and tap water (i.e., varied the conductivity).

Results from these tests show very deliberate trends in the measured TDR traces. The shape of the traces varied according to the number of dielectric interfaces, relative depths of the interfaces, the dielectric properties of the media around the probe, and the conductivity of the fluid.

- *Laboratory flume experiments.* Carlsbad's Sediment Erosion Flume was modified so experiments could be conducted under free-surface conditions. In these tests we packed the TDR probe in a soil core and subjected it to erosion by sequentially lifting it into the flowing stream of water. We conducted tests under low (0.11 m/s), medium (0.21 m/s), and high (0.34 m/s) flowrates. We also conducted tests under conditions of a dynamic bedload (i.e., sediment introduced in the flume upstream of the probe). Results yielded similar trends in the TDR traces as measured under static conditions. This suggests that flow velocity does not have a significant impact on the TDR response.

- *Field experiments.* Prior to field-testing, we determined that longer probes would be needed and designed and constructed a 1 m-long probe. We constructed a larger tank and performed preliminary testing on the probe. We are also designing the stream channel anchor for the probe and modeling the stresses on the probe.

- *TDR trace modeling.* Key to the success of this project is the ability to extract stream data from the measured TDR traces. We use frequency-based analysis, pioneered in the electronics industry to model and interpret the traces (Heimovaara, 1994; Feng et al., 1999). In this analysis we

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model the probe as a composite of sections, with each section defined by a dielectric interface. We model the transfer function relating the input to output TDR signal section-by-section by considering the frequency-dependent dielectric properties of the medium, signal attenuation, and the reflection and transmission of the signal at each interface. We successfully implemented this multisectional model in MATLAB and are currently using it to model measured TDR traces in a forward sense.

- *Total system design.* We designed a base-line power system for the TDR system, comprising a 75 W PV module, sealed battery (4-day storage), charge controller, lightning arrestor, enclosure, connectors, and cables. The unit includes a free-standing 6 ft tripod mount onto which the PV, antenna (cell or satellite), and enclosures are attached. We also completed analysis of the data-transmission loads (remote system back to a data-collection and -storage point) for a variety of operating conditions. This analysis considered the transfer rate and the transmission costs associated with a variety of satellite and cellular phone options.

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Research and Development of Mathematical Algorithms to Define and Quantify Critical Infrastructure Interdependencies

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Reliable operation of infrastructures depends on the surety of other infrastructures. Those researching critical infrastructure surety need to understand and quantify infrastructure interdependencies. Research efforts to date aimed at quantifying infrastructure interdependencies centered on the identification of direct physical connections between particular components in one or more infrastructures. While a valid approach, it limits understanding to defined physical connections, requires valid datasets for each infrastructure, and requires constant updating of both the database and the connections as infrastructures change, which is exacerbated by the private, competitive nature of the majority of the nation's infrastructures.

Sandia proposes a three-tiered methodology founded in the development of mathematical algorithms that can be used to define the relationships among infrastructures. First, we utilize domain expertise to define obvious functional relationships within and among infrastructures. Second, we will apply available data against a series of functional forms to determine if perceived relationships can be properly defined. Finally, we will use learning methods to develop additional relationships. Once we develop algorithms, we will implement them in a series of generally accessible demonstration tools. We will perform verification and validation utilizing existing data and events to properly characterize uncertainty. This project will focus on the electric-power, natural-gas, oil, water, and communications infrastructures.

These algorithms constitute a transferable body of knowledge on infrastructure interdependencies, substantially increasing the accuracy and decreasing the analytical cost of infrastructure monitoring, assessment, and design. This method allows for inclusion of multiple and nonintuitive infrastructure connections. It reduces reliance on privately held infrastructure data. Further, it reduces the need to maintain and update physical configuration databases as infrastructures change. Once these algorithms are developed, they can be incorporated into current models, including indications and warning tools and agent-based simulation models.

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Research focused on two interrelated efforts. The first effort involved research toward extending understanding interdependencies between the electric-power and gas infrastructures at an aggregate level, through a thorough investigation of the literature and existing data sources for these infrastructures, as well as expert elicitation. The second area involved the development of graph-based models of interdependent infrastructures that are sufficiently detailed so as to effectively capture their evolving condition over time while maintaining computational tractability.

With respect to the existing literature, we conducted research to determine how performance is described from a mathematical perspective. This step defined a framework for describing infrastructure performance and interaction and for classifying infrastructure models. We found proposed indicators of the health of the power supply system and identified system sensitivities. The research identified diverse mathematical representations currently used in analyses of the electric-power infrastructure. No single existing formulation appears to capture all of the relevant dynamics of generation, transmission, distribution, and load. The majority of models identified represent the physical system, to the exclusion of operational decisions upon which service delivery is dependent. These insights provide vital information for the development of mathematical models in later research.

We gained insights into the performance of these infrastructures and identification of algorithmic relationships through exploration of available and regularly updated databases, facilitated by the development of a meta-database structure. We developed the database structure, containing critical meta-data on infrastructure datasets, including content structure and descriptions, data location, data-quality characterization, update frequency, and latency. We will link this database with (local and actual site) databases that will provide key input values for algorithm evaluation.

Expert elicitation on the infrastructures provided further value. Analysis of the timeliness of causal actions relative to system failures indicated two areas of potentially fruitful research in the electric-power infrastructure. Mathematical analysis of growing quantities of geospatial weather-incident data may aid understanding of the likelihood of damage to transmission and distribution assets, where current analysis of data requires direct input of system experts. Mathematical analysis of the relationship between supply and demand, especially given the accessibility to market-specific forecasts and data, provides the capability to understand the potential for

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and location of contingencies in interdependent infrastructures (such as natural gas) that are more substantial than the electric-power infrastructure's current description of single contingencies. We developed a similar supply-demand relationship for the natural-gas infrastructure, taking into account both the dependence of the infrastructure on electric power for transmission functions, such as pipeline compression, and the historically strong correlation between sectoral demand for natural gas and the price paid by residential customers.

With respect to the second area of effort, we developed a unified framework, based on graph theory, to model and analyze interdependent infrastructure networks over time. We based the framework on the following core ideas. Each network is represented with nodes and arcs. Uncertainty in capacity of each component in the infrastructure network is represented by probability distributions of arc capacity; these may be correlated due to geographic proximity and network topology. Interconnections between infrastructure networks can be represented through additional linking nodes and arcs and the use of correlation between arcs in different infrastructure networks. We can use a time-space network to represent the temporal evolution of these interdependent infrastructure networks, incorporating correlation in the capacity of arcs over time.

This framework, reusable for multiple infrastructures, provides both the central methodology needed to calculate probability distributions for satisfied demand and a basis to optimize investments. We developed a prototype, to which we will apply real-world case studies, that illustrates the types of insights that can be gained from an analysis of this character.

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38668

Functionalized Nanoelectrode Arrays for In Situ Identification and Quantification of Regulated Chemicals in Water

C. I. H. Ashby, M. J. Kelly, W. G. Yelton, K. B. Pfeifer, D. J. Muron, W. Einfeld, M. P. Siegal

Most chemical species that are currently regulated by the national water-quality standards and other compounds, such as endocrine disrupters, that are under consideration for regulation are redox-active species that can be identified and quantified by electrochemical techniques. Standard microelectrodes and even commercial nanoband electrodes require the addition of extra chemicals to condition the water before analysis and so are not useful for most real-time, in situ sampling. They require trained personnel and cannot be used either for distributed remote analysis in a water system or in a dipstick mode for on-site testing of drinking water. An array of suitably functionalized nanoelectrodes could be incorporated into a small, integrated sensor system that can identify many species rapidly and simultaneously under field conditions without chemical addition with signal-to-noise (S/N) up to 10^3 -fold greater than conventional electrodes. Sandia is investigating the use of carbon nanotubes (CNTs) and other conducting nanowires as sensor-array systems for rapid, noncontaminating field analysis. The chemical character of the nanotube or nanowire surfaces can provide chemical selectivity. Electrochemical deposition of a range of different metals and conducting polymers directly or to functionalize the nanotubes will produce different current/voltage relationships from electrode elements in the array as the analytes of interest are subjected to electrochemical analysis. Enhanced selectivity and sensitivity for specific metals, such as heavy-metal industrial pollutants and radioactive nuclides, can be conferred by electrodeposition of thin organic conducting polymers containing functional groups, such as crown ethers, that selectively bind and preconcentrate the metals of interest for redox sampling. We will also develop organic conducting polymers that can provide electrochemical signatures for organic and biochemical analytes that lack normal redox signatures, such as methyl tertiary butyl ether (MTBE) and halocarbons like trichloroethylene (TCE.)

We learned to precisely control the diameters of multiwall CNTs grown by thermal chemical vapor deposition (CVD). CNTs grown with this method are uniform in diameter ($< \pm 10\%$) both across the entire CNT array and within the lengths of

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individual tubes. Nanotube outer diameters, ranging from 3 to 350 nm, increase exponentially with growth temperature from 610° to 790°C. High-resolution transmission electron micrographs show that CNTs grown at < 630°C demonstrate long-range structural perfection in the nanotube walls, while CNTs grown at > 650°C have highly disordered nanocrystalline graphite walls surrounding a highly ordered innermost wall structure. Such a disordered wall structure will reduce electrical conductivity. Since highly conductive nanotubes may be most desirable for the purposes of this project, we will initially focus on CNTs grown at the lowest temperatures resulting in the smallest diameters (≤ 10 nm). This size is also very compatible with the 6–12 nm pore size in the alumina templates that will be used to control electrode spacing.

We made major progress developing anodized aluminum (Al) nanopores for CNT growth templates. In particular, we found that we could sputter-deposit neodymium (Nd)-doped Al onto substrates, using a niobium (Nb) adhesion layer, to result in nearly optically smooth Al coatings. Pure Al deposits as an extremely rough film. We showed that this Nd-doped Al anodizes very reliably and should lead to the ability to fabricate high-quality nanopore templates. We are also using the nanoporous alumina templates to control the direct deposition of metallic nanowires and of nanowires made of conducting polymers. Development of methods to precisely pattern and increase nanopore spacing by stress-indentation of the Al before anodization is in progress. The increased nanoelectrode separations possible through this approach should relax demands on measurement electronics speed to achieve optimum array performance and enable use of the nanoelectrode arrays with common commercial hardware.

We modified the goals of this project by expansion to include direct formation of metallic and conducting polymer nanowires as a simpler alternative to chemical modification of CNTs. We expect arrays of these materials to achieve many of the advantages proposed for the functionalized nanotubes. Using nanoporous templates made of both alumina and ion-track polymer membranes, we fabricated and tested gold (Au) nanoelectrode arrays with commercial hardware. Their performance is as expected at the sampling rates possible with commercial hardware designed to work with conventional macroplanar electrodes. A 10 nm Au nanowire electrode array operating under macroplanar diffusion conditions performed better than a conventional macroplanar Au electrode under the same conditions. Macroplanar and nanowire electrodes have also been formed by electrochemical deposition of poly-3-

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methyl thiophene on polished Al or in a nanoporous alumina template. Conducting-polymer nanowire arrays exhibit good working electrode behavior. We are now investigating the thermodynamics, kinetics, operating range, and stability of these arrays. To date, laboratory evaluations of these electrodes have been limited to pulsewidth domains that can not adequately evaluate their true performance potential. We are assembling hardware capable of shorter pulsewidths to test the performance of nanoelectrode arrays under radial diffusion conditions as required for optimum performance.

A novel integrated nanoelectrode array architecture has been invented that should permit greatly improved performance at the slower sampling rates achievable by many commercial instruments.

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Refereed

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38669

Hybrid Infrastructure Cryptography

M. D. Torgerson, W. D. Neumann, M. J. Collins, T. J. Draelos, D. R. Gallup, A. J. Lanzone

In resource-constrained environments, such as ad hoc wireless networks, existing cryptographic protocols are not suited to the security needs of the environment. Symmetric key protocols provide bandwidth and computationally efficient security solutions; however, they are difficult to manage and require an increased level of end-to-end security. Public-key protocols make key management in large networks possible, but they are computationally and bandwidth intensive, plus they require a large support structure to operate. Diffie-Helman-type key exchange algorithms are an attempt to bridge the gap between public and symmetric key techniques. These types of key exchange algorithms are orders of magnitude too slow to use in a dynamic environment. No cryptographic technology currently exists that is able to provide scalable, real-time security for large dynamic networks.

Sandia is investigating the possibility of merging the two types of protocols to provide a new type of cryptographic infrastructure that strikes a balance between the two extremes. The new architecture will provide computationally and bandwidth-efficient methods of authentication and key exchange, and will be manageable when compared to traditional symmetric key infrastructures. Our work has direct application in distributed trust models and will have far-reaching implications in all types of resource-constrained communications. In particular, the ideas have applicability for providing inexpensive cryptographic solutions for certain subsystems of the real-time control networks. Also, the methods support application to current and proposed advanced research efforts at Sandia in the area of securing dynamic wireless networks.

Our efforts to combine public-key and symmetric-key cryptographic protocols led to a number of notable discoveries. These discoveries have already produced one technical advance.

- We developed a new method of speeding up existing discreet log-type digital signatures and key exchange algorithms. The method yields a speed-up factor of more than 8 for a standard implementation of a digital signal algorithm (DSA)-type signature. The new method requires almost no secure storage as compared to possibly tens of thousands of bytes for competing methods. The method has been

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incorporated into the hardware design of a Sandia-developed low-power authentication chip. It has also been incorporated into Sandia's Cryptographic Library, and a TA was filed.

- We developed an efficient method of extending one-time public-key signatures to r -time signature schemes without the reduction in security typically noted with such extensions. These public-key signatures are nearly as efficient as typical symmetric-key signatures. (An r -time public-key signature scheme allows the signer to pass out public information that can be used by anyone in the future to authenticate a single, as of yet undetermined message to be sent by the signer, and r messages can be authenticated before new signature information needs to be passed out.)

- Due to our examination of various simple networks and their trust requirements, we developed a method of obtaining efficient private channels within a private network, which led to the development of a new provably secure, highly efficient cipher and mode of operation. Together these have particular applicability for real-time control systems where many communications are aggregated to a single point.

- We made significant progress on the implementation of a network-modeling tool that will allow testing and comparison of various security algorithms in various network models.

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38672

Validated Modeling of Distributed-Energy Resources at Distribution Voltages

M. E. Ralph, J. D. Boyes, J. W. Stevens, III, J. W. Ginn, S. Gonzalez

Lack of validated models of distributed-energy resources (DER) is a significant barrier to their deployment. To date, the impact of aggregated DER has been modeled primarily on transmission systems. However, sources that are presently being commercialized and those in the foreseeable future will operate at low voltage and connect via transformers to local distribution systems. In this project, Sandia will develop and experimentally validate models of transient and steady-state source behavior for incorporation into utility distribution analysis tools. Development of these models has not been prioritized either by the distributed-generation industry or by the inverter industry.

The technical challenge is that although the electrical behavior of rotating machines such as diesel generators has been well characterized, no utility-compatible models are available for power-electronics inverters. Inverters are the utility interface for microturbines, fuel cells, photovoltaic (PV) inverters, variable-frequency wind generators, and virtually any system using electrical-energy storage.

We selected the Xantrex PV 20208 inverter as the first DER to be modeled. This 20 kW grid-tied PV inverter is a mature, commercially available product, one of which is presently generating power at Sandia's Distributed Energy Technologies Lab (DETL).

A goal of the project is to incorporate the new DER models into software tools presently used by utilities for distribution-system planning.

We simulated the operation of the PV 20208 inverter at Sandia using PSCAD. Model features included voltage and current regulation, semiconductor-switch firing controls, the modulation scheme used to generate a sinusoidal output, and voltage shifting for detection of islanding. We obtained the inverter and installed it at DETL. We developed a model of the DETL power grid for use in distribution system simulations. Because transformer characteristics can dominate local grid impedance, we began analysis and testing of distribution transformers. We recorded nonlinear load data at a local commercial data center.

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Water Desalination

*T. E. Hinkebein, L. Evans, J. E. Miller, J. A. Voigt, T. M. Nenoff,
J. L. Krumhansl*

The world's water supply is finite and too small to meet our future needs. Desalination is one way to increase water supplies. Sandia's in situ crystallization team is focused on the removal of salt from inland groundwater, primarily brackish water. We hope to develop methods that use conventional municipal water-treatment facilities. Success will avoid the costly need for planning and building desalination plants, facilities, and disposal units. The scientific concept behind our project is to use precipitation and/or ion exchange of inorganic compounds at near-environmental water conditions. The materials developed in this project will be low cost and environmentally friendly. To achieve this objective, we are (1) scientifically searching for energetically favorable methods for removing the salts, and (2) interested in developing materials that upon disposal will have low leach rates for disposal in landfills or can be recycled upon demand.

We are also focusing on the removal of salt from saline waters through the use of forward osmosis (FO) and a designer solute. By focusing on the use of FO to remove salt from the water, two important drawbacks associated with reverse osmosis (RO) may be avoided: high-pressure costs and membrane fouling. The FO process is predicated on the identification of a designer solute. This material must provide a high osmotic potential and be compatible with the chosen membrane. The membrane for our process must meet three criteria. It must be nonreactive with the osmotic agent, it must be stable at the temperature of the osmotic agent, and the flux across the membrane must be maximized, preferably with near 100% selectivity.

- *In situ crystallization.* Accomplishments include literature searches, and studying phosphate cation getters, clay anion getters, material characterization, and sodium/chloride (Na/Cl) adsorption studies. We continue working on the economic feasibility of desal with these materials.

- *Chlorine getters.* We focused our efforts on hydrotalcite (HTC) two-dimensional (2-D) clays. These materials crystallize rapidly through precipitation at room temperature and are easily anion-exchangeable. The process has two paths. First, the HTC is synthesized hydrothermally, then thermally treated to intermediate "amorphous" plates. The intermediate phase is then introduced to the Cl-containing solution and reformed into

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layered Cl-HTC. We can use the Cl-HTC in two additional ways: (1) it can be reheat-treated, eliminating the chlorine as a side product and regenerating the “amorphous” intermediate HTC phase, or (2) heat-treat the entire Cl-HTC, which collapses the layered material into leach-free ceramic. Chlorine can be recovered as off-gas hydrochloric acid (HCl). Second, the HTC is synthesized in bulk. The material is introduced to the Cl-containing solution. At room temperature, an *in situ* anion exchange occurs, resulting in the Cl-HTC.

- *Sodium getters.* We focused our efforts on zeolites and successfully synthesized the zeolite sodalite-analog at 70°C in a few hours from saltwater. This initial preparation method required that we modify the reaction pH with the addition of sodium hydroxide (NaOH) (to balance the NaCl) addition. Subsequent reaction preps included variation of zinc and phosphate sources to increase the initial pH, without the addition of NaOH base, but still using NaCl. The results have been very promising. Under this method, we continue to synthesize the Zn-SOD (superoxide dismutase), which captures the Na cations, but mixed with an inert layered $\text{Zn}_3(\text{PO}_4)_2 \cdot 4\text{H}_2\text{O}$ phase (as determined by x-ray powder diffraction).

- *New perspective for water desalination and purification.* There are strict demands on the designer solute. It must be nontoxic and easily recoverable. In addition, it must have solubility that approaches zero under near-ambient conditions of temperature and pressure. It must provide a high osmotic potential. Finally, the solute must be compatible with the chosen membrane. We identified and tested a number of salts and identified a likely candidate. Efforts may be required to optimize a membrane for compatibility.

Economic evaluations began with establishing the cost and energy requirements for the current technologies. The theoretical minimum for seawater desalination is 3–4 kJ/kg RO, typically consuming about 20 kJ/kg freshwater of electrical energy. The cost of seawater RO is typically near \$4 per 1000 gallons. For seawater RO, energy and pretreatment can be major contributors to the total cost. For brackish water, fixed costs dominate. Given the opportunity for energy and pretreatment savings, the best opportunity for our process lies in treating seawater.

The energy requirement of FO is determined by two factors: the concentration of the designer solute exiting the contactor and the thermodynamics of the separation process. For our best candidate, we calculated that the minimum energy required for

We focused our efforts on zeolites and successfully synthesized the zeolite sodalite-analog at 70°C in a few hours from saltwater. ... The results have been very promising.

the separation is 6.5 kJ/kg water transferred across the membrane.

The membrane for our process must be nonreactive with the solute. It must be stable at the temperature of the osmotic agent, and the flux across the membrane must be maximized, preferably with near 100% selectivity. There are at least three potential membrane types: (1) microporous hydrophobic membranes (which tend to be lower flux, but selectivity is high), (2) RO membranes (limited flux), and (3) new membranes specifically designed for the direct osmosis (DO) process (fluxes can be maximized up to 20 l/hrm², while maintaining the desired selectivity). Currently, we have assembled a test apparatus and evaluated membranes of each type from various manufacturers with our best candidate for an osmotic agent.

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Refereed

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38674

Revolutionary Systems for Catalytic Combustion and Diesel Catalytic Particulate Traps

J. Cesarano, III, P. O. Witze, J. E. Miller, J. N. Stuecker, T. J. Gardner, P. R. Schunk

Diesel-particulate emission (soot) is a global problem, but current technologies for meeting looming regulations are costly and failure-prone. Nitrous oxide (NO_x) formation from methane (CH_4) combustion in electric power plants is also an environmental concern, but materials and catalyst-reliability issues have prevented the application of catalytic combustors that circumvent NO_x formation. Sandia proposes to utilize a commercially viable, scalable, direct ceramic-fabrication technique as a basis for creating revolutionary systems for diesel-particulate trapping and destruction, and catalytic CH_4 combustion. Traditional fabrication techniques are limited to producing “honeycomb”-structured extrudates and foams. Our technique is not only more flexible in terms of the shape of the ceramic product, but also allows a broader range of materials (and catalysts) to be used.

Our design is a three-dimensional (3-D) cross-hatched mesh, formed from alternating layers of precisely spaced rods (similar to “Lincoln logs”). Direct fabrication inherently ensures that the rods meld together and form a strong bond upon sintering. The sintered meshes will have controlled porosity in three dimensions, but no line-of-sight (LOS) pathways. This macrostructure ensures adequate tortuosity and a high-surface-to-volume ratio while maintaining predictable permeability and low-pressure drop. The incorporation of, or fabrication from, a catalytically active material will allow efficient combustion of CH_4 without NO_x formation. Similarly, the structures will trap soot particles that will then be catalytically combusted, thereby extending the life of the trap indefinitely.

Research challenges include efficient particle-trapping with low-pressure drop, catalyst design for severe combustion environments, mechanical and chemical stability, flow and filtration simulation for optimizing designs, and real-time performance characterization. Our expertise in ceramic processing, catalysis, engine diagnostics, and modeling uniquely positions us to overcome these challenges to create “real-world” systems with broad impact in clean-energy utilization.

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Preliminary results for our catalytic supports show increased catalytic activity when compared to commercial supports. We wrote a technical advance.

Objectives were to develop simple lattice structures with utility for CH_4 combustion, compare the structures to commercial products, and model the flow properties of our structures. First, we selected materials that could be useful in the catalytic combustion of CH_4 . After a comprehensive literature search, we decided to use aluminum oxide (Al_2O_3) as the catalyst-support material and barium/manganese (Ba/Mn) hexaaluminate powder as the catalyst. Al_2O_3 powder was made into pastes and robocasted into 3-D meshes of cross-hatched lattices of rods. We modeled the lattices and analyzed and compared simulations of flowing CH_4 through them to commercial cordierite honeycomb catalyst supports. Simulations suggest that lattice structures induce more turbulence into the gas stream than standard honeycomb. Model structures were fabricated, coated with a catalyst, calcined, and characterized to determine if more turbulence results in higher catalytic activity. We fabricated honeycombs and lattices with the same surface area per unit length. Additionally, the structures had the same mass of catalyst wash-coated onto their surfaces. We flowed a 3% CH_4 gas through the lattice and honeycomb structures and measured the combustion of CH_4 as a function of temperature. Amazingly, the lattice structure improved the combustion of CH_4 15 times at 600°C . To reach the same level of conversion, a honeycomb support needed four times the amount of catalyst applied to its surfaces. We are extremely excited about these results. Our lattice structures may lead to products that improve the combustion of CH_4 while reducing the amount of catalyst necessary and reducing the amount of NO_x formation.

In preparation for the next phase of the project, i.e., fabrication and testing of diesel-particulate traps, we successfully set up a diesel engine with diagnostics for soot particles and pressure drop. We successfully characterized the performance of a commercial diesel particulate trap and have a benchmark to be used for future comparisons.

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Other Communications

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38677

Potential Application of Microsensor Technology in Radioactive-Waste Management—with Emphasis on Headspace Gas Detection

Y. Wang, C. K. Ho, P. I. Pohl, R. C. Hughes, M. L. Thomas, C. R. Bryan, H. Gao

Measurements of headspace gas in waste containers or in waste-disposal facilities are generally required for the demonstration of compliance with Resource Conservation and Recovery Act (1976) (RCRA) or transportation requirements, as well as for an operational safety concern. The existing methods for such measurements are time-consuming and expensive, and increase worker's exposure to hazardous environments. Therefore, a reliable, real-time, in situ gas-detection technique is highly desirable. We expect that Sandia-developed H_2 and volatile organic compound (VOC) microsensors with appropriate further development and adaptation will have a wide range of applications in radioactive-waste management. We propose the following work: (1) test the long-term stability of both H_2 and VOC microsensors and make necessary improvements, (2) optimize the ability of VOC microsensors for the discrimination of individual VOCs that are present in transuranic wastes, and (3) study the feasibility of using microsensors as a screening tool to discriminate two populations of waste drums according to a prespecified total VOC concentration limit. One outcome of this work is a set of microsensors specifically adapted to waste characterization and monitoring. Success in the work could lead to large-scale deployment of these sensors across the Department of Energy waste-generator sites and waste-storage/-disposal facilities. The work will greatly enhance Sandia's expertise in nuclear-waste management by leveraging Sandia's strength in microsensor development; it will highly impact the investment area of monitoring systems.

(1) We concluded an extensive literature review on the existing procedures and requirements for headspace gas sampling and analysis in waste characterization and monitoring. We identified the most relevant gaseous species in transuranic wastes and constrained their typical concentration ranges and regulatory limits as compared to the detection limits of microsensors. We also defined the relevant physiochemical conditions for microsensor testing.

(2) We tested the performance of H2SCAN™ hydrogen (H_2) sensors in the presence of interfering VOCs. We found that the

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presence of these VOCs does have an effect on the H concentration readings of the sensor and that the increase in the reading seems independent of VOC concentrations. This effect is probably caused by the inhibition of the catalytic reaction of H with oxygen (O) on the surface of the sensor's palladium-nickel (Pd/Ni) film.

(3) We conducted a long-term stability test for a VOC sensor loaded with four sensing polymers (poly(isobutylene) [PIB], polyepichlorohydrin [PECH], poly(ethylene-vinyl acetate) [PEVA], and poly(N-vinyl 2-pyrrolidone [PNVP]). We observed a significant drift in the response signals from PIB, PECH, and PEVA.

(4) We initiated a molecular-modeling activity to study interactions of VOCs with sensing polymers and identified the appropriate modeling tools.

(5) We put in place an experimental setup for testing VOC sensors in the Sandia-Carlsbad Laboratory and tested the responses of four sensing polymers (PIB, PECH, PEVA, and PNVP) to temperature changes. We observed nonlinear response.

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38678

Surety Enhancement for Wireless Automated-Control Networks

W. F. Young, M. D. Torgerson, E. L. Witzke, J. M. Depoy, D. P. Duggan, M. J. Berg, M. D. Murphy

Sandia originally focused on developing secure network architectures for process control systems (PCS) utilized by off-shore oil-drilling platforms. However, the terrorist attacks of September 11 quickly moved security of critical infrastructure (CI) elements such as the water and electric-power utilities to the forefront. Cyber assessments of these CI elements pointed to the urgency in correcting security problems in current PCS that include a combination of wired and wireless segments, as well pending PCS implementations. To meet these immediate security challenges, we modified the direction of this project to focus primarily on these types of control systems. The modification required was not extreme, and the changes mainly centered on the particular type of PCS instantiations used for case studies in the research.

Initial work consisted primarily of vulnerability analysis, identification of key characteristics of relevant PCS architectures, operating network (OPNET) model development, and vulnerability validation in the OPNET environment. The goal was to study the vulnerabilities created by the use of wireless communications in the modern PCS environment. This will allow the development of architectural mitigation strategies, which will be validated in the OPNET modeling environment in upcoming work. The end result will be architectural security improvements, dictated by an information assurance (IA) perspective, for modern PCS. These IA-based solutions are vital to the nation's CI.

One milestone, the development of representative system architecture, underwent some slight direction changes and is nearly complete. There are two baseline models, one based on a modern water-treatment PCS and another on a wind-power-generation PCS. Results and findings from ongoing assessment efforts are also guiding these models.

Another milestone resulted in the decision to focus primarily on Internet Protocol (IP)-based networks, with wireless asynchronous transfer mode (ATM) receiving some attention due to the natural extension of ATM security solutions to switched IP-based networks, such as Multiprotocol Label Switching (MPLS). Investigation into the hybrid wired/wireless process control networks either currently utilized or scheduled

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for implementation identifies the increasing use of IP/transmission control protocol (TCP) and mobile IP in modern PCS. The research into vulnerabilities and solutions in wireless ATM networks led to a submission at the ATM Wireless Working Group on the topic of label-based security in the mobile environment. The security implications of the topic directly relate to the emerging MPLS protocol.

The milestone on vulnerability analysis of interaction between wired/wireless links utilized the Information Design Assurance Red Team (IDART) Methodology to discover vulnerabilities in hybrid wired/wireless communication systems. The quick-look portion of vulnerabilities in wireless networking is basically finished. The use of the IDART Methodology represents a key accomplishment of this activity in that this is the first application focused on discovering wireless vulnerabilities. The validation and relative ranking of vulnerabilities are basically complete.

The development of an OPNET model for the wind-power-generation architecture is substantially complete. Within the modeling environment, we incorporated the ability to replicate wireless attacks. This will support analysis of proposed secure architectures during upcoming work.

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38679

Advanced Nuclear-Engineering Analysis Technology

M. F. Young, R. O. Gauntt, V. J. Romero, K. K. Murata

This effort focused on applying Accelerated Strategic Computing Initiative (ASCI) technology developed for the analysis of weapons systems to the state-of-the-art accident analysis of a nuclear reactor system. The Sandia SIERRA parallel computing platform for ASCI codes includes high-fidelity thermal, fluids, and structural codes whose coupling through SIERRA can be tailored specifically to the particular problem at hand to analyze complex multiphysics problems. Presently, however, the suite lacks several physics modules unique to the analysis of nuclear reactors. The Nuclear Regulatory Commission (NRC) MELCOR code, not presently part of SIERRA, was developed to analyze severe accidents in present-technology reactor systems. We will (1) evaluate the SIERRA code suite for its current applicability to the analysis of next-generation nuclear reactors and the feasibility of implementing MELCOR models into the SIERRA suite, (2) augment SIERRA models and integrate the MELCOR code, or portions thereof, into SIERRA as needed to address physics particular to nuclear-reactor issues, especially those facing next-generation reactor designs, and (3) apply the SIERRA framework to a demonstration problem involving a nuclear-reactor system. Completion of this research would demonstrate the feasibility of performing high-fidelity, rapid analyses of safety and design issues needed to support the development of next-generation power-reactor systems.

We evaluated possible demonstration test problems with regard to the physical quantities that would be coupled between MELCOR and the high-fidelity code(s), and at what fidelity (finite-element [FE] node, surface set, etc.). The evaluated problems included the following:

- (1) *Lower-head molten pool with crust formation.* This problem would use MELCOR to set up the initial and boundary conditions (BCs) of a molten pool and GOMA (predecessor of ARIA) to calculate convection and heat transfer in the pool.
- (2) *Pressurized thermal shock (PTS).* This would use MELCOR for thermal conditions in the vessel and two-phase flow of the coolant, and PRESTO for the structural response of the vessel break.
- (3) *Reactor-fuel pool accident.* This would use MELCOR for the fuel-pin behavior, including temperature and clad

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oxidation rates. FUEGO would provide convective gas flow using the fuel-pin temperatures and clad oxidation rates as BCs.

(4) *Heat transfer and convective flow around pebble bed reactor fuel.* MELCOR would provide overall system conditions; CALORE and FUEGO would calculate the coolant flow and fuel temperature.

We reviewed several technologies for use in coupling MELCOR and ASCI (Accelerated Strategic Computing Initiative) codes. The most promising method is to use the DAKOTA (Design Analysis Kit for Optimization and Terascale Applications) executive code. We can use DAKOTA to control MELCOR and ASCI codes together, plus synchronize the code coupling. Transfer of parameters from MELCOR to ASCI codes would most likely be done via user functions in the ASCI codes.

Another method would be to use ENTERO, a system-simulation environment project currently under development. This option would be used in conjunction with DRM (Distributed Resource Management) to use JANUS, or could be used alone if networked workstations were used as the computing platforms. Parallel virtual machine (PVM) is also a solution for machines other than JANUS (JANUS does not run PVM). We evaluated a PVM application coupling MELCOR and RELAP5, a finite-difference high-fidelity reactor code. The coupling was facilitated by use of an executive program to control the PVM master and remotes on different networked machines.

We evaluated the National Aeronautics and Space Administration (NASA) Numerical Propulsion System Simulation Project for ideas and pitfalls. This system is discussed in two papers: "Implementing Monitoring and Zooming in a Heterogeneous Distributed Jet Engine Simulation," by Abdollah Afjeh *et al.*, and "Distributed and Parallel Programming in Support of Zooming in Numerical Propulsion System Simulation," by John A. Reed and Abdollah Afjeh. The papers discuss the problems associated with coupling multifidelity models of flowfields. One major conclusion is that coupled flowfields can be numerically unstable. This suggests that coupling MELCOR and ASCI-generated flowfields is not a good idea for a first test problem and that using a single flowfield from one or the other is an easier approach. The flowfield could then be coupled to other physics models, such as heat transfer or structural response, without as much danger of causing numerical instability.

We evaluated GOMA models for application to the molten pool problem. In discussions with GOMA developers, we

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discovered that there are currently no eutectics in GOMA. This would mean that the very rudimentary eutectics model in MELCOR would have to be coupled to GOMA at the GOMA cell level. Coupling a property routine from MELCOR into an ASCII code using tight coupling is not a first choice for a demo problem, as this approach does not use much of MELCOR's capabilities and amounts to adding property routines to GOMA.

We evaluated FUEGO models for application to the fuel pool problem. This is the most likely candidate for a demonstration problem. We are still evaluating the problem as to what the best coupling method would be. We would transfer parameters from MELCOR to FUEGO via user functions in FUEGO.

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38681

Identification of Chemical Plumes: Range-Resolved IR Lidar Enabled by New Photonic Technologies

T. J. Kulp, R. P. Bambha, S. E. Bisson, D. A. V. Kliner

The need to search an area for chemical emissions is shared by several Sandia strategic business units. Buried facilities can be revealed when they release effluents. Similarly, rapid sensing of gas leaks produced in natural-gas transmission is key to protection of critical infrastructures (CIs).

Sandia proposed technology to fundamentally advance laser remote sensing of chemical plumes in the infrared (IR), where most species absorb at characteristic wavelengths. Range-resolved IR LIDAR (light detection and ranging), using the atmosphere as the backscattering medium, has been difficult because of poor-quality detectors and low atmospheric-scattering cross-sections. These limitations forced the use of topographic backscatter, where the ground serves as a reflector. This method measures only the path-integrated absorption in the atmosphere and suffers from large systematic noise due to laser speckle and variations in surface reflectivity.

We will develop and demonstrate a miniature, range-resolved IR LIDAR. We will develop a novel upconverting detector to shift the frequency of IR signal photons to the visible, where they can be detected with far greater sensitivity. Both the laser transmitter and the upconverter will be enabled by new quasi-phase-matched (QPM) nonlinear materials, which exhibit much higher nonlinearity than standard materials, and by high-power fiber amplifiers. The upconverter can also serve as a high-sensitivity detector for space applications (nonproliferation and materials control [NP&MC]). Moreover, fiber-amplifier and QPM-material development will contribute significantly to emerging threats initiatives.

Our accomplishments fall into two categories:

(1) development of components for an upconverter-based LIDAR system, and (2) development of in-house capabilities to fabricate QPM materials and rare-earth (RE)-doped fiber amplifiers.

- *Upconverting LIDAR development.* We modeled the upconverting detector using the nonlinear optics code SNLO, which showed that a quantum efficiency of 50% in converting 3057 nm light to 789 nm is attainable with a pump power of 70 W. We thus determined that a resonant cavity should be used to build up the intracrystal pump power to the appropriate level.

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We procured the components for a resonant upconverter, including mirrors for a bowtie-ring cavity coated to resonate the pump wave, beam-formatting optics, electronics to control the cavity resonance, and coatings for the periodically poled lithium-niobate (PPLN) crystals. The required PPLN crystals were poled by Sandia personnel at Wright-Patterson Air Force Base (WPAFB).

To demonstrate resonant enhancement of a mixing process, we carried out resonantly enhanced difference frequency generation using existing components. We observed an enhancement of 340 with a cavity designed to have an enhancement of ~ 37 . We are now assembling the resonant upconverting cavity, and evaluation of its performance will take place soon.

We procured the components for the transmitter. The transmitter is a Nd:YAG (neodymium:yttrium aluminum garnet [laser])–pumped optical parametric generator (OPG) seeded by a diode laser. Procured items include a PPLN crystal and oven, a diode seed laser, and optics. The PPLN crystal is poled to generate light near 3057 nm, corresponding to a strong methane absorption. We will use an available Nd:YAG pump laser.

We tested the transmitter and found it to generate $\sim 10\%$ conversion from the pump to the mid-IR (in accord with theory), yielding $\sim 10 \mu\text{J}$ (sufficient to test a portable upconverting LIDAR).

- *Component development: fiber amplifiers.* Fiber development focused on bringing the capability to manufacture fiber amplifiers in house. This fabrication typically entails several steps:

- (1) *Fiber characterization:* measurement of the fiber absorption spectrum, birefringence, size/shape of the inner cladding, and mode-field diameter.

- (2) *Splicing single-mode pigtails to the ends of the gain fiber.*

- (3) *Termination of the fiber ends:* splicing of fused-silica beam expanders to prevent optical damage and feedback, connectorization, and angle-polishing of the ends, and optical inspection.

- (4) *Preparation of the fiber for side pumping:* polishing a groove in the inner cladding and epoxying a micromirror into the groove.

- (5) *Alignment of a pump diode to launch light into the fiber via reflection from the micromirror and immobilization of the diode-fiber assembly.*

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(6) *Packaging*: may include temperature regulation of the pump diode(s), fabrication of the enclosure, assembly and testing of the drive electronics, and thermal management.

(7) *Characterization of the amplifier performance*: measurement of the output power, slope efficiency, linewidth, stability, tuning range, polarization extinction ratio, and threshold power for the onset of nonlinear processes.

We recently completed construction of a new laboratory for fiber-amplifier development, and we are currently setting up the above capabilities in this space. Of the above steps, 1–3 and 7 are now in house and routinely used; portions of the other steps are also set up.

We continued our collaboration with the Naval Research Laboratory, which resulted in two papers, one conference proceeding, and two patent applications in the past year.

- *QPM material development*. Through collaboration with the University of Dayton and WPAFB, Sandia personnel were trained in E-field poling to generate PPLN and other QPM materials. This process involves (1) photolithographic mask layout and procurement, (2) spin-coating, exposure, and development of the photoresist on the lithium-niobate (LN) wafer, (3) E-field poling of the wafer, and (4) wafer dicing and polishing. The training yielded useful PPLN crystals for this project. We procured the components for the in-house PPLN-poling facility.

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44601

High-Level Decision-Support Framework for Critical-Infrastructure Protection Prioritization

A. B. Baker, G. V. Herrera, E. K. Webb, A. K. Moonka, R. E. Hutchison, G. D. Wyss, P. K. Falcone, M. L. Swinson, W. C. Hines, T. D. Woodall, J. M. Harris

Critical infrastructures underpin the domestic security, health, safety, and economic well-being of the U.S. They are large, widely dispersed, mostly privately owned systems operated under a mixture of federal, state, and local government departments, laws, and regulations. While there currently are enormous pressures to secure all aspects of all critical infrastructures immediately, budget realities limit available options.

Sandia's purpose in this project is to provide a clear framework for systematically analyzing and prioritizing resources to most effectively secure U.S. critical infrastructures from terrorist threats. It is to be a scalable framework (based on the interplay of consequences, threats, and vulnerabilities) that can be applied at the highest national level, the component level of an individual infrastructure, or anywhere in between. This study will also provide a set of key findings and a recommended approach for framework application. In addition, this study will develop three laptop computer-based tools to assist with framework implementation—a risk-assessment credibility tool, a notional risk-prioritization tool, and a county-prioritization tool.

We developed a framework for systematically analyzing and prioritizing resources to most effectively secure U.S. critical infrastructures from terrorist threats. It is a scalable framework, based on the interplay of consequences, threats, and vulnerabilities, that can be applied at the highest national level, the component level of an individual infrastructure, or anywhere in between. The framework involves consideration of assets to be secured, the consequences that flow from those assets not being secured, the threats to those assets, and the vulnerability of those assets to threats. The systematic assessment and combination of these inputs within and across critical infrastructures can provide consistent risk measures (characterization of expected losses or expected costs) from potential adversary activities. We can then relatively rank and prioritize these risk measures for improving their security. The process for such risk reduction involves cost-effective consideration of reducing consequences, threats, and vulnerabilities. In the course of this study we found that threat

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effectiveness and innovation among U.S. adversaries appear to be increasing, raising the threat threshold and requiring evolving concepts of threat reduction. At the same time, the complexity of U.S. infrastructure ownership and responsibility makes system-security prioritization extremely difficult. This ownership and responsibility spans all levels of both the public and private sectors, although the vast majority of U.S. critical infrastructure is privately owned. While critical-infrastructure owners are also responsible for infrastructure design, operation, and security, they currently receive relatively limited access to threat information that would affect the security of their specific infrastructures. The siting and operation of their infrastructures also are affected by a jurisdictional patchwork of federal, state, and local laws and regulations, most of which have not been evaluated for their impact on security from terrorist threat.

This study also provided a set of key findings and a recommended approach for framework application. In addition, the study developed three laptop computer-based tools to assist with framework implementation—a risk-assessment credibility tool, a national risk-prioritization tool, and a county-prioritization tool. We based this study's tools and insights on Sandia's many years of experience in risk, consequence, threat, and vulnerability assessments, both in defense– and critical-infrastructure–related areas.

We presented the results and conclusions of this study to the Sandia Laboratory Leadership Team and the National Security Advisory Panel and transmitted them to the Office of Homeland Security.

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44774

Dynamic-Simulation Model of the National Security Consequences

A. B. Baker, T. E. Drennen, D. L. Harris, O. H. Paananen

The main objective of this project is to develop a high-level dynamic-simulation model that would allow policy makers and their staffs to explore the national security (NS) consequences of major U.S. energy-supply disruptions and to do so in a way that also would allow consideration of the energy-policy implications for U.S. greenhouse-gas emissions. This new model is based on Sandia's U.S. Energy and Greenhouse Gas Model (USEGM) and adds the capability to assess the potential economic impacts of energy disruptions and associated NS issues.

The U.S. Energy Security Model (USESM) is designed for use as a learning tool in considering alternative U.S. energy-policy options in response to energy disruptions in the U.S. economy. Energy disruptions using the USESM will impact gross domestic product (GDP), employment, and greenhouse-gas emissions under different scenarios. USESM is designed to complement rather than substitute for or duplicate existing complex models, allowing users to explore "what-if"-type energy, economic, and environmental questions in real time. In addition to energy-disruption impacts, the model allows analysis of policy options that affect overall energy demand, choice of fuel mix, electric power supply portfolios, and resulting U.S. carbon emissions. Detailed, complex models, such as the National Energy Modeling System (NEMS) used by the Energy Information Administration (EIA) of the Department of Energy, provide a framework for such analysis. However, the complexity of those existing models makes it difficult to quickly interpret the model results or to perform real-time evaluations of policy options.

The USESM combines two problem-solving paradigms—dynamic simulation and input/output (I/O) analysis—into one tool. In this way the USESM can alter both the demand and supply sides of the energy-consumption equation and provide an easy-to-use interface for policy makers.

We researched the issues and literature involved with the concept of energy security and determined, for modeling purposes, that changes in GDP due to a change in energy supply or consumption is the measure of energy security.

The USESM is an extension of the USEGM. This project successfully converted the USEGM from one software platform

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to another, PowerSim Constructor to PowerSim Studio, to take advantage of features in the latter.

The USESM successfully combined the modeling paradigms of dynamic modeling, using a system dynamics tool, and I/O analysis as defined by the economist Wassily Leontief. This combination is done within PowerSim Studio 2001 and now serves as a reusable template for both supply and demand issues related to energy in the U.S. economy. The I/O model is disaggregated to 55 economic sectors as defined by the IMPLAN (PC-based economic analysis system) U.S. dataset for 1999. It permits an examination of energy consumption and employment at that level of disaggregation.

The combination of I/O and dynamic simulation permits a policy maker to view the disaggregated consequences of disruptions in energy supply for several fuels using I/O. That disruption is passed to the dynamic simulation to propagate changes to the GDP. These changes can then be passed back to the I/O module to complete the cycle.

In a broader context, the successful inclusion of I/O into a dynamic-simulation model opens the possibilities for other types of analysis, specifically for issues relating to critical infrastructure.

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46072

Electricity-Generation Production Cost Model*T. E. Drennen*

Sandia seeks to develop a dynamic simulation model that calculates electricity production costs (in cents per kWh) for a wide variety of generating technologies and under a wide range of technology and policy scenarios. Electricity production costs are dependent on a number of key factors, including operating capacity, capital costs, operation and maintenance costs, fuel costs, interest rates, expected years of operation, and expected years needed for plant siting. The model interface will mimic that of Sandia's highly successful U.S. Energy and Greenhouse Gas Model (USEGM), allowing the user to quickly explore the sensitivity of the key variables. The user will be able to compare production costs at any specific capacity factor. Such a capability would permit more effective utilization of scarce federal electricity research and development (R&D) funding as well as development of alternative electricity options for defense and civilian use. We could then examine several types of questions. Under what conditions can nuclear power compete economically with gas combined-cycle plants—does it take \$5 per Mbtu gas and installed capacity costs of less than \$1500 per kW? Or, what would be the required capital costs (and/or capacity utilization with storage) for solar photovoltaic (PV) modules to compete with pulverized coal facilities?

Likely users of this model include executives and staff in the Congress, the Administration, and private industry (power-plant builders, industrial electricity users, and electric utilities). The model will improve understanding of the economic viability of various generating technologies and possibly their emissions tradeoffs. As such, it may help direct R&D toward developing more cost-effective, environmentally friendly electricity-generation sources. Collaboration with one or more private-sector power-plant builders may be sought to make this model a widely used, state-of-the-art, generation cost-modeling tool.

The overall accomplishment is the completion of the Electricity Generation Cost-Simulation Model (GENSim). Once we complete the final report, we will submit the model for copyright and widely show and distribute it as a policy tool. Initial reviews of the draft versions of the model are quite positive. The great thing about this model is the ease with which one can show policy makers and other interested parties the key assumptions behind calculating levelized costs for future electricity-generating plants. The model allows a wide variety of sensitivity and externality analysis.

The user can compare the likely costs based on two different sources of data—one governmental and the other from industry.

Sandia seeks to develop a dynamic simulation model that calculates electricity production costs (in cents per kWh) for a wide variety of generating technologies and under a wide range of technology and policy scenarios. ...The user will be able to compare production costs at any specific capacity factor. Such a capability would permit more effective utilization of scarce federal electricity research and development (R&D) funding as well as development of alternative electricity options for defense and civilian use. ...The model will improve understanding of the economic viability of various generating technologies and possibly their emissions tradeoffs. As such, it may help direct R&D toward developing more cost-effective, environmentally friendly electricity-generation sources. ...The overall accomplishment is the completion of the Electricity Generation Cost-Simulation Model (GENSim).

49167

Radiolytic Reduction of Carbonaceous Gases During Coal Gasification for Hydrogen Production

D. A. Powers

The President has set a goal of reducing emissions of carbonaceous gases to zero by 2070. Electricity generation by nuclear power can contribute to this reduction. There will still need to be mobile fuels for transportation that do not emit carbonaceous gases during combustion, such as hydrogen (H). A method for H production proven on an industrial scale is the steam treatment of coal. To be useful for the production of H without carbonaceous gases, the steam treatment of coal must include a method to eliminate the carbon monoxide (CO) and carbon dioxide (CO₂) also produced by the chemical process. Here, Sandia proposes that radiolytic processes associated with a nuclear-energy source also used to produce the steam be harnessed to rid the effluents from the steam reaction with coal of undesired gaseous oxides of carbon (C), sulfur (S), and nitrogen (N).

Radiolysis of the gas phase yields highly reactive chemical species. By adjusting the chemical conditions, it is possible to convert nitrogen oxides to the benign N gas, and sulfur oxides to S that can be filtered from the gas. It is also known that in the presence of magnetite, carbonaceous gases can be reduced radiolytically to elemental C particles that can be filtered. Sandia seeks to develop a radiolytic reaction scheme to strip nitrogen oxides, sulfur oxides, and carbonaceous gases from the gas stream produced by the steam reaction with coal. We will develop the reaction scheme using a chemical model that builds on the available data on kinetics of thermal and radiolytic reactions. This work will be benchmarked against data on the radiolysis of carbonaceous gases. We will base development of the reactor design on conventional plug-flow tubular reactors connected radiolytically to a pressurized-water nuclear reactor of conventional design.

Sandia undertook analyses to ascertain if radiolytic methods using the current-generation nuclear power reactors could be used to reduce “greenhouse” gases from the products of steam oxidation of coal to produce an effluent stream that was purified hydrogen. Greenhouse gases in the gases produced by steam oxidation of coal include nitrous oxide, nitrogen oxide, nitric oxide, sulfur dioxide, hydrogen sulfide, carbon dioxide, and carbon monoxide. Steam oxidation also yields substantial

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amounts of inorganic particulate that can scavenge reactive radicals.

We assumed that the effluent stream from a fluidized bed of coal in steam could be directed through a core of a conventional nuclear reactor and be subjected to intense irradiation by gamma rays and neutrons. These gamma rays and neutrons will produce a cascade of energetic radicals—notably electrons—that could reduce the greenhouse gases. Oxides of nitrogen could be reduced to elemental nitrogen gas, sulfur oxides and hydrides could be reduced to elemental sulfur, which would be filtered from the stream, and carbon oxides could be reduced to carbon.

We found that particulate material in the stream had to be filtered to avoid radical scavenging. Kinetic reaction schemes for the reduction of nitrogen oxides and sulfur oxides could be defined that did not unduly degrade the quality of the hydrogen product. We developed a careful review of the thermodynamics and kinetics of sulfur reactions at intermediate temperatures. Reduction of carbon oxides required that an oxygen trap more kinetically active than hydrogen had to be included to avoid oxidation of hydrogen back to water vapor. We identified some suitable, reversible hydrogen traps. We investigated ferrous oxide and manganous oxide. Reversing the oxygen trapping by ferrous oxide requires a high-temperature source. Manganous oxide can be reversed at lower temperatures, but still requires temperatures above those of the currently operating nuclear power reactors.

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49367

Proton Beam Shield*M. G. Mazarakis, T. J. Renk*

Sandia studied a defensive weapon consisting of a proton beam that is propagated from a ground-based accelerator located near a power plant or aboard a ship. The beam is directed toward an incoming missile or airplane and delivers sufficient energy to destroy the target. We studied two options: the first, a proton shield, creates a proton cloud up to 1 km away from the accelerator. The cloud was composed of energetic protons of 50 million eV kinetic energy, dense enough to detonate the high explosives of an incoming missile or incapacitate an airplane. The second weapon is a longer-range one, 1–10 km, that can intercept with the speed of light and detonate the high-energy explosives (HE) of a missile or incapacitate an airplane. The project concentrated mainly on the most critical issues of the weapon that need study: namely, proton-beam material interaction and lethality against HE and aviation fuel, repetition (rep)-rated proton ion source for the accelerator, and finally, the best accelerator structure for the required 1 GeV, 10 kA, high-brightness beam.

(1) The lethality of the proton-beam weapon against an HE-loaded missile, airplane, or other fast-moving or stationary object appears to us quite certain. The energetic-proton particles will deposit enough energy per gram in the explosive to detonate and destroy the incoming target.

The energetic-proton cloud interaction with an aviation fuel, being kerosene (fuel of jet airliners) or gasoline (fuel of lighter planes), is more complicated. The ignition of such a liquid fuel can occur only in a vapor state and strictly depends on the air-to-vapor ratio composition of the mixture since the aviation fuel does not contain its own oxidizer as the HE do. Furthermore, the required gasoline-to-air ratio in mixture capable of igniting and detonating is very tenuous. Very small amounts of gasoline vapor are necessary in a large volume of air to ignite. For example, the crash of TWA Flight 800 off Long Island in 1996 was linked to an explosion in the center fuel tank. This appears to have occurred because (a) there was almost no fuel in the tank, about 50 gal out of a 13,000 gal capacity, and (b) the plane waited on the tarmac at Kennedy Airport for over 2 hours in July, leading to heat buildup in the plane and vaporization of the fuel in the tank. Therefore, our studies conclude that it will be very difficult to destroy a fuel-loaded jetliner or a smaller airplane with the energetic-proton cloud version of the proton-

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beam weapon. The flammability conditions are very demanding and the fuel-to-air ratio of an explosive mixture very small. Nonetheless, we studied and planned upcoming experiments to investigate the detonation of microballoons containing mixtures of various air-to-fuel compositions and pressures judged to be in the flammability region. For these experiments we will utilize the GABLE II proton-beam accelerator at the Naval Research Laboratory.

On the other hand, the directed and well-focused beam option of the weapon could effectively detonate a fuel-full airplane tank since it could drill a hole and ignite the leaking and evaporating fuel into the air surrounding the airplane. Therefore, a proton-beam defense weapon will be effective in destroying an incoming missile or airplane with or without explosives (as in the case of the 9/11 terrorist attacks). The energetic-proton cloud version will detonate the explosives while the well-focused proton beam will detonate both HE and/or aviation fuel.

(2) The best candidate for the development of a rep-rated, high-current, high-voltage proton source appears to be a gas diode similar to the one in operation at RHEPP-1 (repetitive high-energy pulse power) operating at much higher rep-rate frequency and voltage. However, the produced beam emittance needs to be greatly improved first before being considered as the choice source of the well-focused, directed proton-beam option. The emittance requirements of the energetic-proton cloud, if any, are much more relaxed. The successful development of such a source will require resources and manpower much larger than that affordable by this project.

(3) Following a careful study of the available accelerator technologies, it appears that a new induction voltage adder, the linear transformer driver (LTD), may be the best accelerator architecture for our purpose. The salient feature of the approach is switching and inductively adding the pulses at low voltage straight out of the capacitors through low-inductance transfer and ferromagnetic core isolation. Average accelerating gradients as high as 5 MV/m could be achieved in the near future if a serious effort is focused on the development of high-energy-density capacitors and compact switches.

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Other Communications

Mazarakis, M. G., B. N. Turman, T. J. Renk, and R. B. Asher. 2002. Proton beam defense weapon. Presentation to DARPA, 8 January, Washington, D.C.

Mazarakis, M. G., T. J. Renk, and B. N. Turman. 2002. Proton beam shield. Presentation at the Naval Research Laboratory, 6 September, Washington, D.C.

49770

Frameworks for Nuclear Process Transparency and Control

M. W. Harrington, S. M. Deland, P. E. Rexroth, R. J. Wyant

A critical element in achieving global nuclear management is the ability to collect and analyze information in timely fashion to ensure that fissile materials are always secure from theft and legitimately used safely. Proliferation resistance is achieved in three steps: (1) extrinsic systems that focus on verification of legitimate use, (2) passive systems that prevent diversion of nuclear materials, and (3) risk-based methodologies that assess new designs and continuously reassess existing systems.

This project focused on the first and second steps by establishing a range of options for extrinsic systems that can effectively provide the required information and glean information from intrinsic process-control systems for successfully completing the third step.

Sandia's first objective is to survey the field of detectors, sensors, and communication currently in use and identify the advanced sensors, instrumentation and control (I&C) capabilities, automation technologies, and information systems under development that can improve the transparency and control of nuclear processes. This project is tightly coupled to the Quantitative Proliferation Assessment of International Nuclear Facilities project, in that the methodology needs information about the performance of current equipment, and the methodology can provide guidance for utilization of advanced technology. The second objective of the project is to utilize this information and establish conceptual frameworks that illustrate the effective implementation of the technology to achieve global nuclear transparency and control. To accomplish our objective, we will draw from the fields of monitoring systems, satellite detection, video data analysis, robotics, and nuclear facilities. A diverse team will examine concepts of automatic targeting, semantic processing, configurable data management, data integrity/validation, and cognitive modeling with the purpose of providing the required data to support a real-time proliferation risk-modeling methodology.

Our focus was to examine one real nuclear facility, for example, a light-water reactor with mixed-oxide (MOX) recycle and spent fuel in a nonweapon state shipping spent fuel to a weapon state for resupply with fresh MOX fuel.

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We developed the criteria for populating a transparency technology tool (box) list, which is critical to the framework.

We formulated this “tool box” of technologies and techniques that can be used for validating the location, quantity, and utilization of fissile material.

We began configuration of the data for the fuel-cycle facility that will be characterized in a risk-informed proliferation analysis (RIPA) influence diagram.

We established a glossary of terminology for a transparency framework for the control of the fissile material.

We also accomplished the following: (1) created a problem set model, (2) established a technology analysis for examining the available fuel-cycle component technologies and related technology, and (3) began researching transparent conditions as related to other systematic social, economic, and technological situations or settings.

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51534

A Fully Integrated Sensor-Based Critical Facility and Border Defense System

R. O. Griffith, F. Gelbard, M. E. Tadros, R. W. Stinnett, J. E. Brockmann, L. D. Brandt, T. D. Woodall, S. J. Martin, G. J. Smith, T. H. Karas, R. D. Horton, S. P. Gordon

Facilities such as ports, airports, and border crossings are critical elements of the nation's infrastructure and play a key role in homeland defense. In addition to acting as choke points for the flow of people, goods, and materials, the facilities themselves may be targets for terrorist attacks aimed at causing massive disruptions to the U.S. economy. To prevent terrorists, weapons-of-mass-destruction (WMD) materials, and other contraband from entering the country and to protect these facilities from attack, we must employ a layered defense system. These layers might include defensive systems outside of the recognized borders of our country, as well as perimeter defenses at national borders and entryways such as ports, airports, and border-crossing facilities. Sandia has broad expertise in physical-security systems, sensor systems, modeling and simulation, and distributed information systems. Specific sensors exist or can be developed to detect a wide range of threats, including chem/bio/rad materials, explosives, weapons, and specific known individuals. However, sensors alone are useless if they are not employed within a supporting architecture that allows the collected information to be rapidly processed and understood to guide effective actions within the context of a layered defensive system. This study will assess whether pursuing enhanced or newly developed sensor systems to monitor various entry modes and threats, algorithms for the interpretation and use of collected data, and defensive systems for facility protection are technically feasible and can be incorporated into useful products.

We identified three specific sensor technologies as having high impact in border protection: microoptical radar (MOR) three-dimensional (3-D) facial recognition, an integrated-sensor suite for shipping containers, and nonintrusive sensors for bulk checked-baggage inspection. In addition, we proposed a system-level simulation of the four critical border elements as a way to explore the performance requirements of various sensor technologies and to explore tradeoffs among the various types of sensor systems.

We prepared a Grand Challenge and submitted it to the Mission Council for funding consideration. The proposal was accepted.

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51540

Introspection, Integration, and Intercession (I³): Toward Self-Healing Critical Infrastructures

S. Y. Goldsmith, J. H. Ganter, B. K. Cook, D. C. Barton

The national security of the U.S. depends on the steady operation of an interconnected and complex “system of systems” that includes telecommunications, electric power, transportation, oil and gas, manufacturing, and financial infrastructures. Both fixed elements and external forces (e.g., market conditions) combine to create flows that aggregate and distribute material, information, energy, and capital. Both normal delivery and failure of services are emergent behaviors resulting from complex interactions—they are not easily predicted from the properties of components. Characterizing and adjusting these behaviors requires a multilevel strategy that detects initial and changing conditions through sensors, predicts responses at multiple time scales with models, alerts decision makers with situational analysis and options, and responds to optimize, protect, or repair the system.

Infrastructures have formed in response to technological and economic forces. They are hierarchically organized, geographically distributed networks of producers, transporters, and consumers. Dependencies among component systems are numerous and involve feedback coupling at many levels. Malfunctions in elements of one system may cause cascading malfunctions in elements of other systems. Coordination of an infrastructure system requires that the flow of information among distributed decision actors accounts for both upstream and downstream effects on other infrastructure elements. Tradeoffs are common but poorly characterized. The nation must rapidly develop an understanding of, and capability to protect and repair, distributed assets that are increasingly vulnerable to both local and widespread threats.

We propose to investigate opportunities for Sandia to contribute to the emerging field of self-healing infrastructure systems. We will emphasize critical infrastructures upon which Department of Energy missions are particularly dependent. We will design and create exploratory prototypes based on Sandia strengths in secure-agent architectures, micro- and macrosimulation, modeling, complexity, systems analysis, and decision making within uncertainty.

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In collaboration with researchers at the Massachusetts Institute of Technology (MIT), we began our analysis with a review of the current state of interdependency modeling. These models provide the crucial understanding of interoperation and propagation of failures in large-scale infrastructures. The I³ strategy uses implicit and explicit models to perform online prediction of inadmissible states. We reviewed multilevel coordination strategies and juxtaposed them with current agent-based architectures.

We made the following specific accomplishments:

- (1) A comprehensive bibliography of interdependency models.
- (2) A joint Sandia–MIT workshop on self-healing infrastructures.
- (3) A fresh analysis of the proposed I³ strategy for creating self-healing systems.

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Engineering Sciences

The Engineering Sciences investment area encompasses the core engineering disciplines that support the Nuclear Weapons Strategic Business Unit and other Sandia priorities. The goal is to develop a validated, science-based, simulation environment. This requires the integration of experimental, simulation, and test activities required for pertinent physics discovery and validation. The challenge is to provide engineering understanding through simulation unprecedented in physical and geometric fidelity, and spatial and temporal resolution. This will advance the understanding in the engineering disciplines critical to Sandia's national security mission. Research emphasis includes micro- and nanoscale phenomenology, technologies supporting Sandia thrusts in the War on Terrorism, and technologies critical to advanced weapon concepts.

“Small-Scale Multiaxial Deformation Experiments on Solder for High-Fidelity Model Development” models the failure of solder joints with a focus on understanding the underpinning physics. Deformation of engineering materials is complex. The ambient-temperature deformation of low-melting-point alloys is complicated by competing, thermally activated mechanisms. The resulting small-scale, multiaxial experimental and modeling

methodology will be an enabling technology for other applications such as the microstructural evolution of multiphase alloys. This research will support advances in weapons development and other critical engineered materials technology. The modeling work was conducted in collaboration with researchers at the University of Michigan.

10765

Energetic-Material Burn and Detonation at the Mesoscale

A. M. Renlund, W. M. Trott, S. H. Kravitz, A. S. Tappan, M. R. Baer, K. L. Erickson, G. T. Long

The success or failure of an ignited energetic material (EM) to propagate a burn or detonation is determined by material properties and reactions at the mesoscale. Burn models cannot adequately account for surface-area burning effects without understanding burning at high pressure in small fissures. Similarly, rarefactions from sides and from grain boundaries are efficient at quenching shocks, leading to failure of a detonation wave at some critical diameter. Whether or not a detonation can be sustained at small diameters (submillimeters) may depend on engineering the EM without traditional grains while incorporating microporosity into the material. Winning the thermal race between reaction propagation and heat losses to substrates remains a key technical hurdle in designing highly miniaturized components capable of transforming stored chemical energy of EMs into useful work.

This project applies innovative experiments to observe burning and detonation at the mesoscale. We rely on advances in material processing both to create appropriate substrates and enclosures and to deposit and pattern EMs to enhance the likelihood of reaction propagation. Indeed, sample preparation and selection of appropriate EMs were major efforts. Diagnostic development to allow accurate measurement of reactive processes at these physical scales is also a focus area of this project.

State-of-the-art simulations of deflagration and detonation are now incorporating effects of microstructural elements. These experiments will provide insight into the controlling mechanisms associated with the reliability and safety of energetic components and address issues for future applications of EMs in a new class of miniaturized components.

Microstructural effects play a crucial role in the initiation and growth of EM reactions. For example, surface area is the controlling factor in burn rate. The ability to define the microstructure by engineered design at the mesoscale provides the greatest opportunity for studying the physical phenomena of ignition and propagation. In this project, we sought ways to define specific porosity of EMs by devising methods for depositing and patterning EM films, then studying their ignition and burn or detonation performance. Our interest was in the

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performance of EMs in tubes or channels with a diameter or cross section below 300 μm . The limiting factor in our progress was our ability to create and pattern EM films. Our method of choice was physical vapor deposition by thermal evaporation. We relied on a custom system that allows some control but severely limits production. Patterning after deposition was affected by thermal processing that could lead to recrystallization of the EM film and loss of pattern definition. We concluded that the best solution was to purchase a dedicated production deposition system that could extend the flexibility of production by allowing us to use different sources and deposition methods. We are now purchasing this instrument separately with capital equipment funds. We continued to examine means of pattern definition using microelectronic fabrication techniques. We defined patterns for porosity with either connected or isolated void volumes that allow us to vary the surface area of the EM.

A large part of our recent progress was in developing diagnostic methods for monitoring burn or detonation at this small scale. We successfully demonstrated how we can use the motion of a piston, initially in contact with a pressed bed of EM powder, to monitor burning of 250 μm -diameter samples of EM. We also optically observed evidence of deflagration-to-detonation transition in similar geometries. Ignition in both these cases used laser heating of tungsten in contact with the EM sample.

A key accomplishment was the fabrication and testing of an “integrated” ignition system with the EM sample. We designed an ignition system on a Si or sapphire substrate consisting of 10 electrical contact pads with semiconductor bridges (SCBs) defined between each pair of pads. The SCBs were 100 μm in square cross-sections. This ignition substrate served as the mating lid to an EM-containing Si substrate with nine 300 μm -wide by 100 μm -deep channels. Ignition sites were 500 μm -wide circles near one end of the substrate. We filled EM powder into the channels and aligned the mating SCB lid with an SCB over each ignition circle. We were able to ignite and propagate reactions with several EM powders. We monitored reaction by high-speed photography through the transparent sapphire lid. Achieving intimate contact between the EM and the SCB remains a fabrication and assembly issue.

We transferred further development of the techniques to study and develop microenergetic devices to a project with both internal nuclear weapons funds and work-for-others funding from the Department of Defense. We will continue to focus our attention on the deposition and patterning of EMs, on diagnostic

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development, and on using modeling tools to help define and engineer efficient EM devices.

Refereed

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10788

Small-Scale Multiaxial Deformation Experiments on Solder for High-Fidelity Model Development

W. Y. Lu, T. J. Lim, H. E. Fang, P. T. Vianco, B. L. Boyce, T. E. Buchheit

Deformation of engineering materials is complex; the ambient temperature deformation of low-melting-point alloys is complicated by competing, thermally activated mechanisms. The interrelation between temperature, stress state, deformation, microstructural coarsening, and localization is not understood. Sandia examined three areas, with a focus on understanding the underpinning physics. (1) The failure of solder joints is often preceded by the formation of localized coarsened bands, but there is no fundamental understanding of the energy criteria that govern coarsening or localization. Uniaxial tension and shear experiments did not reveal the underpinning mechanisms; it is not known whether resolved shear, hydrostatic, or deviatoric strains are the critical factors and how they interrelate with thermal activation. (2) Deformation-mechanism maps are widely applied in continuum-level deformation models. However, these maps do not differentiate between the effects of shear and tension. A thorough understanding of the role of multiaxial stress states on deformation mechanisms will lead to an understanding of critical deformation conditions. (3) As joint size decreases, mechanical behavior changes from true polycrystalline behavior to a scale where bulk size-independent constitutive relations no longer hold. Current models do not incorporate a length scale that would allow exploration of this effect. Experiments at a range of length scales, decreasing to the point where breakdown of continuum is found, will provide a foundation for the development of deformation models that account for size effects.

High precision and rigorous control of microstructures are necessary to succeed in these investigations. The physical understanding developed will directly impact the Accelerated Strategic Computing Initiative (ASCI) and Enhanced Surveillance Campaign (ESC) programs, and the resulting small-scale multiaxial experimental methodology will be an enabling technology for other applications, e.g., the microstructural evolution of multiphase alloys, which heretofore have not benefited from such local experiments.

Our recent investigation focused on the solder lead-tin (^{63}Pb - ^{37}Sn)-deformation mechanism and the coarsening of

Microstructural evolution, cyclic at 5% and 100°C.

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solder microstructure. We made specimens with controlled initial microstructural characteristics and subjected them to creep and cyclic loading. Throughout the experiments, we measured *in situ* grain size and tracked the evolution of the microstructure using scanning electron microscopy (SEM).

We experimentally characterized the multiaxial creep behavior of solder at room temperature and 100°C under three modes of loading: pure tension, pure torsion, and mixed tension and torsion. The specimen geometry chosen for multiaxial creep testing of solder was a thin-walled tubular specimen. The solder portion of the tube was only 0.64 mm long, contained between two copper (Cu) or brass tubes. The thickness of the tube in both the solder and Cu/brass regions was 0.64 mm, and the overall diameter of the tube was 6.35 mm. Experimental dataset was fit using the Garafalo hyperbolic sine relationship of creep. Values obtained for the activation energy and stress exponent are consistent with published values for Region-I creep behavior. The Von Mises equivalent stress appears to be a useful predictive parameter for describing multiaxial minimum creep-rate data. We documented micrographic montages of regions containing ~ 750 Pb-rich grains on the polished outer surfaces of the tubular specimens after stabilization prior to loading. The microstructural evolution is apparent both after primary creep and after secondary creep. There was no clear qualitative difference in the evolution of the tension and torsion specimens.

We conducted isothermal cyclic loading tests in torsion at room temperature and at 100°C. Specimens were solid cylinders with a diameter of 2.5 mm and a solder section that is 2.5 mm long. We performed thermal cycling experiments, between – 35°C and 135°C, for both creep loading and thermal-mechanical fatigue (TMF) in shear. We used shear lap specimen (with a solder section that is 2 mm long, 0.5 mm wide, and 0.5 mm thick) for TMF experiments. We recorded cyclic stress-strain curves. In observing microstructural evolution, microcracks developed along phase boundaries or within Sn-rich phase during early cycling. It is apparent that the damage in high-temperature specimens does not accumulate as quickly as in room-temperature specimens. We made phase-coarsening measurements during cycling and compared our experimental results to an existing model by Vianco. The model-predicted growth of Pb-rich phase under loading, i.e., strain-enhanced coarsening, appears to be high. For the test conducted, we found general coarsening was not sensitive to the strain rate, and the coarsening rate was about the same for both thermal cycling and isothermal fatigue.

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We observed localized coarsening under torsional-loading conditions. In cases of mixed tension and torsion, where the tensile component contributed at least 25% of the total Von Mises stress, there were no indications of localized coarsening.

Refereed

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26520

Uncertainty Propagation in Models of Thermofluid Systems

H. N. Najm, M. T. Reagan

Uncertainty quantification (UQ) in models of thermofluid systems is necessary for model validation with respect to experimental results and for the development of predictive engineering models. Consequently, the development of improved UQ techniques to investigate the propagation of uncertainty in models of thermofluid systems is relevant to Sandia's Defense Programs mission regarding validation of fire models and weapon design and optimization. This project is a collaboration between Sandia and Johns Hopkins University. The project involves the development, implementation, and evaluation of four UQ approaches using combinations of spectral stochastic and Monte Carlo (MC) techniques. This is to be done in the context of one-dimensional (1-D)/2-D reacting flow, with uncertainties in rate constants, thermodynamics, and transport properties. MC is the simplest but least efficient approach. It also does not provide information on the sensitivity of uncertainties in model outputs to specific parametric uncertainties. An intrusive spectral (IS) approach, which promises improved efficiency and enables sensitivity information, reformulates the governing equations using polynomial chaos expansions to arrive at equations for the spectral stochastic mode strengths. A nonintrusive spectral (NIS) approach, where post-processing of MC statistics, based on computations of the original deterministic equations, provides the sensitivity information at the cost of reduced efficiency. The fourth variant is a hybrid IS/MC approach, which may lead to a very efficient implementation. Earlier work on this project involved development and implementation of these formulations. Current work involves extensive comparisons between them, and evaluations of their merits as applied to thermofluid systems, with an eye toward determining optimal ranges of application of each. This is a high-risk research plan that we expect to highlight unknown challenges in the application of each of these techniques to thermofluids.

...the development of improved UQ techniques to investigate the propagation of uncertainty in models of thermofluid systems is relevant to Sandia's Defense Programs mission regarding validation of fire models and weapon design and optimization. ...This is a high-risk research plan that we expect to highlight unknown challenges in the application of each of these techniques to thermofluids.

(1) We adopted a serial/shared-memory and a distributed-parallel deterministic reacting-flow solver.

(2) We developed a hybrid spectral reacting-flow formulation and implemented it for H_2 - O_2 ignition.

(3) We used Sandia's DAKOTA code for sample generation for NIS UQ for both homogeneous ignition and 1-D H_2 - O_2 flames. We compared ignition results to available literature and

to IS computations. Results showed convergence of NIS statistics to the IS result and the superior IS efficiency. In 1-D, results highlighted poor chemical model robustness for H_2O_2 prediction, where the coefficient of variation was 100%. We also identified the rate parameter of the reaction $\text{H}_2\text{O}_2 + \text{OH} = \text{H}_2\text{O} + \text{HO}_2$ as a dominant source of uncertainty in the results. We now have a complete DAKOTA implementation around our deterministic reacting-flow solver.

(4) We implemented and demonstrated IS codes for UQ in nonreacting natural convection in a heated cavity with a stochastic wall temperature boundary condition (BC). We used these codes to study uncertainty in flow and temperature fields, and to compare against NIS computations of the same flow. We found a quadratic dependence of the mean cavity Nusselt number on the standard deviation of the wall temperature field. We also found good agreement between IS and NIS, with better efficiency available from IS.

(5) We implemented and demonstrated an IS construction for modeling a reaction-diffusion system, using operator split-time integration and involving explicit diffusion and implicit chemistry integration. The chemical source term uses a second-order Taylor expansion in terms of all stochastic parameters and fields, allowing for uncertain reaction-rate parameters and thermodynamic properties. The diffusion source term allows for uncertain transport coefficients.

(6) We implemented the IS construction for the full low-MACH-number reacting-flow problem in a message-passing interface (MPI)-based distributed parallel code. This includes operator split-time integration of stochastic species equations and projection solution of the stochastic momentum equations. Testing and final debugging for a 1-D H_2 - O_2 flame are in progress.

*We now have a complete
DAKOTA implementation
around our deterministic
reacting-flow solver.*

Refereed

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26521

Filtered Rayleigh-Scattering Diagnostic for Multiparameter Thermal/Fluids Measurements

S. P. Kearney, S. J. Beresh, T. W. Grasser, R. W. Schefer

Simulation-based life-cycle engineering and the Accelerated Strategic Computing Initiative (ASCI) program have resulted in models of unprecedented size and fidelity. The validation of these models requires high-resolution multiparameter diagnostics. Within the thermal/fluids disciplines, the need for detailed, high-fidelity measurements exceeds the limits of current engineering sciences capabilities and severely tests the state of the art; therefore, a diagnostic development effort is warranted. The focus of this project is the development and application of filtered Rayleigh scattering (FRS) for high-resolution, nonintrusive measurement of velocity, temperature, and pressure.

With FRS, the flow is laser-illuminated and Rayleigh scattering from naturally occurring sources is detected through a molecular filter. The filtered transmission may be interpreted to yield point or planar measurements of three-component velocities and/or thermodynamic state. Different experimental configurations may be employed to obtain compromises between spatial resolution, time resolution, and the quantity of simultaneously measured flow variables. This capacity for multiparameter, nonintrusive instrumentation represents an unprecedented advance beyond presently available techniques in the Engineering Sciences Center and in the larger scientific arena. Potential Accelerated Strategic Computing Initiative (ASCI) code validation applications include simultaneous three-component velocity, temperature, and pressure measurements in compressible flows to support SACCARA/PREMO validation, and full-field temperature measurements in reacting or nonreacting flows for FUEGO and SIERRA/CALORE validation.

We accomplished the following: (1) FRS temperature imaging in laminar and turbulent air jets and in a premixed methane/air flame, (2) FRS imaging of scalar mixing in a turbulent helium (He)/air plume, (3) time-mean single- and two-component FRS velocity measurements in a MACH 3.7 free jet, and (4) completion of CARS temperature measurements at the Combustion Research Facility (CRF) to be used to validate the FRS temperature measurements in premixed and diffusion flames. We also conducted initial estimates of uncertainties and model calculations to assess the

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viability of ratioed FRS measurements for reduced-bias temperature measurements in nonpremixed flames.

We tested the initial performance of our FRS thermometry system in a high-temperature, low-speed air-jet facility, which provided a well-characterized, high-temperature flow where initial system development could be carried out without the added complexity of a reacting flow. The jet could be run in both stable and unstable modes. The stable laminar jet exhibited a large, uniform-temperature core that can be used as a calibration source for the FRS measurements. The stable jet core temperature was measured at 800 K using a thermocouple prior to acquiring a series of 200 FRS temperature images with an in-plane spatial resolution of $175\text{ }\mu\text{m} \times 175\text{ }\mu\text{m}$ and an out-of-plane resolution of $500\text{ }\mu\text{m}$. The FRS-measured core-temperature profile, evaluated from an average of 200 images, displayed a mean core temperature of 816 K with a standard deviation of 10.6 K for a two-standard deviation (95% confidence interval) uncertainty of 21 K, or 2.5% of the measured absolute temperature. This level of uncertainty is more than adequate for thermometry at combustion temperatures. We used the same FRS imaging system to measure local chemical composition in a binary He/air jet, extending the range of the FRS technique to an additional parameter—species concentration.

We also made FRS thermal imaging measurements in the combustion product region of a premixed methane/air flame using a Hencken-type flat flame burner. Our FRS system performs well for acquisition of both instantaneous (10 ns averaging time) and time-mean temperature measurements in this reacting flow. Typical random errors (precision) in time-mean (average of 100 instantaneous thermal images) data from this reacting flow are observed to be on the order of $\pm 25\text{ K}$ – 30 K , or 1.5% of the typical combustion product temperatures. We calculated instantaneous (single-laser-pulse) temperature precisions to be on the order of $\pm 100\text{ K}$, which is satisfactory for many turbulent combustion applications. Thermometry in the Hencken burner also allowed us to investigate the impact of measurement bias due to varying flowfield chemical composition. These bias errors can be as large as 150 K toward low temperatures if the impact of local chemical composition is not considered. We utilized premixed flame calculations using the Sandia OPDIF code to estimate ratioed filtered to unfiltered Rayleigh-scattering signals for potential use in a ratioed FRS technique to reduce the chemistry bias. For measurements in diffusion flames, these calculations show that the local chemistry bias is significantly lowered in all cases and is almost

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eliminated in flames where the fuel molecular weight is comparable to air.

We accomplished FRS planar velocimetry measurements in a lab-scale supersonic jet, including both time-mean and instantaneous measurements for one-component velocities and time-mean two-component velocities. These data compare favorably with expected velocity magnitudes; a more rigorous comparison is in progress to ascertain and then reduce the measurement uncertainty. A second FRS measurement system is currently being constructed for upcoming experiments in the hypersonic wind tunnel, such that these activities may occur concurrently with continuing lab-scale experimentation.

Refereed

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26522

A Physically Based Approach to Modeling Ductile Fracture

P. A. Klein, J. W. Foulk, III, D. J. Bammann, B. R. Antoun, S. X. McFadden, G. R. Feijoo

Sandia's work in this project will result in a new computational tool for modeling crack growth in ductile materials. Ductile fracture is probably the most common mode of fracture in solids where material fails by a combination of excessive bulk deformation and cracking. The initiation and growth of cracks in ductile materials consumes energy due to the evolution of bulk plastic and damage processes as well as the creation of new free surfaces. A computational model of these processes must reproduce the physical dimensions and stresses in the fracture process zone because the response and evolution of the dissipation mechanisms is inherently scale- and strength-dependent. The development of this computational tool begins with a fundamental, thermodynamically sound description of the failure process that encompasses both ductile failure and fracture mechanics. The development of a thermodynamic theory that includes the dissipation of both the bulk material and the surface energy of a cohesive zone requires the development of a new kinematical description of the failure process to couple these concepts at a basic level. In situ scanning electron microscope (SEM) observations of the initiation and evolution of fracture zones will reveal the scale over which the failure mechanisms act in Defense Programs alloys 6061 aluminum (Al) and 304L stainless steel (SS) and in copper (Cu). These observations are essential for motivating micromechanical models of the decohesion process that incorporate the effects of mode mixity in the loading, temperature, loading rate, and load reversals. We must incorporate the effect of load reversals into the computational model to model fatigue.

We completed the second round of quantitative *in situ* SEM fracture experiments on all three test materials. This round of tests involved side-grooved specimens intended to promote the tendency to fracture and to allow better observation of the ductile crack tip. The purpose of these experiments is to observe surface features surrounding the crack tip during fracture of three-point bend specimens using a straining stage mounted to a JEOL 840 SEM. The specimens, which measured 2.0 x 0.25 x 0.25 in., were cut from compact tension (CT) samples of 6061 Al and 304L SS that had been fatigue-precracked in a servo-hydraulic test frame. Observing the onset of fracture *in situ*

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provided valuable insight into the development of the crack-tip plastic zone and the subsequent initiation and growth of the crack. Previous tests performed with the straining stage did not involve side-grooved specimens. As a result, they developed large “shear lips” on the surfaces, which obscured observation of the fracture-process zone. The specimen dimensions (beam height, beam thickness, and precrack length) used for the tests presented here were chosen based on three-dimensional (3-D), finite-element (FE) calculations of the three-point bend geometry, showing the through-thickness variation in the ratio of the pressure to the deviatoric component of the stress field.

This second round of testing involved both symmetric and asymmetric bending specimens. The symmetric specimens produce mode-I loading, while the asymmetric specimens produce mixed-mode conditions. The tests generated data that we will use to validate the mixed-mode cohesive model that we developed. The mode-I tests with the side-grooved 6061 specimens resulted in extensive crack growth. We performed many load reversals during the tests to provide validation data for the cohesive relations under cyclic loading conditions. Despite the side-grooving, the 304L specimens failed to produce extensive crack growth. We also made continuing progress in developing a method of making high-resolution, quantitative measurements of plastic strain in the vicinity of the crack tip. We based the technique on electron backscatter diffraction (EBSD). This method is based on correlating the lattice incoherence that is introduced by dislocations with microscopic plastic strain. We mounted the EBSD measurement apparatus in a newly acquired SEM and calibrated the instrument. The broken specimens will now be sectioned and analyzed to map levels of plastic strain in the vicinity of the crack tip.

In our modeling efforts, we completed formulation of mechanism-based cohesive-zone relations specific to fracture in ductile materials. The standard approach of specifying *a priori* traction-separation relations based on reversible cohesive interactions is not appropriate for the inelastic processes active in a ductile fracture-process zone. We addressed three major shortcomings of the standard approach. First, mechanism-based description of cohesive-zone deformation is more readily expressed in terms of deformation mechanism maps, which describe deformation rate in terms of the applied stress and material state. Second, the inelastic response of the zone must incorporate load and material history. Finally, the state of the bulk material surrounding the crack tip at the initiation of the cohesive zone must itself be incorporated into the subsequent

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zone response. To address these issues, we developed cohesive zone relations based on the deformation rates of the cohesive zone in terms of the applied tractions and material state. The deformation mechanisms and material state variables were related to the constitutive model used to describe the surrounding bulk material. We finished formulating an initial version of these cohesive-zone relations, developed a numerical integration scheme for updating the tractions and material state variables, and tested the response of the model under simple loading conditions.

...we developed cohesive zone relations based on the deformation rates of the cohesive zone in terms of the applied tractions and material state.

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26523

Radiation Aging of Stockpile and Space-Based Microelectronics

H. P. Hjalmarson, J. R. Schwank, S. C. Witczak, M. R. Shaneyfelt, C. E. Hembree, P. A. Schultz

Enhanced low-dose-rate sensitivity (ELDRS) effects can reduce the lifetime of electronic components in weapon systems and in space systems. Earlier work suggested that pre-irradiation elevated temperature stress (PETS) and latent interface trap buildup (LITB) may be associated with ELDRS. Sandia's focus in this project is to use an experiment-theory collaboration to develop a complete computational model of these three important radiation-effects phenomena—ELDRS, PETS, and LITB. We combined two earlier studies. One is the experimental effort suggesting that the ELDRS problem can be related to LITB for transistors that have undergone PETS. The other is a theoretical effort advocating a hydrogen (H) dimerization mechanism as the explanation for the ELDRS problem. The goal of this project is to develop a unified explanation for these three phenomena. The project may be important in assessing whether commercial-off-the-shelf microelectronic components will be adequate for use in the stockpile.

We found that the silicon nitride (SiN) passivation layer causes ELDRS. Initially, we made this connection by doing ELDRS experiments after removing the passivation layers; we strengthened the evidence by doing ELDRS experiments on devices that were identical except that one batch had nitride passivation layers and the other did not.

In further work, we found that the dose-rate behavior depends on which type of passivation layers is used. We did this by studying devices with either SiN or phosphosilicate passivation layers. We also surveyed devices provided by various vendors. We concluded that ELDRS is always caused by the passivation layers, but it is also affected by additional processing, an effect that we will study in upcoming work.

We extended the H theory to explain ELDRS in terms of H released from the various types of passivation layers. In addition, the revised theory predicts that nitride passivation will also lead to LITB, one of the puzzling radiation effects being studied in this project. In the theory, we include sources for both ionized and neutral H; we assume the H undergoes bimolecular reactions, both dimerization and retrapping at the H sources.

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26524

Large-Deformation Solid-Fluid Interaction Via a Level-Set Approach

D. R. Noble, P. R. Schunk, S. R. Subia, D. J. Segalman, S. W. Attaway, J. R. Weatherby

Solidification and blood flow seemingly have little in common, but each involves a fluid in contact with a deformable solid. In these systems, the fluid-solid interface moves as the solid advects and deforms, often traversing the entire domain of interest. Currently, these problems cannot be simulated without innumerable, expensive remeshing steps, mesh manipulations, or decoupling of the solid and fluid motion. Despite the wealth of progress recently made in mechanics modeling, this glaring inadequacy persists.

Sandia seeks a new technique that tracks the interface implicitly and circumvents the need for remeshing and remapping. The fluid-solid boundary is tracked with a level-set algorithm that changes the equation type dynamically, depending on the phases present. This novel approach to coupled mechanics problems promises to give accurate stresses, displacements, and velocities in both phases simultaneously.

This effort involves high-risk research in Eulerian solid mechanics of bodies defined by an implicit interface, not defined by a mesh contour. An equally difficult task is to equate the solid and fluid stresses at this implicit interface. Simulating fluid mechanics requires a Eulerian formulation to avoid mesh entanglement. Solid mechanics formulations, however, tend to be Lagrangian, as it is easier to track material interfaces, compute strain, and apply boundary conditions (BCs). We will handle the complete problem in a Eulerian context using level sets to define the solid-fluid interfaces. We will apply the advances made in level-set methods for multiphase fluids to this more difficult problem involving multiple physics.

High-payoff applications are as numerous as the complex moving geometry problems that we seek to address every day. A small subset includes solidification and polymerization with accurate residual stress determination and biological applications like cell deformation and blood rheology. Many of these problems cannot be adequately addressed using existing methods, but may be quantitatively simulated using the methods we propose.

We made accomplishments in three major areas. First, we developed embedded BCs that are capable of describing multidimensional interfacial discontinuities within finite

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elements (FEs). Second, we developed, implemented, and tested two multidimensional Eulerian solid-mechanics formulations. Third, we developed a hybrid technique where the fluid-structural interactions were loosely coupled with an overlapping mesh method in which Lagrangian solid mechanics was coupled to Eulerian viscous-fluid mechanics. We now think that the hybrid methods will be useful for a certain class of physics applications such as gravure coating and dendrite dynamics that do not need a fully Eulerian approach.

A critical ingredient for level-set-based simulations of multiphase mechanics is the capability of imposing the interfacial physics along surfaces that are moving through the computational mesh. We developed and implemented two different algorithms for imposing this interfacial balance. As a result, interfacial physics can be imposed along multidimensional surfaces that cut through FEs for the first time in a Sandia code. One of these methods is applicable to a wide variety of applications and has been tested on problems in heat transfer as well as fluid-structure interactions. We verified the results against both exact solutions and arbitrary Lagrangian Eulerian (ALE) simulations and proved them to be accurate.

We developed, implemented, and tested two Eulerian solid-mechanics formulations. The first formulation uses the Cauchy momentum equations in both phases along with variables describing the solid-material velocity vector, an acceleration vector of the deformation gradient tensor, the fluid velocity, and the pressure. The deformation gradient requires a material reference state, so the formulation advances that state through the grid with a statement of Lagrangian invariance. The velocity and acceleration vectors are computed based on local time-rates-of-change of the displacement field. We implemented these equations in GOMA and tested simple ball-drop cases with mixed success. The formulation still has issues regarding discontinuities in the vector fields across the fluid-solid interface. Some of these issues may be solved by utilizing the sharp-interface work discussed above or by using extension velocities and displacements.

The second Eulerian formulation uses continuous fields in both the phases (velocity, stress, pressure, level-set, and velocity gradient unknowns), but changes the definition of the stress, depending on the phase. In the fluid phase we have a Newtonian stress tensor, and in the solid phase we have a hypoelastic stress tensor. Difficulties arise at the boundaries, though, due to viscoelastic boundary layers. We think that performance may be improved by implementing sharp interfacial physics in lieu of the diffuse physics currently in use.

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This will eliminate the viscoelastic boundary layer and hopefully improve convergence. Another difficulty that arises is specification of the correct BCs for the hypoelastic solid mechanics.

Overlapping mesh techniques are ideal for applications that involve solid materials that move through a significant portion of the fluid domain but are not excessively deformed. We developed and implemented a loosely coupled overlapping technique with Lagrangian solid mechanics and Eulerian fluid mechanics. The method is shown to simulate much larger deformation than that possible with ALE methods without expensive remeshing and remapping steps. However, the loose coupling has hurt convergence, and efforts are currently under way to make the method more tightly coupled through the use of bordered algorithms that can connect the solid and fluid matrices.

The method is shown to simulate much larger deformation than that possible with ALE methods without expensive remeshing and remapping steps.

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26781

Effect of Dielectric Photoelectric Effect on Surface Breakdown

R. E. Jorgenson, L. K. Warne

Sandia wrote a Monte Carlo (MC) code to simulate the early stages of high-voltage breakdown that occurs in nitrogen (N) across a dielectric surface. The application of this research is to understand breakdown caused by lightning in nuclear weapons components, which often involves surface breakdown. During surface breakdown, as electrons collide with neutrals in a gas, photons of various energies are released. Some of the photons have high-enough energies that they cause neutrals ahead of the streamer (a breakdown wave) front to ionize and thus advance the front. These are the only photons of importance in volumetric breakdown. Sandia accounted for these photons in the MC code using the data of Penney and Hummert. When a dielectric surface is introduced, however, the lower-energy photons, which are released in a collision that excites rather than ionizes the neutral, must also be considered because they can release electrons from the dielectric surface ahead of the front via the photoelectric effect. Because these lower-energy photons propagate further in the gas and because there are more of them than the photons that ionize the gas directly, we anticipated that they could play a major role in advancing the surface streamer. This hypothesis was supported by discussions in recent literature. When we began this project, no quantitative measurements on the effect had been done.

We assembled data from the literature on subprocesses that we determined to be important in the breakdown mechanism described above and incorporated them into the MC code, concentrating on N for the gas and Teflon or polyethylene as the dielectric surface. The important subprocesses are creating a photon due to a collision between an electron and an N neutral, transporting the photon through N to the dielectric surface, and releasing an electron from the surface due to photoemission. To calculate the photon energy due to a collision, we used published apparent cross-section data for various emission bands of N. The photon is assumed to be emitted uniformly with respect to direction, and we are interested only in the photons that will hit the dielectric ahead of the streamer front, thereby advancing the streamer. Ahead of the breakdown, we assume the N to be in the ground state; the photon has a probability to be absorbed on its way to the surface, based on its energy and the absorption spectrum of N. Once the photon hits

Top view of electrodes in Texas Tech University experiment.

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the surface, an electron has the probability of being released based on photoemission data, consisting of quantum yield versus photon energy. The simulations that we performed indicate that photoemission does not have a major effect on the growth of the number of electrons as a function of time. Therefore, it is not anticipated that photoemission will affect the breakdown voltage.

Texas Tech University performed a series of breakdown experiments across a surface made of Lexan. A short time prior to the main breakdown current pulse—on the order of tens of nanoseconds to several microseconds—they observed small-amplitude current pulses, which they termed *prebreakdown pulses*. These prebreakdown pulses had amplitudes on the order of 100 mA compared to the main breakdown-pulse amplitude of 150 A. Accompanying these prebreakdown pulses were light emissions from the surface of the Lexan. The light emissions were most intense near the anode. The prebreakdown and main breakdown-pulse discharges developed close to the surface, even when the electrodes were configured to push the breakdown path off the surface. They also measured the breakdown voltage between the two electrodes with and without the Lexan surface and saw no significant difference in the breakdown voltage.

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Multiscale Thermal Modeling

E. S. Piekos, C. C. Wong, D. R. Noble, S. Graham, Jr.

Successfully predicting the performance and reliability of many devices hinges on accurate knowledge of their thermal response in normal and abnormal environments. Unfortunately, the assumptions underlying common numerical tools and material property data used for predicting thermal behavior fail in the microscale regime. In this regime, phonon interaction with surfaces and microstructural entities, not the usual phonon-phonon scattering, dominates thermal resistance. Heat flow thus becomes dependent on direction and feature size. As devices shrink, these effects will become increasingly important as highly localized heating is caused by reduced thermal conductivity. This project is aimed at providing tools for increasing our understanding of microscale heat-transport phenomena and translating this understanding into efficient models for representing these effects in commonly used macroscale codes.

This research concentrates on exploring thermal transport in thin silicon (Si) films using both experiments and numerical simulation. Experimental efforts use microfabricated heaters and probes to measure the effect of various microstructural and processing effects on the thermal conductivity of single and polycrystalline Si films (i.e., with film thickness, grain size, dopants, temperature) of interest to Sandia. These data form a physical reference for the development of models intended to predict the impact of microstructural and length-scale effects on thermal transport in microscale devices. While the general framework of these models will be applicable to a wide number of devices that are dominated by phonon transport, the efforts of this work will be applied first to thermal microelectromechanical systems (MEMS) that use polycrystalline Si as the functional material. The development of both modeling tools and thermal property-microstructural data has been requested by and will be invaluable to the development of thermal actuators by Sandia weapons designers and MEMS fabricators.

We constructed a proof-of-concept Lattice-Boltzmann (LB) model. Due to the numerous constraints on the LB model and conflicting conclusions in the literature regarding the dominant transport mode, we adopted a Monte Carlo (MC) model for further development due to its flexibility in representing complex phenomena with fewer *a priori* assumptions. We coded the MC model using a measured dispersion relation and included all acoustic phonon modes. We developed an

This project is aimed at providing tools for increasing our understanding of microscale heat-transport phenomena and translating this understanding into efficient models for representing these effects in commonly used macroscale codes. ...The development of both modeling tools and thermal property-microstructural data has been requested by and will be invaluable to the development of thermal actuators by Sandia weapons designers and MEMS fabricators. We constructed a proof-of-concept Lattice-Boltzmann (LB) model.

isothermal boundary condition (BC) and implemented phonon-phonon scattering. We identified numerous errors and omissions appearing in the relevant literature. Near room temperature, where the currently represented scattering mechanisms are dominant, the MC results show excellent agreement with experimental data collected during this work without adjusting the scattering coefficients obtained using previous data on much thicker materials. At lower temperatures, the MC results show a higher thermal conductivity than the experiments, which is expected due to the absence of isotope and impurity scattering in the model. These mechanisms tend to lower thermal conductivity, and MC models for them are currently under development.

The length-scale effect on the thermal conductivity of undoped single-crystal Si films was experimentally determined using steady-state electrical resistance thermometry. We measured films of 0.34 μm , 1.0 μm , and 1.5 μm thickness between 100 K and 320 K. The resulting data compare well with previous work by other researchers, where available. The data show that boundary-scattering effects are most prominent at temperatures below 100 K. However, the effect of film thickness on thermal conductivity is still quite significant near room temperature for 0.34 μm film, with a reduction in thermal conductivity of 40% when compared to bulk Si. This reduction as compared to bulk Si reduces to only 10% at room temperature for the 1.5 μm film, whose thermal resistivity is dominated more by anharmonic phonon interactions.

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A Robust, Coupled Approach for Atomistic-Continuum Simulation

J. A. Zimmerman, E. B. Webb, III, R. E. Jones, P. A. Klein, D. J. Bammann, J. J. Hoyt

With the growing focus on predictive modeling and simulation, Sandia must develop the capability to model deformation and failure in multiple-scale settings. We are developing a robust approach to coupled atomistic-continuum simulation, capable of both quasi-static and finite-temperature/dynamic analyses. Sandia currently does not have this simulation capability. Our methodology will simulate systems at finite temperatures correctly, which involves the transfer of energy from the continuous spectrum of vibrations in the atomistic region to the separate modes of a scalar temperature field and “long” elastic waves in the continuum. Existing schemes found in the literature make no attempt to differentiate between the exchange of thermal and elastic energy. We are creating a comprehensive framework to relate the dynamic motion of atoms with the kinetics of a continuum. Our approach introduces high-fidelity physics to capture nanoscale processes while using continuum mechanics to model the elastic deformation for the majority of a system with microscale dimensions.

An essential requirement of our work is the development of definitions for continuum quantities that can be evaluated locally within an atomistic region. Historically, continuum variables are defined only in terms of equilibrium thermodynamics. The instantaneous, individual atomic contributions to these averages do not have the same physical interpretation as the corresponding “point-wise” continuum quantities. We are developing physical measures of stress, deformation, and temperature that are calculable in an atomistic simulation and have well-defined meanings when evaluated in the continuum limit.

This work will ultimately allow analysis of inherently multiscale problems such as stiction and wear in microelectromechanical systems (MEMS), nanoindentation, and fracture in microdevices.

We studied definitions of stress used in atomistic simulations and identified four key literary works that present such definitions. We wrote internal documents summarizing these works and used group meetings for discussion and evaluation of the quality of these expressions from a theoretical standpoint. We performed atomistic simulations to compare the expression developed by Hardy with the standard atomic stress

The hybrid decomposition method divides up the entire 2-D domain into individual, equally sized unit cells, but partitions the cells among eight CPUs (denoted by color) to account for the spatially varying density of atoms. Within the circled region the density is high and only a few dozen cells are partitioned per processor, whereas outside this region the density is low, and a few thousand cells are treated per processor.

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originating from the virial theorem. Hardy's expression equates the Cauchy stress field to the sum of atomic-force interaction terms plus a kinetic tensor term involving atomic velocities relative to a momentum-averaged velocity field.

We compared Hardy's method to small-volume averages of the virial stress using molecular simulations of face-centered cubic (FCC) crystals. The interatomic potential used was the embedded atom method (EAM) by Foiles, Baskes, and Daw. We first uniaxially strained the crystal by 5% at room temperature and evaluated stresses at various points in the system using different cut-off radii. While both approaches converged to the same approximate value, the Hardy formulation "smoothes" the fluctuations more effectively than the virial expression. The nature of these fluctuations differs for the two expressions. For the virial stress, they occur due to the effective change in density calculated from a continuously varying volume containing discrete points of mass. The Hardy stress fluctuates due to differing amounts of force contribution for each interacting atomic pair as the localization volume changes. We verified this by comparing the two expressions for a crystal at zero temperature and pressure. Since each atom's virial stress is zero for this case, the volume average is also zero at all volume sizes. However, the Hardy value for stress fluctuates about the zero value, with a magnitude decreasing as the cut-off radius increases. The differing nature of these fluctuations greatly impacts stress evaluation for regions of inhomogeneous structure, such as at a free surface. Although the magnitude of fluctuations is comparable for both expressions, the period of the virial fluctuation is clearly tied to the size of the averaging volume (it equals twice the cut-off radius), while the period for Hardy stress fluctuations is considerably smaller and the same for both cut-off radii. The Hardy value decays in the region between the top atomic layer and the "effective" surface of the crystal, while the virial increases in magnitude, dropping to zero within only 0.5 Å of the effective surface. Given this behavior, the formulation by Hardy seems most suitable for coupling atomistic quantities to continuum variables.

We have begun considering issues associated with performing coupled atomistic-continuum simulation on massively parallel platforms. One challenge is the differing methods used to decompose a problem over multiple processors. Atomistic simulations use a spatial decomposition, whereas finite-element methods require decomposition based on optimal slicing of the internodal connections. For the coupled simulations, we began developing a hybrid approach in

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which the cells of a spatial grid are partitioned over the available processors. This approach allows the number of spatial grids to be set independently of the available number of processors and the decomposition to reflect special boundary conditions. Our hybrid approach extends the simplicity and efficiency of a regular spatial decomposition to more general and changing atomistic simulation geometries.

We began to implement tools within our continuum simulation code to perform atomistic simulations. We constructed a module to generate atomic systems of various crystal structures and elemental properties. We are in the process of developing the underlying mechanisms for interacting atomistic and continuum regions. Once done, we will perform zero-temperature, quasi-static nanoindentation simulations to evaluate our method.

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Microscale Rarefied-Gas Dynamics and Surface Interactions for EUVL and MEMS Applications

D. J. Rader, J. N. Castaneda, J. R. Torczynski, M. A. Gallis, L. E. Klebanoff, W. M. Trott, T. W. Grasser

Momentum and heat transfer to solid surfaces immersed in noncontinuum transitional (rarefied)-gas flows continues to be an active topic of research. Gases exhibit noncontinuum effects when the characteristic length scale of the system becomes comparable to the gas mean free path. Thus, rarefaction becomes important when either system-length scales become small (e.g., microelectromechanical systems [MEMS]) or when gas pressures become low (e.g., semiconductor manufacturing). To predict momentum and heat fluxes, it is essential to understand the details of the gas/surface interaction; unfortunately, despite considerable effort, reliable interaction mechanisms are still lacking. Only two relevant experimental studies are found in the literature, and these two studies presented limited data that are not in complete agreement.

A combined experimental/modeling study is under way to better understand the critical role of gas-surface interactions in rarefied-gas flows. Sandia will make extensive, precise, well-characterized experimental measurements in a quiescent transition-regime gas between two parallel plates held at unequal temperature. We will conduct tests with a broad range of diagnostics for a variety of gases (monatomic, diatomic, polyatomic) using carefully controlled, well-characterized surfaces of different types (metals, ceramics) and conditions (rough, smooth). We will make precise measurements of system pressure, plate temperatures, and heat flux between the plates. We will use electron-beam fluorescence to measure gas density and temperature profiles between the plates.

We will compare the experimental results to modeling predictions to identify areas of model strength and weakness, paying particular attention to validating current gas-wall interaction models and to developing new wall models, if needed. This work will have immediate benefit for current extreme ultraviolet lithography (EUVL) particle protection work, help validate rarefied-gas model performance, and, in the long term, help develop the modeling and experimental tools that will be needed under the Microsystems and Engineering Sciences Applications (MESA).

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The principal challenge in this work is to field experimental tests that substantially improve upon the limited data currently available in the literature. During the experimental design phase of this project, it became clear that improvements over previous work could be achieved only by careful attention to detail in four key areas: (1) plate-temperature uniformity and control, (2) gas-pressure uniformity and control, (3) the ability to make measurements as close to the plates as possible, and (4) the ability to perform simultaneous measurements of gas heat flux and gas density (temperature) profiles. Thus, the completion of the experimental and system design, which is expected to meet our strict experimental requirements, represents a significant accomplishment.

An important element of the original proposal was that we would adapt an existing Gaseous Electronic Conference (GEC) vacuum chamber for the experiments. Upon detailed scrutiny of the specific experimental requirements, however, it became clear that even a modified GEC chamber would not be suitable. Thus, we designed, ordered, and received a new test chamber shell. While this has caused the milestone schedule to slip a few months, we anticipate that the expanded capability of the new design will greatly improve system flexibility and allow for significantly more-efficient and -precise data acquisition.

Most of the supporting hardware and diagnostic systems also have been designed, ordered, and received, including high-precision pressure sensors, pressure/flow controllers, plate positioners, and temperature sensors. Because of the high degree of accuracy required for these tests, calibration pathways had to be identified for each component. For example, we secured a precision bench-top bath to allow on-site temperature-probe calibrations.

A key accomplishment was the selection of electron-beam fluorescence as the primary *in situ* diagnostic for measuring gas-density profiles between the plates. Electron-beam fluorescence provides a single diagnostic that will work with both monatomic and diatomic gases over a wide range of gas densities. More-sophisticated analysis of the fluorescent emission signal will ultimately allow measurement of the gas-temperature profiles and the local gas molecular velocity distribution.

One key remaining task is the design and fabrication of a structure that holds the test plates at a uniform, precise temperature while providing an accurately known heat flux. The challenge here is that the required heat flux is extremely low and consequently difficult to measure. A novel design that meets these requirements is currently under consideration. In

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rarefied flows, significant departures from noncontinuum are observed at the gas-surface boundary, and it is this region that is of greatest experimental interest. Unfortunately, the physical dimension of any *in situ* diagnostic beam (or intrusive probe) will limit how close to the surface a measurement can be made. For a converging beam, a significant improvement in near-wall resolution can be obtained by using slightly curved (opposed spheres) instead of flat plates. To alleviate concerns that a curved plate might confound data interpretation based on one-dimensional flow, we performed direct-simulation Monte Carlo calculations that showed negligible nonuniformity in the temperature profiles near the centerline.

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High-Fidelity Frictional Models for MEMS

E. D. Reedy, Jr., M. P. de Boer, F. Bitsie, R. E. Jones, O. B. Ozdoganlar, B. R. Antoun

Frictional losses play a dominant role in microsystem performance and reliability, but are not yet well-enough understood to enable high-fidelity modeling and simulation needed for weapon component design and qualification. Surface interactions currently treated in a global sense using classical friction laws are insufficient for microelectromechanical systems (MEMS) in which single asperities and their interplay with interfacial roughness are the primary energy-dissipation mechanisms. First, Sandia will construct a three-dimensional (3-D) computer model of the interface on the basis of surface topography, constitutive frictional relations for the asperity contacts, and surface tractions due to van der Waals forces. Second, we will evaluate and optimize novel MEMS friction test structures to explore a wide pressure-velocity space, developing necessary metrologies that yield information on slip for nanometer displacements. This will enable us to resolve microsecond time frames as needed to determine velocity and stick-slip effects over many orders of magnitude. Third, we will model the frictional response at the mesoscopic scale. This modeling/experimental approach will allow us to connect frictional response across the length scales and will form the basis for microdomain-specific contact algorithms to be incorporated into the evolving multiphysics SIERRA code infrastructure. Successful completion of the project will yield validated grid-scale models for MEMS interfaces that accurately treat dissipation mechanisms.

Activity centered on establishing the experimental and analytical infrastructure needed to address our ultimate goal of developing an in-depth understanding of friction at the MEMS scale.

Our objective is to measure the friction laws of single-asperity contacts using the atomic-force microscopy (AFM), use computer-based models to predict the characteristics of the MEMS test devices, and then compare to the MEMS and larger-scale data. We are using the AFM to measure the topography of typical MEMS surfaces and to determine single-asperity friction laws by rubbing AFM tips of known curvature on flat silicon (Si) surfaces. We showed that we can uniformly apply pressure to make static MEMS-scale friction measurements in air using an inchworm actuator. However, air damping can be

Successful completion of the project will yield validated grid-scale models for MEMS interfaces that accurately treat dissipation mechanisms.

an important loss mechanism in MEMS. To eliminate air-damping effects in dynamic friction measurements, we began to assemble a chamber that allows testing in a vacuum. The MEMS structures will be viewed by optical microscopy and by long-distance optical interferometry through a window. In friction testing, both normal (out-of-plane) and tangential (in-plane) forces must be known to obtain accurate measurements. With our MEMS test structure configurations, normal forces are easily calibrated. However, tangential forces can be obtained only indirectly by knowing displacements. Therefore, accurate and high-resolution displacement measurements are essential. In-plane measurements are typically accomplished by bright field microscopy, with a corresponding resolution of approximately one micron. This resolution can be improved by a factor of 20 times or more using Moiré metrology (interpolating phase contrast between object and reference gratings). We quantified an in-plane Moiré metrology MEMS test structure and demonstrated an automation technique for the measurement. We have also begun to make macroscale friction measurements using microtribology instruments.

Efforts to develop frictional models for polysilicon (poly-Si) MEMS are progressing on several fronts. We are performing both PRESTO and ADAGIO finite-element (FE) simulations of two hemispherical asperities that are pushed into or past each other. These calculations serve several purposes. First, they allow us to verify our modeling techniques by comparing calculated results with analytic contact mechanics solutions. More importantly, this simple test geometry allows us to begin to understand the relative importance of the phenomena that generate MEMS friction. We expect that frictional resistance is closely linked to the shearing of strongly adherent regions of asperity contact, but other mechanisms, such as contact forces opposing the motion of asperities past each other, could also contribute. The two asperity calculations will also help us understand the contribution of local adhesional forces to asperity deformations and the potential for asperity yield and fracture. We also performed a few preliminary FE simulations using meshes generated from AFM data and are currently writing a CUBIT script to define an FE mesh from raw AFM data that can be appropriately refined to better model asperity contact. We are also studying the numerous analytical models that predict contact and frictional forces for rough surfaces that interact at a relatively large number of deforming asperities. Predictions using these models are being applied to AFM-measured poly-Si surfaces to provide baseline predictions for comparison with more sophisticated models that will take into

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account the relatively low number of contacts that occur between MEMS-scale surfaces. These same analytical models, specifically those derived from Greenwood and Williamson (1966), are being employed in an FE-based interface model. The Greenwood-Williamson paradigm is used as a homogenization technique that allows for the micromechanics of asperity deformation to be accounted for in a coarse mesh describing the nominal geometry of MEMS parts, thus saving the prohibitive computational expense of meshing the actual rough surfaces on the parts for system-level simulation. We verified the consistency and robustness of this multiscale computational model with simple tests.

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38687

Soot Formation, Transport, and Radiation in Unsteady Diffusion Flames

C. R. Shaddix, S. P. Kearney, T. C. Williams, L. G. Blevins, R. W. Schefer, J. M. Suo-Anttila

Fires pose the dominant risk to the safety and security of nuclear weapons, nuclear transport containers, and Department of Energy (DOE) and Department of Defense (DoD) facilities. The thermal hazard from these fires primarily results from radiant emission from high-temperature flame soot. Therefore, it is necessary to understand the local transport and chemical phenomena that determine the distributions of soot concentration, optical properties, and temperature to develop and validate constitutive models for large-scale, high-fidelity fire simulations.

The work in this project aims to make a vital improvement in Sandia's ability to predict heat flux from fires by performing experiments in steady and pulsed diffusion flames, using both simple hydrocarbon gases (methane and ethylene) and a JP-8 surrogate fuel mixture. We are refining and perfecting in situ laser diagnostic techniques for critical gas species and the velocity field for sooty flames, together with extractive analysis of soot morphology (via transmission electron microscopy [TEM] grid sampling) and soot optical properties. We will attempt novel laser techniques for temperature measurements in flames. Spatially and temporally resolved measurements of thermal radiation will allow detailed comparisons between estimated and measured heat flux.

We designed, constructed, and optimized a new, pulsed slot burner flame facility. We conducted detailed surveys of both methane and ethylene flame response as a function of pulse intensity and frequency. We designed and fabricated a quartz electromechanical sonic microprobe for local sampling of soot. We assembled a solenoid-piston-actuated TEM grid sampling probe to analyze soot morphology and microstructure. We purchased sensitive, fast-response thermopiles and specified an associated light-pipe arrangement for performing spatially resolved measurements of thermal emission from the radiant flames. We performed OH absorption and laser-induced fluorescence (LiF) measurements, together with polynuclear aromatic hydrocarbon (PAH) LiF, soot laser-induced incandescence (LII), and near-infrared (NIR) soot emission.

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We performed shakedown of the new burner with methane and ethylene fuels, which resulted in stable steady and pulsed flames.

We designed a quartz electromechanical sonic microprobe for local sampling of soot from the diffusion flames, which to our knowledge has never previously been achieved. This design utilizes a fast-acting solenoid valve to rapidly plunge a fine wire into and out of the quartz probe opening, preventing clogging from the soot. Calculations suggest that this probe should be successful in sampling soot with a spatial resolution of approximately 2 mm and will sample over 2 mg of soot per minute in flame zones with 1 part per million (ppm) of soot. This sample flowrate is well within the requisite volume needed to perform accurate measurements of the soot extinction coefficient in a transmission cell reciprocating nephelometer (TCRN). The probe has been manufactured.

We fabricated an air-piston-actuated TEM grid sampling probe for use in collecting soot samples for subsequent analysis of soot morphology and microstructure via standard and high-resolution TEM imaging. Also, we purchased two different types of fast-response thermopiles to perform measurements of the radiant emission from the flames. Long, thin light pipes will be placed in front of the thermopiles to make spatially resolved measurements. We initiated discussions with external researchers concerning their recommendations for a surrogate fuel mixture for JP-8 and for a fuel vaporizer design and suggestions that the filtered Rayleigh-scattering approach to making temperature measurements in sooty flames may fail for soot levels on the order of a ppm. We identified an alternative technique, two-color thermometry, using tunable diode laser measurements on water vapor, as a technique that may be able to make these measurements in very sooty flames.

We conducted detailed surveys of both methane and ethylene flame response as a function of pulse intensity and frequency. As a result of these surveys, we established best canonical operating conditions for performing the full suite of experimental measurements. Measurements that have been performed in these canonical flames include OH laser absorption and OH LiF (giving the flame oxidation zone and overall shape of the flame at any given instant), PAH LiF (showing active zones of pyrolytic chemistry leading to soot), soot concentration via LII (qualitative, at this point), and NIR emission (yielding a semiquantitative measurement of thermal radiation from the flame). Strong impacts of external vortex roll-up on soot formation and emission are evident in the data that we have collected.

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Electrical-Impedance Tomography for Opaque Multiphase Flows in Metallic Vessels

S. G. Liter, K. A. Shollenberger, J. R. Torczynski

Electrical-impedance tomography (EIT) is a minimally invasive measurement technique that can be used to quantitatively map material distributions in visually opaque systems. While much progress has been made on EIT for nonconducting vessels, significant research and innovation remain before it will be realized for its most important industrial application: conducting (metal) vessels (reactors, pipes, etc.).

This project had two primary objectives: (1) to develop a new EIT diagnostic capable of quantitatively measuring material distributions of liquid-gas two-phase flows in industrially relevant electrically conducting vessels, specifically, in Sandia's pilot-scale slurry bubble-column reactor (SBCR), and (2) to combine EIT with an established gamma-densitometry tomography (GDT) system to quantitatively measure distributions of solid-liquid-gas three-phase flows in Sandia's SBCR.

- *New diagnostic.* We developed an EIT system and used it to measure material distribution profiles inside Sandia's SBCR. The new EIT system is a modification of an existing EIT system used with nonconducting vessels. The EIT system consists of electronic control and data-acquisition hardware and software and eight electrodes. We positioned seven discrete electrodes along an insulating rod, capable of spanning the interior diameter of the SBCR. Modifications included new data-acquisition and -control software along with multiple significant hardware upgrades. The EIT system operates by applying a constant excitation voltage onto each of the seven electrodes along the rod, in turn, with the vessel wall always serving as ground (eighth electrode). We then measured the resulting voltage and current on all electrodes for each applied excitation voltage. We used these measurements to reconstruct the electrical conductivity field, from which we inferred the material distributions (e.g., calculated using the Maxwell-Hewitt relationship between bulk conductivity and void fraction).

- *Two-phase measurements.* We first used the EIT system in a solid-liquid bench-top experiment to measure the height of a packed bed in a liquid-filled standpipe. EIT bed-height measurements agreed to within $\pm 2\%$ of the bed height as measured with a meter stick for six different heights. Next, quantitative measurements of the gas-volume fraction in water-

Schematic of EIT system interfacing with the SBCR.

We developed an EIT system and used it to measure material distribution profiles inside Sandia's SBCR. ... We first used the EIT system in a solid-liquid bench-top experiment to measure the height of a packed bed in a liquid-filled standpipe.

air flows were made in Sandia's SBCR for eleven different flow conditions, specifically, column pressures of 15, 30, and 45 psia with superficial gas velocities of 10, 15, and 20 cm/s, and pressures of 15 and 30 psia with a gas velocity of 25 cm/s. We compared these measurements against results from an established GDT system and observed agreements ranging from within 0.03 to ± 0.12 for gas-volume fractions on the order of 0.24 to 0.45, with EIT results consistently below GDT results. We are still analyzing data. Two possible explanations for the large discrepancies include the use of a simplified reconstruction algorithm due to project constraints, and the electrode rod being more invasive than expected from literature reviews, thus resulting in a locally liquid-rich wake region surrounding the rod and electrodes.

- *Three-phase measurements.* We used EIT with GDT to measure solid-water-air three-phase material distributions in the SBCR. EIT distinguishes the liquid phase from other nonconducting phases, and GDT distinguishes the gas phase from other nonattenuating phases. We can then determine the solids fraction knowing that solid-, liquid-, and gas-volume fractions must sum to unity. We performed experiments with three solids loadings: 0%, 4%, and 8% by volume. For each loading, we took measurements with a superficial gas velocity of 10 cm/s at two pressures, 15 and 30 psia. We are still analyzing data.

The EIT diagnostic is capable of measuring material distributions in multiphase flows in metal vessels. We can improve quantitative accuracy through further modification of the hardware electronics and electrode construction, as well as electrode placement within the measurement domain. Three-phase measurement accuracy cannot be better than the two-phase measurement accuracy; therefore, experiments with greater solids loading would be desirable.

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Refereed

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Grand Challenges

The Grand Challenges investment area investigates innovative ideas with the potential for dramatically impacting national-level concerns and for creating technologies and processes required for the twenty-first century. Grand Challenges engage lab-wide multidisciplinary research teams that establish critical mass in participation and funding to focus on world-class research. High-risk, potentially outrageous ideas are considered for investigation. In addition, all Grand Challenges research efforts must identify linkage to supporting Sandia's business goals.

Solid-state light-emitting diodes (LEDs) that emit across the visible spectrum have developed rapidly. LEDs have opened possibilities for generating white light for general-purpose illumination at efficiencies far higher than existing conventional light sources. The conversion to high-efficiency solid-state lighting has the potential to save up to \$100 billion per year on electrical-energy costs. This technology will also create completely new applications based on solid-state lighting compactness. "A Revolution in Lighting: Building the Science and Technology Base for Ultraefficient Solid-State Lighting" will establish

the fundamental science and technology bases required to realize this vision of ultraefficient solid-state illumination. This endeavor will also result in the development of infrastructure and associated synergistic technology of vital importance to national security needs. Five patent disclosures have been filed.

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Molecular Integrated Microsystems (MIMS)

L. M. Napolitano, K. S. Potter, E. F. Hasselbrink, C. J. Brinker, D. R. Wheeler, S. M. Brozik, D. Y. Sasaki, T. J. Shepodd, A. K. Singh, A. R. Burns, S. A. Casalnuovo, S. A. Kemme, D. A. Loy, B. C. Bunker, A. P. Thompson, B. G. Potter, Jr., J. S. Schoeniger

Microfabrication tools and processes developed for the microelectronics industry make it possible to miniaturize devices including chemical analysis systems, navigational components, and mechanical locks. Sandia's experience with microsystems has shown that direct miniaturization of conventional architectures can provide significant benefit through increased portability, low power consumption, and improved speed of operation. We believe that the full benefit of miniaturization will be achieved only when microscale addressability is used to control nanoscale materials properties and molecular interactions. In this project, we are pursuing a revolutionary approach to microsystems in which microscale patterning of functional materials is combined with local addressing (electrical, optical, thermal fields) to provide fully programmable systems and architectures. The overall goal of this project is to combine molecularly tailored nanomaterials with addressable microdevice architectures to demonstrate the first-ever programmable MIMS devices for protein and peptide analysis and encoded optical interconnects. We built on the technical advances made in our previous work as we begin developing engineering approaches required to design and construct proof-of-principle devices that will meet our target capabilities. We developed new molecular sorting and detection approaches, including EK (electrokinetic) trapping and switchable polymer coatings. Here we were able to demonstrate the first-ever programmable preconcentration of proteins in solution. We developed new fluidic architectures around newly discovered Mobile Monolith Technology. Our programmable optics work explored a set of photosensitive materials that show extremely promising optical response. In each case we continue to build on our understanding of the underlying phenomena as we optimize our fabrication approaches.

The primary focus of this project was the development and demonstration of the μ ProLab architecture for sorting proteins. μ ProLab represents a completely unique approach for sorting complex protein mixtures that are important for biothreat and human health problems. (A smaller effort successfully demonstrated a programmable optical architecture. The

...we are pursuing a revolutionary approach to microsystems in which microscale patterning of functional materials is combined with local addressing (electrical, optical, thermal fields) to provide fully programmable systems and architectures. The overall goal of this project is to combine molecularly tailored nanomaterials with addressable microdevice architectures to demonstrate the first-ever programmable MIMS devices for protein and peptide analysis and encoded optical interconnects. ...we were able to demonstrate the first-ever programmable preconcentration of proteins in solution. We developed new fluidic architectures around newly discovered Mobile Monolith Technology.

μ ProLab utilizes molecular integrated microsystems (MIMS) technologies for on-chip sample preconcentration, separations, and fluid routing within a programmable architecture that provides protein-sorting capabilities not currently available. The unique μ ProLab features include (1) a demonstrated 1000-fold intensification of dilute protein signatures, (2) fluid routing that allows (for the first time) multiple separation chemistries on a single chip, and (3) reconstitution of analyzed samples to allow re-analysis of small samples or signal integration for increased detection sensitivity.

The goals were to (1) down-select to the most promising technologies among those previously discovered or invented in this project, (2) develop a materials integration strategy to implement those technologies in the μ ProLab architecture, and (3) demonstrate μ ProLab architectures that can be used to measure the performance of the new MIMS technologies. The MIMS project accomplishments successfully delivered on each of these technical goals while at the same time developing solid business and technical plans for a fully integrated MIMS demonstration.

We used μ ProLab requirements to drive materials integration needs. Important developments include (1) chip-level integration of polymer preconcentrators, (2) development of cast-in-place polymers for on-chip EK trapping and separations, and (3) development of cast-in-place monoliths for programmed μ fluid routing. We integrated all critical components into chip-level components. Finally, we achieved our goal of demonstrating and measuring the performance of integrated architectures, including coupled preconcentration/separation and coupled separation/fluid routing; we will complete the second goal in upcoming work.

The External Advisory Committee met in February, applauding MIMS' progress and recommending that this project be extended so that the power of the MIMS μ ProLab architecture can be demonstrated on an important problem in biology.

The External Advisory Committee...(recommended) that this project be extended so that the power of the MIMS μ ProLab architecture can be demonstrated on an important problem in biology.

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A Revolution in Lighting: Building the Science and Technology Base for Ultraefficient Solid-State Lighting

J. M. Gee, L. E. S. Rohwer, R. J. Shul, J. J. Figiel, A. J. Fischer, J. P. Wilcoxon, W. W. Chow, S. R. Kurtz, A. F. Wright, R. M. Biefeld, J. R. Creighton, H. K. Moffat, C. H. Seager, E. D. Jones, A. A. Allerman, C. C. Mitchell, J. A. Emerson, M. E. Coltrin, D. D. Koleske, D. M. Follstaedt, J. Y. Tsao, K. E. Waldrip, J. R. Wendt

The rapid development of solid-state light-emitting diodes (LEDs) that emit across the visible spectrum has opened the possibility of generating white light for general-purpose illumination at efficiencies far higher than existing conventional light sources. The conversion to high-efficiency (~ 50% at the wall-plug) solid-state lighting has the potential to save up to 100 billion dollars per year on electrical energy costs. It will also create completely new applications based on solid-state lighting's compactness, ruggedness, large intensity variation, directionality, reduced heat output, programmable color rendering, and amenability to high-frequency modulation for communication purposes.

To develop a high-efficiency solid-state white-light source, it will be necessary to (1) improve LED and/or vertical-cavity surface-emitting laser (VCSEL) efficiency to the 50% range, (2) extend the color spectrum of these high-efficiency optical emitters into the yellow, green, blue, and possibly also ultraviolet (UV), and (3) substantially reduce the cost. The goal of this project is to establish the fundamental science and technology base that will be required for this vision of ultraefficient solid-state illumination to become a reality. Sandia is pursuing a balanced research program to address the following topics: solid-state materials theory and characterization; optimization of III-nitride growth and substrates, metallic-oxide chemical vapor deposition (MOCVD) chemistry, reactor design, and control; luminescent conversion materials; and solid-state lighting packaging. In so doing, we will position Sandia to be the national leader in these areas, and thus to play a major role in the future Department of Energy-funded initiative now being planned. This endeavor will also result in the development of infrastructure and associated synergistic technology of vital importance for national security needs in the important III-nitride material system and other associated technologies (semiconductor nanoclusters, etc.).

LEDs—the future of lighting?

The conversion to high-efficiency (~ 50% at the wall-plug) solid-state lighting has the potential to save up to 100 billion dollars per year on electrical energy costs.

- *Material characterization and solid-state theory*

- We studied and explained the kinetics of hydrogen (H) thermal and E-beam annealing and H motion in drift field.

- We experimentally and theoretically characterized carbon (C) doping. We found C to self-compensate at high concentrations.

- *Low-defect epitaxial growth and substrates*

- Significant improvements in Sandia-invented cantilever epitaxy process led to fully coalesced films with low defect density.

- We developed a nucleation sequence for growth on planar sapphire substrates that significantly reduces defect density.

- *III-nitride MOCVD chemistry*

- We performed a wide variety of reactor-scale experiments. All data point to chemistry in the high-temperature boundary layer as the origin of parasitic reactions during aluminum gallium nitride (AlGaN) MOCVD.

- We found the first direct confirmation of particle formation during AlGaN MOCVD and are quantitatively characterizing the particles with Mie scattering. The density and size of particles were sufficient to account for loss in the AlN growth rate.

- *In situ process control*

- We examined five different techniques for temperature measurement during GaN MOCVD. We filed a technical advance (TA) disclosure on a promising new option using self-referencing emissivity correction.

- We upgraded the *in situ* multibeam optical stress sensor (MOSS) system in our MOCVD reactor. We developed a theory to account for the oscillation anomaly in the MOSS signal.

- *Reactor design and modeling*

- We examined fluid instabilities theoretically and experimentally. We developed a model to provide a guideline for designing growth reactors in which buoyancy instabilities are suppressed. We verified the analytical model in experiments.

- We developed numerical modeling tools to model the coupled fluid flow, temperature distribution, and homogeneous and heterogeneous chemical reactions in a complex reactor geometry. We investigated a new reactor geometry that used baffled injectors and exhaust to provide constant velocity injection of the reactants into the reactor.

- *UV LEDs and VCSELs*

We found the first direct confirmation of particle formation during AlGaN MOCVD and are quantitatively characterizing the particles with Mie scattering. The density and size of particles were sufficient to account for loss in the AlN growth rate.

— We demonstrated a 15 times improvement in near-UV LEDs fabricated on both planar and cantilever sapphire substrates compared to previous Sandia-best LEDs. The LED on planar substrate used the improved growth recipe with the delayed onset of 2-D growth. The near-UV LED on cantilever substrate used a fully coalesced cantilever film of 2 mm posts separated with 5 mm trenches.

— We investigated the effect of strain on light emission in (Al,In)GaN quantum wells and initiated the theoretical investigation of light emission from InGaN quantum dots (QDs) in a GaN matrix.

— We provided E-beam-exposed patterns for photonic lattices to our industrial collaborator. Photonic lattices fabricated in the cladding layer above an InGaN LED exhibited improved light extraction compared to adjacent planar regions.

— We used a 3-D semivectoral model to examine light extraction in LEDs with photonic lattices. We found enhanced light extraction for photonic lattices using spacing corresponding to second- and fourth-order Bragg diffraction.

- *Luminescent materials*

— We obtained and characterized luminescence from cadmium selenium (CdSe) nanocrystal samples from Sandia and Los Alamos National Laboratory and observed strong luminescence.

— We improved the characterization procedure for measurement of absolute external quantum efficiency. We determined quantum efficiency around 33% for 3 nm CdSe clusters capped with ZnS.

— We performed a survey of conventional phosphors and compared results with the phosphors provided by Lumileds Lighting. We initiated development of phosphors via the spray pyrolysis technique with an Albuquerque firm.

— We initiated development of encapsulation and spin-casting of semiconductor nanocrystals. We demonstrated encapsulation of semiconductor nanocrystals in polymer (polymethylmethacrylate [PMMA] and polystyrene) films.

- *Encapsulation*

— We examined alternative catalysts to platinum (Pt) to accelerate the curing of the silicone. Pt catalysis would be poisoned by the semiconductor nanocrystals and some of the conventional phosphors.

— We submitted two TA disclosures on QD synthesis integrated with encapsulation.

We demonstrated a 15 times improvement in near-UV LEDs fabricated on both planar and cantilever sapphire substrates compared to previous Sandia-best LEDs.

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Interfacial Bioscience Grand Challenge (IBIG)

J. S. Schoeniger, M. D. Rintoul, M. J. Stevens, R. Behrens, Jr., S. M. Brozik, A. K. Singh, R. C. Hughes, D. Y. Sasaki, M. M. Young, A. R. Burns, P. Novak, M. Z. Hadi, T. W. Lane, P. S. Crozier, G. H. Kruppa, A. Slepoy, J. M. Faulon

This project focuses on developing bioanalytical tools for elucidating structure-function relationships in membrane proteins (MPs). It was motivated by (1) the need to improve understanding of structure-function issues in MPs, (2) the inadequacy of current methods, and (3) the importance of MPs in processes, such as pathogenesis and intoxication, relevant to the action of biological agents. Despite the significant progress in recent years, there is no compelling evidence that the majority of MPs will be amenable to analysis using standard structure tools (x-ray crystallography, nuclear magnetic resonance [NMR]). IBIG was originally technology-focused and was structured into three technology development cores: structure, imaging, and simulation.

- *Structure core accomplishments.* The structure core focuses on implementing the mass spectroscopy/mass spectrometry method, called *tandem MS/MS (MS3D)* method, for MPs. We implemented a pipeline that goes from actual physical protein to derived geometric constraints, involving protein cross-linking, purification of monomer from dimer, proteolysis, MS, data reduction to produce automated peak lists, and data analysis. To achieve these goals, we overcame a large number of the protein chemistry and bioanalytical barriers that make work with MPs difficult. The External Advisory Committee (EAC) described the capability we developed as “unique.”

- *Simulation core accomplishments.* The simulation core focuses on developing tools to determine MP structures based on diverse constraints. We implemented a code that, for alpha-helical bundle MPs, enumerates the helical bundles consistent with a set of experimental constraints. We also implemented Monte Carlo/simulated annealing codes to further refine these helical bundle structures and are extending these codes to “flesh out” the helical bundle to include amino-acid side chains and loop regions. Finally, we demonstrated a state of the art in molecular dynamics (MD) simulation code for MPs, with timings of 1 ns of simulation time per day on an ensemble of > 40,000 atoms.

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The External Advisory Committee (EAC) described the capability we developed as “unique.”...we demonstrated a state of the art in molecular dynamics (MD) simulation code for MPs, with timings of 1 ns of simulation time per day on an ensemble of > 40,000 atoms.

- *Imaging core accomplishments.* Following the recommendation of the first EAC, the imaging core focused on developing tools targeted at answering specific biological questions. We demonstrated high-resolution (< 1 nm resolution) atomic-force microscopy (AFM) on two-dimensional (2-D) crystals of MPs, and the detection of single-molecule pores using transmembrane impedance measurements. Finally, we imaged isolated cholera-toxin multimers bound to membranes, demonstrating a state-of-the-art capability that can be used to study MP oligomerization.

- *Biology core accomplishments.* The biology core has now conducted extensive studies on the prototypical MP rhodopsin. Specific accomplishments include successful identification of cross-linked peptides from rhodopsin. We also constructed expression systems for bacterial signaling MPs and key proteins involved in mammalian neurotransmission.

Finally, we imaged isolated cholera-toxin multimers bound to membranes, demonstrating a state-of-the-art capability that can be used to study MP oligomerization.

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Biomicrofuel Cell

D. A. Loy, M. Okandan, S. H. Kravitz, D. Ingersoll, C. J. Cornelius, S. M. Brozik, M. H. Beggans, J. H. Fleming, A. W. Walker, C. A. Apblett, C. H. Fujimoto, C. L. Staiger, B. A. Simmons, D. B. Fein, K. R. Zavadil, M. J. Kelly, D. W. Peterson, J. J. Hudgens, C. F. Schmidt, G. S. Grest, A. Santos, A. E. Zivkovich, S. K. Eisenbies, D. A. Stoner, A. R. Straumanis

This project will develop new, compact power sources that can directly and efficiently convert biological fuels, such as glucose or sucrose, into electricity. This project addresses the need for new, autonomous power supplies for chemical/biological (C/B) and ground-based sensor platforms, communications, and microelectronics applications. While current fuel cells have demonstrated clear advantages over batteries in energy density, they still rely on fuels such as hydrogen (H) or methanol that may be inconvenient for many applications. Sandia will develop fuel-cell technologies with biological systems as the renewable energy source. The challenges facing biofuel cells include (1) design of a high-power-density, low-power (< 100 mW) fuel cell compatible with biofuels, (2) preparation of mechanically stable, embossable polymer electrolyte membranes (PEMs), (3) engineering of the appropriate biological interface, (4) development of long-lived, precious-metal or enzymatic electrodes that will completely oxidize the biofuel, (5) design, preparation, and integration of new fuel- and oxidant-selective membranes, and (6) integration of the complete system. This project was recognized by its External Advisory Committee (EAC) as being unique in its systems approach to biofuel cells. They also recognized that the project is poised to yield significant and broadly applicable advances in (1) PEMs and (2) new electrocatalysts that will help realize a U.S. H economy, (3) innovative micro-fuel-cell and biomicromachine architectures, and (4) more sophisticated and robust enzymatic systems. We propose to increase the focus on new PEMs, accelerate the discovery of long-lived electrocatalysts, improve the energy utilization of biofuels, and drive toward a versatile biofuel-cell system. Furthermore, to provide a power supply for C/B weapon and ground-based sensor platforms, we are proposing a modified, more-aggressive project structure that will yield a working prototype biofuel cell.

- Developed new membrane materials that swell less than 5 wt.%. We must still increase the conductivity of our membranes to be comparable to Nafion @ 30 wt.%.

This project addresses the need for new, autonomous power supplies for chemical/biological (C/B) and ground-based sensor platforms, communications, and microelectronics applications. ...This project was recognized by its External Advisory Committee (EAC) as being unique in its systems approach to biofuel cells. They also recognized that the project is poised to yield significant and broadly applicable advances....

- Developed electron mediators for precious-metal and enzyme-conversion approaches. We obtained promising lifetime study results for precious-metal/glucose systems, initiated tests on glucose conversion with enzymes, and started sucrose electrochemistry investigations.

- Designed and fabricated a prototype plant harvester and designed a microneedle harvesting device that is expected to be fabricated before the end of the upcoming fiscal year.

- Developed a new manufacturing paradigm for microfuel cells that enables fabrication of microfuel cells from pre-assembled membrane electrode assemblies. Demonstrated 15 mW/cm² from H and powered light-emitting diode (LED) with cells.

We also considered the positive EAC report to be a significant achievement. The EAC report verified that the project will provide important information to the fuel-cell community and has exciting approaches:

“The biomicrofuel cell represents an application that, in the absence of a Sandia organization and the Grand Challenge approach, would be especially formidable, if not impossible.”

“In addition to the product deliverable, the route itself will generate important and valuable information and technology advances along the way for the fuel-cell community as a whole.”

“Your objectives are well beyond ‘incremental improvements,’ and your technical approaches are very exciting.”

“You are to be commended on how well you have organized and integrated the effort.”

“The biomicrofuel cell represents an application that, in the absence of a Sandia organization and the Grand Challenge approach, would be especially formidable, if not impossible.”

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War on Terrorism

F. T. Mendenhall, M. B. Murphy, M. D. Ladd, J. R. Yoder, R. W. Stinnett, L. G. Stotts, M. C. Reineke, L. J. Ellis, R. A. Griffiths, C. L. Lewis

The motivation behind this project is to neutralize enemy denial and deception by using heterogeneous, disposable, integrated, long-duration, covert sensors arrayed together to track high-value, time-critical targets. This project will not achieve this vision, but it can make substantial progress. This work builds on Sandia's technical capabilities (e.g., unattended ground sensors [UGS] such as tactical UGS [TUGS] and Steel Eagle) to integrate a network of sensors with delivery and exfiltration capabilities for detecting, identifying, and characterizing mobile and time-critical targets. Such a system requires small, low-cost, low-power sensors that may be integrated into a large, reconfigurable network that is capable of multisensor data exploitation and fusion. The development and demonstration of such a network is well suited to Sandia's experience in fielding end-to-end systems, including ground sensors, autonomous robotic vehicles, and intelligent systems.

The project focused on fielding a network set of approximately 10 sensors to collect and fuse data on a specific mobile target and to learn those lessons that can be discovered only under field conditions.

We demonstrated a small group of networked sensors to detect, locate, and locally track a transporter erector launcher (TEL). We met with our External Advisory Committee, who expressed strong support for this project. We identified key technological obstacles that must be overcome for Sandia to provide sense, decide, act, and communicate (SDAC) technology, as defined in the Advanced Concept Group (ACG) TALON report for the War on Terrorism. This project and the Department of Energy's investment in Microsystems and Engineering Sciences Applications (MESA) should put Sandia in a position to produce prototype and field-study hardware systems in the 3–5-year timeframe.

The purpose of the demonstration was to study multiple sensor systems integrated into a cooperative network. We fielded a network of 10 air-deployable seismic-acoustic sensors, 5 mobile images, 8 local area networked (LAN) seismic-acoustic sensors, several networked miniaturized intrusion detection system (MIDS) sensors, one target tracker, and one autonomous tagger in a one-square-mile test area. This is a

This work builds on Sandia's technical capabilities (e.g., unattended ground sensors [UGS] such as tactical UGS and Steel Eagle) to integrate a network of sensors with delivery and exfiltration capabilities for detecting, identifying, and characterizing mobile and time-critical targets. ...The development and demonstration of such a network is well suited to Sandia's experience in fielding end-to-end systems, including ground sensors, autonomous robotic vehicles, and intelligent systems.

significantly larger array of sensor than we expected to accomplish at this point. The addition of an autonomous tagger allows us to examine questions of network sensors taking immediate action without human intervention. Data collection on these sensors has started and will continue. This test-bed allows us to explore questions of mixed-mode sensors, network communications, data fusion, mission planning tools, and mission operation center requirements.

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Materials Science and Technology

The Materials Science and Technology investment area researches materials that behave in a predictable manner during all phases of their life cycle. Research investigations focus on advancing Sandia's commitment to microsystems—these microsystems will utilize optical, electromechanical, magnetic, and chemical functions to sense, think, act, and communicate. Research efforts also support the revolution in nanoscale science and technology, science-based materials and processing, and predictable performance of complex systems. This research offers the opportunity to build tailored materials and structures atom by atom. Technological developments are expected that will rival the impact of the transistor.

Solidification is an important aspect of welding, brazing, soldering, and casting. For these processes, solidification affects and, in many instances, controls the final properties of the product. “Diagnostics for Joining Solidification/Microstructural Simulations” is identifying key physical phenomena in, and expanding and refining our mechanistic descriptions of, solidification in the iron-chromium-nickel system. Sandia developed and will continue to refine new and expanded experimental techniques, particularly those needed for *in situ* measurement of the kinetic features

of the solidification process. This work will support development of engineered materials with many defense applications. Two patent disclosures have been filed.

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Next-Generation Output-Based Process Control: An Integration of Modeling, Sensors, and Intelligent Data Analysis

R. A. Neiser, Jr., A. J. Mayer, R. C. Dykhuizen, J. W. Cates

The goal of process-based quality is to accept War Reserve (WR) product without inspection. For simple processes, traditional feedback control of process input variables might achieve this goal. However, input-based (upstream) control systems are a major source of Defense Programs (DP) production problems for complex processes because it is impractical, if not impossible, to understand and control all of the factors that affect process output. The primary goal of recent work at Sandia was to sufficiently refine the techniques developed in previous work so they could be transferred to DP production flame-spraying of neutron generators (NGs). A second goal was to demonstrate that this basic approach could be used to control other thermal-spray coating processes.

The primary work areas in this project were to continue testing and improving the robustness of the feedback-control techniques developed previously, continue working with NG production personnel to transfer this technology to DP production, and test the control techniques on a different thermal-spray process.

The basic control algorithm chosen for the wire flame-spray process is based on a proportional-integral control scheme. We modified it to account for the fact that the two process inputs (flowrate of combustion gases and flowrate of air) are not independently related to the two process outputs (particle temperature and particle velocity). A third degree of freedom (DOF), the combustion-gas equivalence ratio, was not required for this control system and is reserved for future use. The system's response time is several seconds and is limited by the characteristics of the gas mass flow controllers and the length of the gas lines from the gas controller to the torch. The major sources of drift in particle temperature and velocity identified to date have characteristic times longer than the system response times, so this control approach seems adequate.

We conducted several important tests of process robustness. A key assumption in the control process is that the particle stream measured by the sensor is spatially stable and that the temperature and velocity gradients of the particle stream are small enough that slight inaccuracies in the relative location of the sensor and the particle stream do not cause the control

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algorithm to inadvertently drive the gas settings to inappropriate values. A variety of tests demonstrated that the wire curvatures and the positional accuracy of the sensor that can be attained on a regular basis are adequate to provide results that are insensitive to the slight positional shifts and shallow gradients observed along the centerline of the jet.

We tested the control algorithm using a second thermal-spray process. The powder flame-spray process is similar to the wire flame-spray process in that material is fed into an oxy-fuel flame, where it is melted and accelerated. However, significant differences in torch geometries result in substantial differences between the two processes. As a result, the relationships between gas flows and particle temperatures and velocities are very different in the powder flame-spray process. Despite these differences, we were able to fairly quickly develop a control algorithm that yielded stable particle temperatures and velocities.

We developed, tested, and deployed into WR production a feedback-control technique that dynamically adjusts process inputs (i.e., gas flows to a thermal-spray torch) to hold process outputs (i.e., average particle temperatures and velocities) constant. The basic approach was to first identify and correct as many as possible of the factors that caused process variability. Second, we developed a real-time sensor and control algorithms, which we used to identify and compensate for any remaining drifts in the process. Finally, we tested the control technique for robustness to ensure that it would not unexpectedly and inadvertently adjust the process to unreasonable conditions. The techniques developed during this project can be used to improve the reproducibility and quality of thermally sprayed coatings; however, they should not be used without first having a thorough understanding of the process to be controlled.

The techniques developed during this project can be used to improve the reproducibility and quality of thermally sprayed coatings; ...

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10735

Physical Basis for Interfacial Traction-Separation Models

N. R. Moody, E. D. Reedy, Jr., M. S. Kent

Many weapons components contain interfaces between dissimilar materials where cracks can initiate and cause components to fail. In recent years, many researchers in the fracture community have adopted a cohesive zone model for simulating crack propagation (based on traction-separation [T-U] relations). While Sandia is implementing this model in its Accelerated Strategic Computing Initiative (ASCI) codes, an important obstacle to using a cohesive zone modeling approach is that currently, T-U relations are chosen in an ad hoc manner. The goal of the present work is to determine a physical basis for mesoscale-level T-U relations. We are performing experiments that will elucidate the dependence of such relations on adhesive and bulk properties. Work will focus on epoxy/solid interfaces, although the approach is applicable to a broad range of materials. Sandwiched-layered double-cantilevered beam (SDCB) and free-surface film nanoindentation fracture-toughness tests will generate a unique set of data spanning length scales, apply mode mixities, and yield (plastic) zone constraint. We will define the crucial roles of crack-tip plastic zone size and interfacial adhesion by varying epoxy-layer thickness and using coupling agents or special self-assembled monolayers (SAMs) in preparing samples. We will probe the nature of the yield zone in collaborative experiments run at the Advanced Photon Source (APS). This work will provide an understanding of the major mesoscale phenomena governing polymer/solid interfacial fracture and identify the essential features that must be incorporated into a T-U-based cohesive zone failure model. We believe that models using physically based T-U relations will provide a more accurate and widely applicable description of interface cracking than models using ad hoc relations. Furthermore, these T-U relations will provide an essential tool for using models to tailor interface properties to meet design needs.

Sandia has determined thickness, mode mixity, and constraint effects on interfacial fracture toughness; used a T-U relationship to simulate crack growth; and imaged crack-tip deformation zones. These results advanced our understanding of epoxy/solid interactions, development of fracture test techniques, design of fracture samples, and the development of techniques to perform crack-growth simulations to assess potential T-U relationships. We determined interfacial fracture

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energies for films ranging from 500 μm to 24 nm in thickness and required the use of four film fracture-test techniques. In all cases, fracture occurred cleanly along the film-substrate interface. Superposition of results showed that fracture energies decreased monotonically with film thickness to a lower-limiting mode I value of 0.5 J/m². This value is significantly higher than the work of adhesion for uncured epoxy oligomers on a methyl-terminated aluminum (Al) surface and indicates irreversible specific interactions such as hydrogen bonding.

We employed SAMs to determine how interfacial adhesion controls susceptibility to fracture of epoxy on Al. The epoxy bond layer consisted of a 100:46 ratio of Epon 828 resin and T403 hardener coated to a nominal thickness of 500 μm . We controlled adhesion using mixed SAMs terminated with a mixture of methyl groups and either bromine atoms or amine groups. The latter two both react covalently with the epoxy adhesive used in this work. Compositions ranged from 100% methyl-terminated to 100% termination with a reactive group. We used a number of methods to verify the quality of the surface treatment (density and composition) and consistency, including contact angles, x-ray photoelectron spectroscopy (XPS), and secondary ion-mass spectrometry (SIMS). We developed a special method to coat very thin films of epoxy on the SAMs, avoiding the tendency for dewetting. This accomplishment allows a complete study of thin-film fracture toughness over the entire range of interface strength. The measured interfacial toughness increased by more than a factor of 10 as the interfacial interactions were varied from being purely weak van der Waals bonding to strong chemical bonding. When we fabricated submicrometer-thick films using the same SAM systems, failure occurred in the film or along the film-overlayer interface. The results showed that use of these SAMs greatly increased film adhesion.

In a complementary modeling effort, we performed interfacial crack-growth simulations using (1) a cohesive zone-separation criterion based on the molecular work of separation and a critical separation distance of 1.0 nm, and (2) large-strain constitutive models for the deformation within the highly deformed crack-tip process zone. Calculated results for an elastic-perfectly plastic model show extensive crack-tip blunting and fail to generate the observed large increase in interfacial toughness relative to the molecular work of separation. Recent work indicates that the analysis may need to include rapid hardening at large strains (simulating orientation hardening) to generate a substantial increase in interfacial toughness relative to the molecular work of separation.

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We used x-ray scattering and imaging techniques to study structural evolution near crack tips using a microfocused beam at the APS in the absence of load. The spectrum did not vary detectably with position of the beam relative to the crack tip over the q range investigated, which seems to indicate that the deformation was limited to a much smaller length scale around the crack tip. Further work expanding the study to a higher q range (where the peaks are more distinctive of changes in the crystalline structure) and smaller spot size is in progress. We applied x-ray tomography to study the structure in an epoxy near a notch tip. Thus far, we obtained data only in the absence of load. The image quality obtained was excellent, indicating that the method has promise. In future work, we will repeat the imaging as a function of load until the samples fracture.

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10740

Diagnostics for Joining Solidification/ Microstructural Simulations

C. V. Robino, G. A. Knorovsky, J. A. Brooks, J. R. Michael, A. C. Hall

Solidification is an important aspect of welding, brazing, soldering, laser-engineered net shaping (LENSTM) fabrication, and casting. For these processes, solidification affects and, in many instances, controls the final microstructure and properties of the product. The current trend toward utilizing large-scale process simulations and materials response models for simulation-based engineering is driving the development of new modeling techniques. However, the effective utilization of these models and simulations is, in many cases, limited by a lack of fundamental understanding of the subprocesses and interactions involved, and experimental validation of model predictions is required. This project focused on identifying key physical phenomena in, and expanding and refining our mechanistic descriptions of, solidification in the iron-chromium-nickel (Fe-Cr-Ni) alloy system. A secondary focus was on developing new quantitative experimental approaches for characterization of solidification phenomena. The Fe-Cr-Ni alloy system displays a wide range of behavior; is of substantial interest both internally and externally, and strongly leverages previous work.

Sandia developed new and expanded experimental techniques, particularly those needed for in situ measurement of the morphological and kinetic features of the solidification process. The new high-speed, high-resolution video techniques and data-extraction methods developed in this project identified several unexpected features of the solidification process, including the observation that the solidification front is often far more dynamic than previously thought. To demonstrate the utility of the video techniques, we made correlations between the in situ observations and the final solidification microstructure. We developed, implemented, and used experimental methods for determining the solidification velocity in highly dynamic pulsed-laser welds to validate and refine laser-welding models. Using post-solidification metallographic techniques, we discovered a previously unreported orientation relationship between ferrite and austenite in the Fe-Cr-Ni alloy system and characterized the conditions under which this new relationship develops. This work expanded both our understanding of, and our ability to characterize, solidification phenomena in complex alloy systems and processes.

This image of a metallic solid-liquid interface is a single frame taken from a high-speed video of a gas-tungsten arc weld in stainless steel. Observations like this are used to better understand solidification mechanisms and processing in complex engineering alloys.

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In recent work, we directed our efforts toward two principal areas: (1) refining and applying the newly developed, high-resolution optical techniques for studying solidification, and (2) defining the conditions under which the newly discovered orientation relationship between ferrite and austenite in Fe-Cr-Ni alloys is formed.

We successfully filmed the solid-liquid interface in a variety of welds at high magnification and high frame rates. We developed algorithms to extract quantitative information about the motion and evolution of the solid-liquid interface. Unlike other experimental techniques, the high-speed, high-magnification video can provide information about solid-liquid interface motion in engineering materials in actual welding environments. Primary and secondary dendrite arm spacing, measured dynamically at the surface of the weld pool, was associated with features deeper in the pool by using comparisons with post-welding metallography.

We also investigated the weld-rippling phenomenon. Based on measurements of the solid-liquid interface velocity associated with the weld-ripple formation, we determined that this velocity changes during the ripple formation. It was also evident that the instantaneous growth direction at the solid-liquid interface changes during the ripple event. Optical metallography showed that the ripple features observed on the surface are present throughout the volume of weld bead. Electron microprobe analysis confirmed that compositional variations are also associated with weld ripples. We correlated Cr and Ni concentration changes with solute redistribution models based on solidification velocity.

We made time-resolved measurements of the liquid pool diameter in small laser spot welds. We compared these data directly to predicted values of liquid pool diameter generated from a physics-based model of laser spot welds. At higher laser powers, the experimental data matched the predicted values closely over the duration of the spot weld. While the model correctly predicted the final diameter of the laser spot weld at lower laser powers, the predicted diameter did not match the measured diameter over the entire duration of the weld. This suggests that additional phenomenological refinements need to be incorporated into the model. The primary improvements required in the model are a better definition of the laser heat flux and verification of the material properties used. The experimental techniques used to measure the laser spot welds in this investigation are relatively straightforward and provided a tremendous amount of information. In particular, the ability to

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capture the dynamic phenomena associated with the laser spot weld provides a basis for significant improvement in the model.

We characterized the solidification modes and solid-state transformations of laser-deposited Fe-Ni-Cr alloys. Solidification velocities and cooling rates were sufficient in some cases to change the solidification mode from that predicted from calculated phase diagrams. In ferrite/austenite (F/A) solidified deposits, all the ferrite exhibited a unique orientation relationship with the austenite, either Kurdjumov-Sachs (K-S), Nishiyama-Wasserman (N-W), or the newly discovered Headley-Brooks (H-B) relationship. In some cases, we found that subsequent thermal cycles reduced the amount of ferrite retained from the original deposit. In other structures, we altered the concentration profiles by on-heating and on-cooling transformations. Although the calculations indicated that solidification occurs in the F/A mode, we found that the laser deposits of these alloys exhibit a range of solidification modes. These were dependent on both composition and processing conditions. An unexpected observation was that in all the F/A solidification structures examined in an alloy with a Cr/Ni equivalent ratio of 1.53, the ferrite and austenite exhibit a unique orientation relationship of either K-S, N-W, or H-B. However, only one orientation relationship was found to exist in any single austenite grain.

We believe that the work conducted in this project has expanded both our understanding of, and our ability to characterize, solidification phenomena in complex alloy systems and processes.

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10741

Effects of Microstructural Variables on the Shock-Wave Response of PZT 95/5

R. E. Setchell, J. A. Voigt, B. A. Tuttle, E. L. Venturini, M. U. Anderson

Sandia is responsible for the design and production of explosively driven power supplies. These devices utilize shock-wave depoling of the ferroelectric ceramic lead zirconate titanate (PZT) 95/5 to provide a high-voltage output. Production of these devices will change within a few years to PZT 95/5 material prepared at Sandia using a new “chem prep” process. This process, still under development, can vary the porous microstructure within the final ceramic by adding different types and quantities of organic pore formers prior to bisque firing and sintering. Early empirical studies showed that the porous microstructure can have a profound effect on device performance: The rate for failures due to high-voltage breakdown at low temperatures was acceptably low only in materials made within a narrow density range. However, little was known about how microstructural features actually influence the constitutive mechanical, electrical, and phase-transition properties that govern the dynamic depoling process. This project represents the first systematic study of the basic physics of microstructural effects on PZT 95/5 electromechanical behavior under shock loading. We performed comparative shock-wave experiments on PZT 95/5 materials in which both the quantity and the type of added organic pore formers were varied. Pore geometry ranged from rods to spheres, with characteristic dimensions of less than 10–140 μm . Bulk densities ranged from 6.94 g/cm^3 (13.2% porosity) to 7.66 g/cm^3 (4.3% porosity). Experiments examined both the constitutive mechanical properties, as revealed by transmitted wave profiles, and the depoling kinetics during the shock-driven phase transition, as revealed by depoling currents measured in external circuits. The results established that the most important microstructural parameter is total porosity, which improves electrical performance and minimizes the risk of a late-time failure mechanism when reduced. However, a different, early-time failure mechanism is probably enhanced at very low porosities. We showed pore morphology to be relatively unimportant, except possibly at the largest pore sizes.

Initial studies focused on “chem prep” materials in which we varied the total porosity resulting from the addition of a particular type of pore former (Avicel). This pore former is in the form of rods 5–15 μm in diameter and greater than 20 μm in

This project represents the first systematic study of the basic physics of microstructural effects on PZT 95/5 electromechanical behavior under shock loading.

length. We performed gas-gun experiments on materials having densities ranging from 6.98 to 7.65 g/cm³. Most of these experiments used samples having an average density of 7.30 g/cm³, which matched the density of a particular mixed-oxide (MOX) batch that was extensively characterized under the MAVEN program. This material was prepared using spherical pore formers having 50–100 μm diameters. Experimental conditions were chosen to allow current results at this density to be compared directly with the previous results. More recently, we examined “chem prep” materials having a fixed density of 7.30 g/cm³ but prepared using different batches of spherical pore-formers (Lucite) in which the sphere diameters varied from 15 μm to 140 μm . We conducted additional comparative experiments with a high-density, MOX material prepared with no pore-former addition. For each material type, experiments were typically conducted on both unpoled samples and normally poled samples (polarization perpendicular to shock motion). We used unpoled samples to obtain basic shock Hugoniot data in reverse-impact experiments and to examine constitutive mechanical properties in transmitted-wave experiments. We varied impact velocities to change shock pressures and used laser-velocity interferometry (VISAR [velocity interferometry system for any reflector]) to record wave profiles at an interface within the target assembly. We examined depoling kinetics associated with the shock-driven phase transition in normally poled samples by measuring depoling currents in an external circuit. We examined the effects of strong electrical fields by adding a large, resistive load to the external circuit. We also recorded transmitted waveforms in these experiments using laser interferometry.

The 32 shock experiments conducted during this project provided a fairly comprehensive examination of how the porous microstructure in PZT 95/5 influences the material behavior during shock loading. An important conclusion is that the pore morphology in common-density materials has little effect on dynamic material properties. We made comparisons at 7.30 g/cm³ using materials made with both the small Avicel rods and the Lucite spheres having diameters of 15, 80, or 140 μm , or a distribution from 50 μm to 100 μm . We observed slight differences in charge release between “chem prep” and older MOX materials, and wave profiles had extended risetimes in the material made using 140 μm spheres. The threshold for dynamic yielding (when shear strength is lost) was highly consistent for all these materials. In contrast, we found shock properties to be very sensitive to the total material porosity. We

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found Hugoniot states, total charge release, and yielding thresholds to vary significantly over the density range studied. In particular, yielding thresholds increased by more than a factor of 2 as density was increased. The yielding mechanism in this ceramic is likely to include significant fracturing, and subsequent unloading following yielding (which occurs in actual power supplies) can result in damaged material with greatly reduced insulating capabilities. A subsequent onset of electrical conduction results in a late-time device failure, and the probability for such a failure process increases with decreasing density. Increasing density not only avoids this failure process, but also produces higher depoling currents resulting from increased remanent polarization and higher shock speeds. Early studies found that prompt high-voltage breakdowns occurred in high-density samples, however, leading to upper bounds on acceptable density values. Although available documentation on this early testing is sparse, higher initial shock pressures in the high-density materials may have been above a threshold for shock-induced conductivity. Optimizing both performance and reliability in power supplies may require both optimization of PZT 95/5 microstructure and tailoring of the explosively generated shock wave that propagates through the device.

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10742

Mechanisms of Dislocation Grain-Boundary Interaction

D. L. Medlin, J. E. Houston, K. J. Gross

Incorporating the localized atomistic and microscopic effects of internal interfaces on materials properties and long-term behavior is a significant challenge for large-scale materials simulations. Critical to improving such models is developing a basic understanding of the dislocation grain-boundary interactions that ultimately control the interfacial response to strain. Such interactions impact many materials phenomena and properties, including slip transmission, boundary migration, recrystallization, and yield strength, and are a critical element in linking atomic structure to continuum behavior. In this project, Sandia seeks to develop an experimentally based understanding of these dislocation grain-boundary interactions.

In this project, Sandia seeks to develop an experimentally based understanding of these dislocation grain-boundary interactions.

(1) Using high-resolution transmission electron microscopy (HRTEM), we analyzed the structure of grain-boundary dislocations at $\Sigma=9$ boundaries in gold (Au) and aluminum (Al) bicrystals. Although the interfacial structure in the Al case was compact, in some cases we found dissociated dislocations (stacking faults) extending from the Au boundaries. This is consistent with the lower stacking fault energy of Au (32 mJ/m²) compared with Al (160 mJ/m²).

(2) We made significant progress in applying and extending our Shockley Partial Dislocation (SPD) model for interfacial structure.

- Through comparisons with our experimental analysis of $\Sigma=9$ boundaries, we employed the SPD model description outside the previous limiting misorientation range of 50.5°–109.5°. To accomplish this, we considered the structural implications of combining multiple arrays of SPDs.

- We experimentally confirmed predictions of the formation of a layer of hexagonal close-packed (HCP) stacked material near the $\Sigma=43$ boundary in Au.

- We also tested this model by experimentally studying the intersection of a $\Sigma=3$ (112) boundary with a $\Sigma=11$ (131) boundary in Au. Both of these interfaces are well described by simple arrays of SPDs, and the combination of these arrays yields, as predicted, an array of 60-degree lattice dislocations. This establishes a key linkage between lattice dislocations, which are responsible for deformation in the bulk, and grain-boundary geometry.

(3) Through TEM studies, we showed how interfacial steps possessing dislocation content (disconnections) can accommodate grain-boundary coherency strains in a manner similar to misfit dislocations. This is important to establishing the connection between grain-boundary morphology and the resulting long-range elastic strains that ultimately govern the interaction of lattice dislocations with a grain boundary.

Refereed

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10754

Functional Materials for Electrochemomechanical Actuation of Microvalves and Micropumps

J. R. McElhanon, L. L. Whinnery, Jr., D. A. Chinn, S. H. Goods, T. Zifer

It is generally recognized that the development of integrated microsystems for Defense Programs (DP) applications, chemical sensing, and medical devices will require fast, efficient microactuators that can function as valves and pumps. Conventionally actuated devices can affect the operating characteristics of microsystems and cannot be miniaturized without significant loss of performance. Sandia plans to take advantage of electrochemomechanical (ECM) functions of conductive polymers to be used as the work-producing unit in microactuators. We will focus on tailoring molecular structure and composition of conductive polymer gels to optimize physical and mechanical response to electrochemical stimulation. Conductive polymer actuators have significant advantages over other approaches in their ability to produce high force and large displacement using low power. Polymer-gel development will include the design and synthesis of a variety of linear and cross-linked polymer gels. We will develop and implement methods of expansion and contraction and force generated during electrochemical stimulation. We will also measure and optimize hysteresis, reversibility, and lifetime of polymer systems. We will design, build, and test polymer actuator geometry and micro-electrodes to optimize microscale performance, including response rate, displacement, force, and lifetime. ECM response (extension, force, rate, and lifetime) of conductive polymer gels will be systematically characterized with respect to applied potential, temperature, and gel electrode geometry. Our principle goals are (1) to obtain a fundamental understanding of structure/property/response relationships of conductive polymers with respect to the ECM phenomena, and (2) to build a prototypical ECM-based valve that is inexpensive, easily manufactured, and adaptable to integrated microsystems.

- *Extension, morphology, and lifetime.* To investigate the role played by morphology in preparing gel actuators that would undergo greater extensions, we turned our efforts toward engineering porosity into polymer gels using thermally induced phase separation (TIPS). Ideally, a honeycomb or open-cellular structure would have thin enough walls, providing a continuous structure to increase the extension. Engineered porosity of these

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gels should also lead to faster response times and greater forces generated. We prepared a polyoctylthiophene (POT) TIPS-modified gel from commercial POT, using a previously described procedure. The result was a gel having a honeycomb-like morphology. Unfortunately, we observed little enhancement to extension, with approximately 2% extension measured during reversible actuation. Attempts at preparing TIPS-modified polyhexylthiophene (PHT) gels were unsuccessful due to poor solubility in benzene.

Our results indicate that conducting cross-linked and noncross-linked polythiophene gels with varying morphologies; commercial, linear, compressed polythiophene polymers; and polythiophene polymer gels prepared with engineered porosity through TIPS all show similar extension characteristics. Only synthesized, linear PHT exhibited relatively larger extensions of 4%–6%. These data suggest that morphology plays little role in the extension profiles of these conducting polymer systems under the conditions of our experiment. Lifetimes of the gel systems studied appear to be greater for the linear thiophene polymers. The shorter lifetime of the cross-linked polythiophene gels studied, in comparison with their linear analogues, may be suggestive of mechanical failure due to their cross-linked nature.

- *Rate and electrode geometry.* Rates of polymer actuation are similar for all polymer gels examined under our experimental conditions. Extension and contraction occur over minutes. Such rates are too slow for practical functional devices.

One explanation for such slow responses may be localized oxidation of the gel due to electrode geometry. Much of the polymer gel may not be oxidized due to the one-point attachment of the platinum (Pt)-wire electrode. Also, since rate of actuation is diffusion-limited, thinner gels having a more uniform electrode surface may lead to an enhancement in rate and extension. If this new electrode geometry were successful in enhancing rate of actuation, we would consider preparing multiple, stacked, gel arrays. We anticipated that multiple, stacked, thin-gel arrays would lead to enhanced rate and force generation.

Accordingly, we prepared thin samples of commercially available PHT by compressing the material into pellets. The PHT pellets were then uniformly coated with a Pt electrode surface on one side. We subsequently attached a Pt wire with silver epoxy. We made extension measurements under identical conditions using this new electrode geometry for a single PHT pellet. Commercial PHT exhibited an axial dimensional change

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of 6%, analogous to synthesized PHT. No signs of gel failure or degradation for the duration of the test (> 1400 minutes, 70 cycles) were observed. We observed no noticeable enhancement in rate of actuation using this more uniform electrode geometry. As a result, we abandoned attempts at creating multiple, stacked, gel arrays using gels coated with uniform Pt electrode surfaces.

10761

Making the Connection Between Microstructure and Mechanics

E. A. Holm, T. E. Buchheit, G. W. Wellman, C. C. Battaile

The purpose of microstructural control is to optimize materials properties. To that end, Sandia developed sophisticated and successful computational models of both microstructural evolution and mechanical response. However, there is currently no way to couple these models to quantitatively predict the properties of a given microstructure.

This problem arises because current continuum response models, such as finite-element (FE), finite-volume (FV), or material-point methods, do not incorporate a real length scale. Thus, two self-similar polycrystals have identical mechanical properties regardless of grain size, in conflict with theory and observations.

In this project, we took a tiered risk approach to incorporate microstructure and its resultant length scales in mechanical response simulations. Techniques considered include low-risk methods that are likely to work (albeit with shortcomings) as well as higher-payoff, higher-risk methods. Methods studied include a constitutive response model with a local length-scale parameter, a power-law hardening-rate gradient near grain boundaries, a local Voce hardening law, strain-gradient polycrystal plasticity, and a subgrain breakup model. We validated these techniques on a variety of systems for which theoretical analyses and/or experimental data exist, including tension and bending experiments on bicrystals and polycrystals. We used the results to generate improved constitutive models that explicitly depend on microstructure and to provide insight into microstructural deformation and failure processes.

Because mechanical state drives microstructural evolution, we coupled a strain-enhanced grain-growth model with the mechanical response simulation. The coupled model predicted both properties as a function of microstructure, and microstructural development as a function of processing conditions.

Incorporating microstructure into mechanical response simulations benefits Sandia's research, development, and manufacturing missions. Solving this problem will provide a new tool for scientific insight and model development in materials science, engineering science, and process design and control for a variety of internal and external customers.

- Deploy Voce hardening model into polycrystal plasticity finite-element model (PPFEM). The physical mechanism for

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strain hardening is often considered to be dislocation pileup near grain boundaries. We developed a Voce hardening law, in which the hardness of an element is related to its distance from a grain boundary, to model this phenomenon in polycrystal simulations. This model with a distance exponent of -1 reproduced experimental data on polycrystalline copper (Cu). We subsequently deployed this model in Sandia's JAS3D FE code and exercised it on large-scale polycrystals.

- *Develop simplified strain-gradient constitutive model for PPFEM.* We developed a simplified strain-gradient constitutive model suggested by Beaudoin to incorporate nonlocal hardening effects. This model was successful at reproducing grain-size-dependent behavior in polycrystals (Hall-Petch). The model was deployed in Sandia's JAS3D FE code.

- *Analyze coupled microstructural and mechanical evolution in realistic polycrystals.* Because stress state and microstructure are interdependent, we developed a strain-enhanced microstructural evolution model using the front-tracking method. Grains are grown for several timesteps, the evolved microstructure is passed back to the PPFEM simulation for re-equilibration, and the process repeats. We performed the largest and longest coupled simulations of this type and analyzed the results. This work provides insight into important deformation processes.

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10779

Switchable Hydrophobic-Hydrophilic Surfaces

B. C. Bunker, R. P. Manginell, J. G. Curro, D. L. Huber, M. S. Kent, C. M. Matzke

*The ability to perform chemical and biological analyses on a microchip requires understanding how to transport, separate, and detect species in nanoliter quantities of liquid confined in channels with micrometer-scale dimensions. At such small length scales, surface effects play a dominant role. The objective of this project is to investigate mechanisms for switching the chemistry of a surface using temperature-induced phase transitions in organic coatings. The specific polymer investigated, poly *n*-isopropylacrylamide (PNIPAM), exhibits a lower critical solution temperature of 30°C. Below this temperature, the polymer swells in water to make a hydrophilic surface that is protein repellent. Above the transition temperature, the polymer collapses to form a hydrophobic surface that adsorbs proteins.*

Sandia's research activities involved (1) synthesizing tethered PNIPAM films in geometries that support a hydrophobic-hydrophilic transition, (2) characterizing conformation changes in the polymers and the impact of transitions on surface energies, (3) modeling chain conformations, the kinetics of phase transitions, and surface energies using Monte Carlo (MC) and molecular dynamics (MD) simulations, and (4) fabricating and using integrated microfluidic systems in which the phase transition in PNIPAM could be utilized to perform a wide range of switchable functions. Results suggest that while PNIPAM phase transitions do occur and promote significant changes in water-contact angles, the resulting changes in interfacial energy are insufficient to pump fluids through microchannels. However, the transition is sufficient to induce the adsorption and desorption of proteins, leading to the development of a switchable protein trap.

- *Synthesis of tethered PNIPAM films.* To be useful for microfluidic applications, PNIPAM films must be strongly attached to the surface in a configuration that supports a reversible thermally activated swelling transition in water. We investigated four schemes for attaching PNIPAM to either oxide or gold (Au) surfaces, each of which involved the use of self-assembled monolayers (SAMs): (1) grafting of carboxylic acid-terminated PNIPAM chains to hydroxyl-terminated SAMs (forming an ester linkage), (2) forming PNIPAM via *in situ*

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free-radical polymerization on SAMs terminated with an azo-initiator that could be heat- or light-activated, (3) forming PNIPAM via *in situ* polymerization on thiol-terminated SAMs via a “chain-transfer” polymerization process, and (4) *in situ* polymerization of PNIPAM via a “living polymerization” process involving an atom-transfer radical polymerization process. We obtained best results on the high-molecular-weight, low-grafting-density azo-films and the low-molecular-weight, high-grafting-density chain “polymer brush” films produced via chain-transfer polymerization.

- *Characterization of phase transitions.* We characterized the swelling transition in PNIPAM using a combination of ellipsometry, surface-plasmon resonance (SPR) techniques, attenuated total-reflectance infrared (ATR-IR) spectroscopy, interfacial-force microscopy (IFM), and neutron-reflectivity (NR) experiments. Ellipsometry, SPR, and ATR-IR results were consistent with the presence of a PNIPAM film that is swollen in water at room temperature and collapses above the transition temperature by about a factor of 2. We measured film thicknesses for both the azo-film and the polymer brush as a function of temperature using IFM, confirming a change of a factor of 2 in film thickness above and below the transition temperature. The NR results provide PNIPAM density profiles, suggesting that a PNIPAM layer may be present at the immediate surface that is too dense to undergo a swelling transition. A low-density, outer PNIPAM layer appears to be the region supporting the transition observed using the other experimental methods.

- *Theory and modeling activities.* We developed theoretical models to support the experimental characterization and to provide insight into the factors controlling the switching transition in PNIPAM. The first phase of the modeling effort involved simulating the behavior of simple polymers immersed in a simple solvent using a self-consistent polymer reference interaction site model (PRISM) theory. We used the PRISM theory to estimate phase diagrams for “normal polymers” in “normal solvents.” Results showed that phase separation occurs even when solvent-polymer interactions are equivalent to solvent-solvent and polymer-polymer interactions due to nonrandom mixing and compressibility effects that are not included in classical Flory-Huggins theory. We modeled tethered polymers with self-consistent field (SCF) theory. With SCF theory, we generated theoretical density profiles that quantitatively agree with profiles obtained experimentally using neutron reflectivity. The results indicate that interactions of

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polymer segments with the surface are important in mediating swelling transitions in tethered polymer films.

- *Applications in microfluidic devices.* We evaluated PNIPAM films for two applications in microfluidic systems: (1) fluid pumps based on switching of interfacial energy, and (2) reversible adsorption of proteins for on-chip protein separations. For the first application, calculations suggest that if water-contact angles could be switched by 10 degrees or more, the phase transition in PNIPAM could be used to pump liquids in microchannels. Unfortunately, while the advancing contact angle in water changes by up to 25 degrees through the transition, the hysteresis between advancing and receding contact angles currently prevents PNIPAM films from being useful for pumping applications. However, experiments show that protein adsorption can be reversibly switched on PNIPAM films. We developed an integrated microhotplate device with PNIPAM as the active element. Fluorescence microscopy with labeled proteins shows that the trap can rapidly grab and release proteins from solution, opening up a wide range of biosensors, bioseparations, and biomedical applications.

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10789

All-Ceramic Battery

T. J. Boyle, D. Ingersoll, J. A. Voigt, K. Rahimian, R. T. Cygan, M. A. Rodriguez

To achieve autonomy, we need the production of a thin-film all-ceramic battery that uses power sources that generate the necessary power and energy to operate microsystems without substantially increasing the size of the device. Thin-film batteries are an attractive power source for these applications; however, currently they are inadequate to operate the microsystems effectively. Sandia seeks to develop a rechargeable thin-film all-ceramic lithium-ion battery (ACB) using solution route deposition methods. The ACB will have higher-power output, longer run times, and a greatly simplified production scheme in comparison to existing technology. Several ACB prototypes (normal and inverted) have been generated using the above chemistries; however, shorting has complicated the electronic testing. Once sufficiently developed, these ACBs will have the versatility to power any number of small systems, such as microsystems and miniature autonomous robotics.

Our investigation into the development of an ACB yielded the following generalized results:

- *Cathode.* We successfully developed a novel sol-gel route to LiCoO_2 . We used novel $[\text{Li}(\text{ONep})]_8$, $\text{Co}(\text{OAc})_2$ in pyridine/HOAc and found films to be recyclable. We monitored changes by x-ray diffraction (XRD). We developed single-source LiCoO_2 precursors that were also found to be cyclable.
- *Anode.* We developed a novel sol-gel route to SnO_x . We used novel $[\text{Sn}(\text{ONep})_2]_\infty$ in HOAc and identified the various products formed in this process. They were found to be cyclable by electrochemical evaluation.
- *Electrolyte.* We developed a novel sol-gel route to $(\text{LiLa})\text{TiO}_3$ (lithium lanthanum titanate, or LLT). We used $[\text{Li}(\text{ONep})]_8$, $\text{La}(\text{DIP})_3(\text{py})_2$, and $[\text{Ti}(\text{ONep})_4]_2$ in tol/py mixtures. Processing into films required rapid thermal processing (RTP) methods (900°C), and testing is under way. We also developed a novel route to ormolyte thin films.
- *Computer modeling.* We developed computational methods to evaluate the individual components and evaluated the strain between the cathode and bottom electrode. We also calculated optimization of the desired stoichiometry of LLT.
- *ACB construction.* We undertook integration of the layers and observed continuous films by scanning electron

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microscopy (SEM). We observed little mixing by SEM. All films show electrical shorting.

Refereed

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26525

Magnetic-Field Effects on Vacuum-Arc Plasmas

P. A. Miller, M. M. Hopkins

The two main goals of this project are to understand the role of the self-magnetic field on the vacuum-arc ion source in neutron tubes and to realize magnetic shaping of the plasma plume from the ion source, thereby enabling increased plasma utilization efficiency, reduced stress on the electrode films, and reduced electrical drive requirements. Prior to this project, computational and experimental studies of neutron tubes had neglected magnetic field effects.

In earlier work, we fabricated and tested experimental hardware, data-acquisition system, and data-analysis software for magnetic-field tests. The primary diagnostic is an array of 16 Langmuir probes. We performed initial computational tests, selecting the Large-Scale Plasma (LSP) code for all subsequent work. In recent work, we showed experimentally that modest applied fields (< 300 Gauss) strongly influence arc impedance, plasma-plume shape, and total ion output. This field level is comparable to the self-magnetic field of the arc. We modified the probe array with the addition of a rotation capability that allows mapping the plasma plume with 64 probe positions. We found that 2-D LSP magnetostatic calculations agree with some of the experimental measurements and successfully performed 3-D EM calculations on an initial test case. The 2-D calculations show a weaker effect of the applied magnetic field on the arc impedance than seen experimentally. Tentatively, we attribute this difference to the modeling of the real filamentary 3-D arc by a 2-D disk, which is a restriction inherent in the 2-D model. The 2-D calculations generally agree with experiment that a uniform axial magnetic field causes concentration of the plasma plume on axis at distances of 10 mm or greater in front of the ion source. However, those 2-D calculations also show a hollowing of the plasma plume closer to the ion source. The ions acquire a large radial velocity at the electrode, which would tend to generate a hollow plume, but the magnetized electrons can not expand radially, and the resulting charge separation bends the ions back toward the axis within 10 mm. We are attempting to measure this effect and will study tapered field geometries in an attempt to develop a fully annular plume at 10 mm from the ion source. Experimental Langmuir-probe waveforms develop oscillations with increasing magnetic fields, suggestive of plasma instability. We will look for this feature in the fully EM 3-D calculations.

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26526

Microstructural and Continuum Evolution Modeling of Sintering

V. Tikare, M. V. Braginsky, J. G. Arguello, Jr., T. J. Garino

All ceramics and powder metals, including the ceramics components that Sandia uses in critical weapons components such as lead zirconate titanate (PZT) voltage bars and current stacks, MCM electronic technology (METs), alumina/molybdenum (Mo) and alumina cermets, and zinc-oxide (ZnO) varistors, are sintered. Sintering is a critical, possibly the most important, processing step during manufacturing of ceramics. The microstructural evolution, macroscopic shrinkage, and shape distortions during sintering will control the engineering performance of the resulting ceramic component. Yet modeling and prediction of sintering behavior is in its infancy, lagging far behind the other manufacturing models, such as powder synthesis and powder compaction models, and behind models that predict engineering properties and reliability. In this project, Sandia seeks to develop a set of computational tools that will enable us to understand, predict, and control microstructural evolution and macroscopic dimensional changes during sintering. Previous research efforts on sintering modeling failed because they treated some limited aspect of sintering on either the microstructural or the macroscopic continuum scale. Microstructural models treat the evolution of two or three powder particles during sintering to give detailed information about particle shapes and densification rates. However, they fail to treat a macroscopic sintering piece—the shape change, density distribution, stress formation, etc. Continuum models apply continuum deformation mechanics to the sintering body to predict shrinkage and component shape change. However, the deformation equations are poorly understood and not directly linked to real material systems, so application of continuum sintering models to real materials has had limited success. We propose a novel modeling method that can treat the microstructural evolution of thousands of powder particles during sintering and integrate the results into continuum models to predict the overall shrinkage and shape distortions in a sintering component. An equally important result of this work will be a fundamental advancement in the understanding of sintering science.

We continued to improve our model to simulate solid-state sintering and enhance our understanding of sintering behavior of powder compacts. We expanded on the anisotropic sintering work by simulating sintering in powder compacts of simply

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packed elongated powder particles and in close-packed elongated particles. We found shrinkage to be anisotropic in both cases, with shrinkage rates related to the ratio of grain lengths. Furthermore, this was in agreement with our analytical predictions based on the sintering model developed by Johnson.

We also developed a technique for simulating volume diffusion in the sintering model. The volume-diffusion algorithm uses the Einstein equation for tracer diffusion in one dimension and generalizes it to two and three dimensions. Thus, a random walker is allowed to “walk” to any position in the simulation where the probability of that walk is proportional to its length cubed. We verified and validated this algorithm by simulating a random walker in a uniform diffusion field and by simulating diffusion for a pair of semi-infinite solids. Both gave results in agreement with analytical predictions.

We modified the mechanical part of the 2-D coupled mesoscale microstructure-mechanical code. The deformation is now calculated incrementally, while previously, total deformation was calculated every time the stress state was evaluated. This change resulted in more realistic microstructures. We are also modifying the model to include external applied stresses. This latter modification is important because it might provide means for not only verification, but also for fitting stress coefficients (control factors) in the stress-dependent parts of transition probabilities to known dependencies of system parameters under applied stress. We continued working on the stress-dependence of vacancy diffusion, pore migration, and vacancy annihilation mechanisms.

We finished performing a sensitivity and convergence study of the SOVS (Skorohod-Olevsky viscous sintering) constitutive model in JAS3D. Results suggest that the bulk shrinkage can be captured with a relatively coarse finite-element (FE) mesh. However, to capture the details of the distortions (curvatures, etc.), we need a fairly refined mesh requiring significantly large computational models and resources to handle production problems in sintering.

We refined validation calculations using the implemented SOVS constitutive model in JAS3D to quantitatively compare not only bulk shrinkage, but also curvature, in Garino’s bilayered ZnO bar experiment. Results suggest that the linear viscous implementation of the model currently in JAS3D is capable of capturing the response, at least for ZnO.

We identified and defined two additional validation experiments that we will simulate using the current implementation of the SOVS model in JAS3D. We will

We modified the mechanical part of the 2-D coupled mesoscale microstructure-mechanical code. The deformation is now calculated incrementally, while previously, total deformation was calculated every time the stress state was evaluated. This change resulted in more realistic microstructures. We are also modifying the model to include external applied stresses. This latter modification is important because it might provide means for not only verification, but also for fitting stress coefficients (control factors) in the stress-dependent parts of transition probabilities to known dependencies of system parameters under applied stress.

compare results from these calculations not only with the experiment, but also with the predictions of Olevsky's independent implementation in his FE code. This benchmarking exercise should increase our confidence in the capabilities of both codes.

We are fabricating and observing sintering in real samples for validation of the model and studying three sample geometries. The first sample geometry is concentric cylinders of two types; concentric cylinders were of different densities, but with the same powder and concentric cylinders of the same density and with different particle-size powder. The second sample geometry is bilayers bonded together with a slurry of the same powder. The first set of bilayers consisted of the same powder in each layer, but with different green density. The second set of bilayers has layers of different particle-size ZnO, both at the same green density. The final geometry is a bilayer disk of the same powder but with different densities and with a 0.25 in. cylinder that is centered halfway between the bilayer center and the edge and is a pressed pellet of the coarser ZnO. We are characterizing the dimensional changes of these samples during sintering for validation of the sintering model.

We identified and defined two additional validation experiments that we will simulate using the current implementation of the SOVS model in JAS3D. We will compare results from these calculations not only with the experiment, but also with the predictions of Olevsky's independent implementation in his FE code. This benchmarking exercise should increase our confidence in the capabilities of both codes.

Refereed

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26527

Assuring Ultraclean Environments in Microsystem Packages: Irreversible and Reversible Getters

L. L. Whinnery, Jr., S. K. Griffiths, T. J. Shepodd, R. H. Nilson, J. R. McElhanon

Microsystems are currently being evaluated as possible replacements for a number of weapon subsystems with the expectation of improved surety combined with reduced weight and volume. However, there is great concern that long periods of dormant storage may impair the mechanical functioning of microdevices that are exposed to water, out-gassing products (organics, solvents, and silicones), and particulates (talc and dust). Low-temperature operating environments and small moving parts in contact with stationary and mating structures make capillary condensation, ice formation, and corrosion true concerns for microsystems. Past experience provides little guidance, and the desiccants currently used to manage system-wide moisture levels cannot be relied on to provide the more stringent control needed to ensure microsystem reliability.

Sandia is developing a new generation of irreversible, chemically reacting getters specifically targeted toward ensuring the integrity of the local environment within microsystem packages. We intend to incorporate volatile species into a polymer through covalent bonds, thus producing a nonvolatile product. We will combine these reactive getters with getters that rely on absorption media (e.g., zeolites and high-surface-area carbon [C] fibers) to scavenge nonreactive species, like solvents. Our getter systems will rely on device packaging to limit exchange between the microsystem and the global weapon environment. Thus, the internal getters need only provide local environmental control within the microsystem package. If the getters themselves are not tacky, they will be incorporated into a tacky polymer matrix to immobilize microparticles in a harmless location. We will use modeling and analysis of available data to estimate the ingress of undesirable species as well as the gettering rates, capacities, and geometries needed to maintain an acceptable environment within the package. We will develop getters that utilize chemical reactions, adsorption, and physical adhesion to ensure a benign dormancy environment within microdevice packages.

We concentrated on scavenging water, ethanol, and isopropanol with commercially available isocyanate and anhydride polymers. Gettering of a reactive species with maleic

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anhydride polymers involves ring opening of the anhydride polymer to form an ester and carboxylic acid (for reaction with ethanol and isopropanol) or a dicarboxylic acid (for reaction with water). For reaction with an isocyanate polymer, a urethane linkage results from gettering ethanol and isopropanol. Isocyanate reaction with water results in forming an intermediate carbamic acid, which spontaneously decomposes to yield carbon dioxide (CO₂) and a primary amine. We investigated functionalized polymers as the gettering species to minimize the chance of contamination of the local atmosphere with another volatile organic species.

We used weight change to monitor reactions during gettering capacity evaluations (excess solvent). We used infrared (IR) spectroscopy to examine the changes in functional groups accompanying the reaction. A commercially available isocyanate polymer resulted in 73%, 29%, and 36 % conversion for water, ethanol, and isopropanol, respectively. With the intent of trying to get higher capacities (percent conversion), we next looked at polymeric anhydrides. Initial testing with commercially available poly(maleic anhydride-alt-1-octadecene) resulted in 0%, 73%, and 8% conversion for water, ethanol, and isopropanol, respectively. Similar experiments using 4-dimethylaminopyridine (DMAP) as catalyst gave 78%, 69%, and 70% conversion for water, ethanol, and isopropanol, respectively. Stoichiometric reaction resulted in 33%, 47%, and 59% conversion for water, ethanol, and isopropanol, respectively. Preliminary results show that poly(ethylene-alt-maleic anhydride) is an excellent getter for water with an experimental weight gain of 11.7% (82% conversion) after only one week of reaction.

We also worked with Inter Basic Resources to design and build a particle-counting system to evaluate various particle-gettering strategies (tacky polymers, permanently charged polymers). The system is operational, and control experiments are currently under way.

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26528

Biocompatible Self-Assembly of Nanomaterials for Bio-MEMS and Insect Reconnaissance

C. J. Brinker, R. J. Simonson, D. Y. Sasaki, S. M. Brozik, J. Cesarano, III

Living cells integrate, within a very small volume, recognition, amplification, and transduction properties of interest for environmental sensors. Key to practical cell-based sensors is patterned cell immobilization in robust, biocompatible environments that maintain cell viability and accessibility while enabling signal transduction and transmittal. Bulk silica matrices formed by “classical” sol-gel processing have been used for cell entrapment, but alcohol solvents cause protein denaturation, and, upon drying, broad pore-size distributions lead to the collapse of small pores and the complete drying out of large pores, limiting accessibility or causing cell inactivation. Furthermore, bulk gels are difficult to integrate into devices like microelectromechanical systems (MEMS). Recently, Sandia prepared porous silica nanostructures by evaporation-induced self-assembly (EISA). EISA employs surfactants to direct the self-assembly of silica into periodic structures characterized by unimodal pore sizes and one-dimensional (1-D), 2-D, or 3-D connectivity of pore channel networks that are stable during drying. Using inkjet printing, we can pattern these pore network systems on arbitrary surfaces. Unfortunately, all surfactant structure-directing agents used to date are bio-incompatible at concentrations needed for self-assembly. This project explores new biocompatible self-assembly approaches to enable both incorporation of whole cells into MEMS architectures and the writing of functional nanostructures on living reconnaissance agents. The advantages of using self-assembly to create biocompatible host matrices are twofold. First, the templated pores are all the same size. These hydrophilic monosized pore networks will spontaneously fill with water to create a kinetically stable aqueous environment without an auxiliary fluidic system. Second, EISA proceeds in complex mixtures unimpeded by guest molecules or particles, so we can expect to pattern (on arbitrary surfaces) cells immobilized in fluidic architectures incorporating buffer and nutrients to sustain viability for time periods needed for reconnaissance missions. Through genetic modification, cell-based sensors can be developed for specific chemical/biological weapons (CW/BW) or explosive threats.

Sandia prepared porous silica nanostructures by evaporation-induced self-assembly (EISA). ...

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Through genetic modification, cell-based sensors can be developed for specific chemical/biological weapons (CW/BW) or explosive threats.

- *Genetically modified Saccharomyces cerevisiae*. To demonstrate molecular recognition, amplification, and optical transduction in immobilized yeast, we used *S. cerevisiae* containing a promoter sequence fused to a green fluorescent protein (GFP) construct. Expression of the reporter gene in response to a glucose-to-galactose nutrient shift produces an optically detectable fluorescent signal. We demonstrated induction of GFP expression in previously immobilized cells both under thin films and in micromolded channels; fluorescence from immobilized cells was still present in biocomposite films even after 5 days. In all cases, GFP expression characteristics (induction periods and spectral parameters) for the immobilized cells were comparable to those of cells in buffer, indicating that we maintain both cell viability and functionality within self-assembled nanostructured materials.

- *Evaluation of GFP emission for LIDAR feasibility*. We are currently evaluating GFP expression and fluorescent emission using hyperspectral imaging (HSI) to determine the feasibility of both reading combinatorial patterned arrays of responsive cells and remote detection using light detection and ranging (LIDAR).

- *Biocompatible cell immobilization*. Immobilizing whole cells in a porous host matrix allows the cells to be protected, sustained, and confined in a buffered environment while retaining accessibility for nutrient, analyte, and waste-transport requirements. We used EISA with biocompatible materials to immobilize *S. cerevisiae* in porous, ordered, silica thin films that extend encapsulated cell viability to over 48 hours. We used naturally occurring lipids as structure-directing agents and also to protect cells during immobilization, while the use of a low-alcohol, buffered sol allowed for the formation of ordered mesophases while minimizing the exposure of cells to toxic system components. Additionally, we developed a double reservoir system to separate buffered cells from the sol until just prior to patterning to further enhance cell viability.

We observed that when yeast cells are added to a sol, additional lipid is required to form a structured mesophase, and the morphology of the phase differs from that obtained in the absence of cells. The addition of a fluorescently labeled lipid during self-assembly allowed us to see the preferential localization of lipid around cells, consistent with both the cells having a structure-directing role and the lipid forming a protective barrier around the cell.

- *Combinatorial evaluation of biocompatible sol-gel systems*. We initiated a study of sol components and their effect

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on yeast by incorporating a pH indicator into a biocompatible sol and using robotic writing to add acid to the system in varying concentrations. A color change along a line of deposited sol, indicating the presence of a pH gradient, demonstrated our ability to spatially control experimental parameters that are crucial for biocompatibility with living cells. Furthermore, we found that yeast cells entrapped in a biocompatible film using robotic writing maintain viability. We also demonstrated inkjet printing of biocompatible sols containing whole yeast cells.

- *Surfactant removal by biocompatible solvent extraction.*

Although transport of low-molecular-weight dyes through templated pores appears to be unimpeded by the presence of lipid templates, removal of these templates under biocompatible conditions may be desirable to maximize transport to and from the cells. We confirmed, using infrared spectroscopy and ellipsometry, the biocompatible removal of short-chain phospholipid templates and increased condensation of the silica matrix through minimal exposure to 20% methanol in water, condensation of the silica matrix being important for optimized film durability.

- *Gene selection for up or down regulation in response to pathogens and biowarfare agents.* We exposed *S. cerevisiae* in stationary phase to the binding subunit of cholera toxin and a supernatant from media containing anthrax simulants. After exposure, we used deoxyribonucleic acid (DNA) microarray analysis to determine changes in gene expression in response to the target agent. We combined the cholera toxin and supernatant as a single cocktail and used visualization software to identify genes whose induction was specific for one or more agent stimuli versus those whose regulation was more general.

A color change along a line of deposited sol, indicating the presence of a pH gradient, demonstrated our ability to spatially control experimental parameters that are crucial for biocompatibility with living cells. Furthermore, we found that yeast cells entrapped in a biocompatible film using robotic writing maintain viability. We also demonstrated inkjet printing of biocompatible sols containing whole yeast cells.

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26529

Nanoclusters for Supercapacitors

J. E. Martin, R. A. Anderson, T. J. Garino, V. K. DeMarquis, J. P. Wilcoxon, D. L. Huber

High-current and -voltage capacitors, such as those used in weapons systems, use polymer films as dielectric materials. The dielectric constant of these polymer films is very low, limiting the energy storage of the capacitors. Because the energy requirements are high for weapons components, the capacitors are large, occupying a significant fraction of device volume and leaving little room for the diagnostic devices that are now envisioned. One route to freeing up space is to create a capacitor film dielectric with a much higher dielectric constant, which would result in smaller capacitors if the dielectric strength can be maintained. Sandia investigated whether high-dielectric-constant nanoparticles can be used to significantly increase the dielectric constant of a capacitor material and thus energy storage in film capacitors. This idea was motivated by our ability to make narrow dispersity nanoparticles of controlled sizes from 1.6–10 nm that are atomically smooth and have precisely controlled organic-capping-layer thicknesses. These nanoparticles should be able to increase the dielectric constant of a capacitor film by a factor of 5. If such a principle applies to both organic and inorganic dielectrics, we anticipate a large commercial demand for products ranging from supercapacitors to improved automotive ignition components.

Our research led us to a much greater appreciation of the factors relevant to the use of particles in the enhancement of the dielectric constant of a continuous phase, such as a liquid or polymer. Much of the work focused on the problem of preparing gold (Au) nanoparticle dispersions that exhibit low conduction at high particle loadings. Using an aqueous synthesis technique, we made Au nanoparticles in the size range of ~ 10 nm. These clusters were purified by precipitation, capped with an alkanethiol, and freeze-dried to make a very low density powder. We densified this powder in a hydraulic press between the ends of two flat stainless-steel cylinders, which then allowed us to make accurate measurements of the dielectric constant of the powder, which currently is in the form of a thin circular disk. Throughout much of the year we found that as we tried to increase the particle concentration to levels that doubled the dielectric constant of the alkanethiol, current conduction became a problem. Eventually we were able to prepare samples with more uniform capping, resulting in the

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successful doubling of the dielectric constant of the composite without serious current conduction. Some current conduction did remain, which we found could be eliminated by freezing the sample, demonstrating that this conduction must be ionic. A second issue is the synthesis of Au-coated iron (Fe) nanoclusters. These nanoclusters give us the opportunity to use magnetic fields to organize the particles to optimize their effect on the dielectric constant. This would enable us to obtain large dielectric enhancements at low particle loadings. We accomplished this by using a traditional chemical route to the synthesis of Fe, then using a second chemical reduction to nucleate Au on the Fe particles. We next addressed how best to organize the particles to obtain the highest composite susceptibility possible. The expected enhancements are independent of particle size, so we used large particles in these experiments. We used a large number of complex methods of composite synthesis, using three orthogonal magnetic fields, to attempt to enhance the susceptibility of particle composites. We showed, through simulation and experiment, that highly optimized composites could be created by organizing the particles into complex foamlike structures, using a technique of heterodyning various magnetic-field components to create beating particle structures in the polymerizing fluid. Through this means we demonstrated that composite susceptibility can be enhanced by a factor of 3 over that of a random particle composite. Further work is needed in the area of sample purification, in employing magnetic fields to optimally control composite structure, and in the area of dielectric breakdown studies.

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26530

First-Principles Determination of Dislocation Properties

M. Vanschilfgaarde, S. M. Foiles, D. L. Medlin, V. Ozolins

Dislocation behavior determines numerous materials properties. Their motion produces deformation. The interaction of dislocations with interfaces produces the grain-size dependence of strength. Motion of dislocations in boundaries determines the boundary mobility and, thereby, microstructural evolution. Prediction of dislocation core structures at the atomistic level in arbitrary materials and ultimately in the presences of defects is central to developing predictive models of material evolution. It would also represent a major scientific achievement.

The need to treat arbitrary materials, alloys, and dopants requires a predictive first-principles approach. Current first-principles modeling capabilities are not well suited to the description of materials properties. Techniques for determining the electronic structure of large numbers of atoms (order-N methods) work well for insulating materials but not for metallic systems. Further, essentially all ab initio modeling to date employs band-structure techniques with periodic boundary conditions (BCs). Thus, dislocations and other aperiodic defects are difficult to model. Sandia seeks to adapt a combined electronic/lattice Green's technique to the direct calculation of dislocation core structures, which avoids the requirement of periodic BCs. Both Green's functions exploit the short-range character of the Hamiltonians defining them. Thus, far from the core, the corresponding Hamiltonians of the host are well approximated by a slightly perturbed crystal Hamiltonian. The Green's function for the defect is solved using the Dyson equation. We will also pursue additional modeling using an ab initio extension of Peierl's-Nabarro. The result of these calculations can be validated by detailed comparison with high-resolution electron microscopy observations. The success of this project will create a new world-class tool for the fundamental study of dislocation properties.

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(1) We applied the combined *ab initio* Peierl's-Nabarro approach to the problem of dislocation structure, morphology, and energetics in Ni_3Al , Ni_3Ge , and Fe_3Ge . This theoretical analysis provides a model for high-temperature yield stress anomalies that are important in technological applications of these alloys. This work was published in the open literature.

(2) We reformulated the Green's function approach to *ab initio* calculation in the framework of exact muffin-tin orbital

theory. This is an important advance that eliminates an undesirable key approximation from the previous theory, thereby improving computational accuracy of the approach.

(3) We obtained detailed atomic-resolution transmission electron microscopy (TEM) micrographs of extended partial dislocations at the aluminum sigma 3 (112)-type twin boundary. Modeling these extended dislocations will require the *ab initio* Peierl's-Nabarro approach developed here. The experimental data regarding dislocation widths will allow quantitative validation of the *ab initio* approach developed here.

This is an important advance that eliminates an undesirable key approximation from the previous theory, thereby improving computational accuracy of the approach.

Refereed

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32915

Study of Polymer Spin-Coating for Photolithographic Semiconductors in Near-Zero-Gravity Environment

S. M. Thornberg, C. J. Flack, J. R. Brown, T. C. Gamble

A variety of applications use the spin-coating procedure to coat flat substrates or objects with thin films of material. The coating material is disbursed onto the surface of the substrate, then spun off, ideally leaving a uniform layer for subsequent processing procedures. As the material is dispensed onto a spinning wafer, spiral-shaped wave fronts called Eckman spirals can be observed as the fluid migrates outward radially across the wafer. Spin-coating has traditionally been one of the first steps in semiconductor manufacturing.

In collaboration with the University of New Mexico (UNM), Sandia performed an experiment aboard the National Aeronautics and Space Administration's (NASA's) KC-135 Reduced-Gravity Flying Laboratory to study the feasibility of spin-coating in a weightless environment.

The goal of this experiment was to spin-coat a series of silicon (Si) wafers with photoresist in a zero-gravity environment and compare them with wafers prepared using identical experimental parameters in the lab. However, unforeseen difficulties were pervasive throughout the execution of the experiment, which prevented a large population of data from being acquired. Nevertheless, we successfully prepared several wafers on the first flight. Analysis of these wafers confirms that the modifications made to the later experiment eliminated several notable problems present in the original experiment. Also, data extracted from these wafers seem to reinforce what was determined from the earlier experiment, specifically that gravity plays an integral role in the fluid dynamics that dictate the characteristics of the photoresist thin film. We established several main findings though our experimentation:

- The adhesive forces between a photoresist and Si wafer are substantial enough to allow for the spin-coating procedure to be done without the force of gravity.
- Higher spin speeds used in the later experiment allowed the photoresist film to stabilize within the allotted zero-gravity timeframe. This confirmed that the spin-coating procedure can be accomplished successfully in the environment present aboard the KC-135, presenting a basis for possible future experimentation.

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- Gravity seems to play a substantial role in the fluid dynamics that dictate the characteristics of the photoresist film in the spin-coating procedure. This can be shown by the formation of fluid wavefronts (Eckman spirals) during the dispense cycle. In all wafers prepared in the lab, we observed two distinct Eckman spirals. However, we observed only one Eckman spiral in all the wafers prepared in zero-gravity. This may prove to be of significance in the modeling of the spin-coating process, because in all the literature available on the subject, gravity is neglected when deriving the equations that approximate fluid behavior.

Further experimentation is required to determine whether the spin-coating procedure can be made feasible in a zero-gravity environment.

Refereed

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34465

Understanding Metal Vaporization from Transient High-Fluence Laser Irradiation

P. W. Fuerschbach, G. R. Eisler

Laser spot-welding is widely used for precision joining of nuclear weapon components and other high-reliability devices. The production of metal vapor as a consequence of high-intensity laser irradiation is a serious concern in cleanrooms, where contamination of adjacent components, ejection of metal particulates, creation of void defects in the fusion zone, and significant loss of high-vapor-pressure alloying elements are all negative consequences of metal vaporization. Despite the widespread use of laser welding, little fundamental understanding of laser/material interaction in the weld pool exists. Without this fundamental understanding, optimization models cannot be applied to mitigate vaporization problems.

We developed a laser-beam measuring technique using Kapton film to enable direct measurements of the laser-beam spot size on the sample surface to be determined. We validated this technique using the Prometec laserscope and found it to yield very consistent results. We also developed a mass-loss measuring method using a Mettler microbalance that enabled us to determine mass loss as low as 0.5 mg. We examined a matrix of experimental conditions that quantify the dependence of metal vaporization on the incident laser-beam intensity for 304 SS.

Since our goal is to understand the mechanism of vaporization, the onset of large-particle ejection (spatter) was deliberately avoided. In weld trials where we suspected spatter, subsequent measurements clearly indicated that a mass loss had occurred that was atypical in magnitude relative to the other results. Careful defocusing of the laser beam enabled the intensity to be reduced to a level where spatter did not occur and bias the experiment.

We found the mass loss after laser spot-welding to be significant, with up to 70 mg of material vaporized per pulse. The mass loss was observed to correlate well with the measured laser-beam intensity. For some pulse energy levels, the loss appeared to reach a plateau level, whereas in other cases mass loss increased continually with intensity. At low beam intensities where only incipient melting occurred, little or no mass loss was measured.

Employment of a transient three-dimensional computer model to help investigate these experimental results has been

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completed at Penn State University (PSU). The model indicated that laser power and pulse duration were the most important variables in determining the geometry of the fusion zone. The peak temperature and convective velocity in the weld pool increased significantly with incident beam power. We found computed temperatures at the weld pool surface to be higher than the boiling point of the 304 SS. The calculations showed that the vaporization was concentrated in a small region under the laser beam where the temperature was very high. During the heating cycle the evaporation rate increased significantly with time as the pulse time progressed.

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34466

Mechanics and Tribology of MEMS Materials

M. T. Dugger, J. R. Michael, S. V. Prasad, T. E. Buchheit, B. L. Boyce

Micromachines have the potential to significantly impact future weapon component designs as well as other defense, industrial, and consumer product applications. For both electroplated (LIGA [the German term Lithographie, Galvanoformung, und Abformung, for lithography, electroforming, and molding]) and surface-micromachined (SMM) structural elements, the influence of processing on structure and the resulting effects on material properties are not well understood. The behavior of dynamic interfaces in present as-fabricated microsystem materials is inadequate for most applications, and the fundamental relationships between processing conditions and tribological behavior in these systems are not clearly defined. Sandia intends to develop a basic understanding of deformation, fracture, and surface interactions responsible for friction and wear of microelectromechanical systems (MEMS) materials. This will enable needed design flexibility for these devices, as well as strengthen our understanding of material behavior at the nanoscale. The goals of this project are to develop new capabilities for submicroscale mechanical and tribological measurements, and to exercise these capabilities to discover fundamental knowledge of material behavior at this size scale. We will develop novel microforce and displacement sensors using SMM technology and new methodologies for isolating local variations in mechanical response of MEMS materials. We expect that understanding the nanomechanics of surface contact will result in new fundamental contributions to theories of interfacial adhesion as a function of topography. The ability to quantify friction over a wide range of pressure and velocity conditions, and in controlled environments, will enable fundamental understanding of the effect of environment on friction and surface durability. Increased understanding of MEMS mechanics and tribology developed in this project will permit performance and reliability of advanced MEMS components to be predicted with a sound scientific basis.

We characterized the strength of various SUMMiT-V™ (Sandia Ultraplanar Multilevel MEMS Technology V) polysilicon (poly-Si) layers under various strain rates, presence of self-assembled microlayers (SAMS) coatings, fillet radius, and gage volume, and found no statistically significant influence. Friction associated with the probe configuration had a profound effect on the observed strength. An improved

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methodology reduced friction and resulted in strength values consistent with other researchers. We developed a “mechanical” probe station capable of measuring forces on MEMS devices during electrostatic/mechanical actuation. Although capable of less-precise strain-rate control than the micromechanics probes used previously, this capability enables more rapid evaluation of mechanical behavior of poly-Si tensile samples. The National Institute of Standards and Technology’s (NIST) traceable force transducer was also used to verify nanoindenter force calibration. During exploration of alternate MEMS materials, we characterized the strength of alumina and stainless steel fabricated by consolidation of powders in a LIGA–formed mold, providing insight into possible processing shortcomings.

We modified SMM test capabilities to permit quantification of static friction between poly-Si sidewalls. We demonstrated a significant increase in static friction for octadecyltrichlorosilane after exposure to 4260 parts per million (ppm) water vapor at 300°C. We observed no degradation in dry environments, attributing the degradation to hydrolysis of the monolayer. We expanded our friction characterization capabilities with design of a new module that enables contact of individual layers of poly-Si and incorporates high-efficiency actuators to permit more test devices to be included on a module. We established procedures for reproducibly creating samples of shear-oriented octadecyltrichlorosilane for grazing incidence x-ray scattering measurements. We developed novel techniques to prepare a cross section of wear scars suitable for backscatter electron diffraction and transmission electron microscopy (TEM) using a focused ion-beam microscope. We applied this technique to study wear-induced subsurface deformations in electroformed nickel. We observed the formation of two subsurface zones, each with its own characteristic features. We also observed formation of low-angle grain boundaries and spread in the orientation of pole. This information is crucial in predicting the reliability of dynamic interfaces in LIGA microsystems.

*We developed a “mechanical”
probe station capable of
measuring forces on MEMS
devices during electrostatic/
mechanical actuation.
Although capable of less-
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poly-Si tensile samples. ...
During exploration of
alternate MEMS materials, we
characterized the strength of
alumina and stainless steel
fabricated by consolidation of
powders in a LIGA–formed
mold, providing insight into
possible processing
shortcomings.*

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34467

Dynamics of Metal/Ceramic Interfaces

K. F. McCarty, N. C. Bartelt

Sandia's goal in this project is to understand how metal/ceramic interfaces form, evolve, and accommodate the stress that can lead to delamination and failure. We emphasize the use of advanced microscopies such as scanning-tunneling microscopy (STM) and low-energy-electron microscopy (LEEM) to observe interface formation in real time. We use these techniques to measure the interfacial work of adhesion, determine the mechanisms and kinetics of interface formation, and develop understanding of how stress is or is not accommodated. We combine real-time measurements of process dynamics with modeling to determine what physical processes govern system evolution.

We used LEEM to selectively image the different phases that form as the nickel aluminum (NiAl) alloy undergoes oxidation at high temperature. When the NiAl (110) surface is exposed to oxygen (O) above about 600°C, rod-shaped islands of crystalline oxide form. These rods are all aligned along the substrate's (001) direction and can be many microns in length. Since the rods are pseudomorphic with the substrate, as established by selected area diffraction, we believe that they are spinel, NiAl_2O_4 . Real-time observations show that the rods can both grow and shrink by addition and subtraction, respectively, at their ends. This one-dimensional (1-D) behavior leads to surprising dynamics. For example, addition at one end and removal at the other end can cause the rods to translate across the surface. A rod can also shrink and totally vanish. In addition, when two rods move close to one another, one rod can grow at the expense of the adjacent rod. We are in the process of writing a manuscript to be submitted to an archival journal summarizing the "nanorod" growth process.

Importantly, we also observed that the rod phase transforms into a completely different oxide phase, namely, the same gamma alumina ($\text{g-Al}_2\text{O}_3$) phase produced by low-temperature oxidation, the focus of our earlier effort. The spinel-to-gamma-alumina-phase transformation occurs by nucleation at steps on the NiAl surface. In addition, the $\text{g-Al}_2\text{O}_3$ phase contains strain-relieving interfacial dislocations. These dislocations move with time, and we have observed their dynamics. Within an oxide island, the dislocations oscillate back and forth, and the dislocation grows in length as the oxide island grows.

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We recorded the kinetics of rod formation as a function of substrate temperature and O pressure. Using digital image analysis, we are in the process of extracting the environment-dependent rates of rod growth. We have begun to formulate a quantitative model that captures the essential processes (anisotropic growth resulting from anisotropic misfit strain) that occur in the 1-D “nanorod” growth. By comparing the model to experimental data, we will determine the relative importance of the competing processes.

We have begun directly observing the growth and dewetting of metals on a model ceramic material, titanium dioxide (TiO_2). We observed that how copper dewets depends greatly on the state of the oxide’s surface. For example, on a stoichiometric surface, relatively isotropic islands result from dewetting. Prolonged annealing caused the metal islands to evaporate from the surface. In contrast, on a nonstoichiometric (O deficient) surface, dewetting produces very elongated structures. We observed the substrate to encapsulate these islands upon prolonged annealing.

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We have begun to formulate a quantitative model that captures the essential processes (anisotropic growth resulting from anisotropic misfit strain) that occur in the 1-D “nanorod” growth. By comparing the model to experimental data, we will determine the relative importance of the competing processes.

34468

In Situ Characterization of Soft Solution Processes for Nanoscale Growth

N. S. Bell, D. R. Tallant

The study of novel materials and structures with dimensions in the nanoscale (<100 nm) regime is an important emerging field of materials science. The small size of these materials results in quantum confinement and surface contributions that translate into novel optoelectronic properties whose applications are still being realized. Many synthesis techniques for nanomaterials are based on soft solution processes (SSP), which include sol-gel, hydrothermal, solvothermal, micellular or organic templating routes, and electrochemical methods. These processes involve the precipitation of ionic species or metal-organic molecules into nanoparticles or nanostructured networks. To exercise a high degree of control over these processes, it is critical to have a capability for monitoring the development of supersaturation, surface reactions, and formation of phase or precipitate in situ. In this project, Sandia is studying the superposition of different measurement techniques to characterize dynamic colloidal systems in new ways. These studies will probe the chemical interactions during reactions and the organizational characteristics developed in the resulting colloids. Of particular interest are properties influencing colloidal dynamics such as zeta potential and particle-size development.

We synthesized model silver (Ag) nanoparticles using a poly(acrylic acid) dispersant for zeta potential measurement in the DT1200 acoustic spectrometer. This instrument measures attenuation of an acoustic pulse and requires 1 volume % solid particulate to measure properties, and with standard systems it has proven to be very reliable. We are concentrating the synthesized Ag nanoparticles for measurement in the instrument; testing will involve pH titration of the nanoparticles as well as titration with reducing solution to characterize the zeta potential during particle growth.

We are also developing a new method designed specifically for measurement of nanoparticle zeta potential. Current methods for measuring zeta potential rely on optical detection of individual particles and cannot resolve nanoparticulate material. We fabricated a microchannel electrode to evaluate the diffusion profile of an ensemble of nanoparticles mixing with pure solvent under forward- and reverse-bias potentials. Rather than observing scattering behavior of particles or the

In this project, Sandia is studying the superposition of different measurement techniques to characterize dynamic colloidal systems in new ways. These studies will probe the chemical interactions during reactions and the organizational characteristics developed in the resulting colloids.

electrophoretic mobility of a single particle in a microscope, we will use the diffusion profile of nanoparticles to infer the zeta potential of nanoparticles. Initial tests showed that a dilute nanoparticle suspension does not have sufficient absorption to provide a signal, and it is necessary to include a fluorescent dye or surface tag to increase signal. We identified three dyes with the potential to increase signal. Alternatively, a charge-coupled detector with cryogenic cooling could be used to attempt to resolve the nanoparticle mixing and diffusion. Further testing involves proof-of-concept of signal generation and altering particle mobility under applied electric field, followed by introduction of reactant species in a two-channel or three-channel configuration to observe the precipitation process *in situ*.

Key to development of the microfluidic method for determination of nanoparticle zeta potential is the mathematic modeling of diffusion under an applied electric field. This process will be a key component of upcoming work. In addition, we will undertake modifications to the flowcell design as determined from experimental measurements.

We will utilize the methods used to fabricate the microfluidic electrode to form the microfluidic gradient system desired for observing the formation of colloidal crystals in a chemical-field gradient.

We are also conducting experiments to synthesize zinc oxide nanoparticles within thermogels and in solutions with specific adsorbates chosen to promote the formation of nonagglomerated platelets.

The acoustic rheometer development to characterize the dispersion and agglomeration of particles during shear is under way.

Initial tests showed that a dilute nanoparticle suspension does not have sufficient absorption to provide a signal, and it is necessary to include a fluorescent dye or surface tag to increase signal.

34469

Determination of Critical Length Scales for Corrosion Processes Using Microelectroanalytical Techniques

K. R. Zavadil, F. D. Wall

A key factor in our ability to produce and predict the stability of metal-based macro- to nanoscale structures and devices is a fundamental understanding of the localized nature of corrosion. Corrosion processes where physical dimensions become critical in the degradation process include localized corrosion initiation in passivated metals, microgalvanic interactions in metal alloys, and chemistry in adsorbed water films in atmospheric corrosion. This project focuses on two areas of corrosion science where a fundamental understanding of processes occurring at critical dimensions is not currently available. Sandia will study the critical length scales necessary for passive film breakdown in the inundated aluminum (Al) system and the chemical reactions and transport in ultrathin water films relevant to the atmospheric corrosion of Al. Techniques are required that provide spatial information without significantly perturbing or masking the underlying relationships. Al passive film breakdown is governed by the relationship between the area of the film sampled and its defect structure. We will combine low-current measurements with microelectrodes to study the size scale required to observe a single initiation event and record electrochemical breakdown events. We will correlate the resulting quantitative measure of stability with metal grain size, secondary phase size, and distribution to understand which metal properties control stability at the macro- and nanoscale. Mechanisms of atmospheric corrosion on Al are dependent on the physical dimensions and continuity of adsorbed water layers as well as on the chemical reactions that take place in this layer. We will combine microelectrode arrays with electrochemical sensing and electrostatic-force microscopy to monitor the chemistry and ion transport in these thin layers. These measurements will be the basis for calculating oxidant partition coefficients and ion mobilities. We will use the techniques developed and information derived from this work to understand and predict degradation processes in electrical and structural components.

To quantify the relationship between electrode area and pitting behavior, we constructed and tested both single electrodes and electrode arrays from pure Al wires ranging from 5 mm to 500 mm in diameter. We studied pitting behavior

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as a function of electrochemical environment, scan rate, and electrode area. We developed a statistical framework of pit initiation to quantify and interpret the observed pitting behavior. We found that the pit nucleation phenomenon was best described by a homogeneous process on small electrodes (i.e., 125 μm and smaller) and a heterogeneous process on larger electrodes (i.e., 500 μm), implying that pit nucleation is random on microelectrodes but is causally linked to oxide defects on the larger electrodes. We estimated the density of these defects to be on the order of 10^{-5} mm^{-2} . We developed and demonstrated a microcapillary-based test cell that will allow these experiments to be extended to studying isolated regions of macroscopic single crystals and polycrystalline ingots, and also allow measurement of electrochemical signatures associated with pit initiation. We designed and fabricated next-generation microelectrode arrays for chemical sensing in thin adsorbed water layers. We fabricated arrays using patterned metal deposition on quartz and using polycrystalline silicon (Si) processing to push the limits of these close-spaced electrode arrays to a 2–5 μm lateral spacing. We developed techniques for direct and indirect (using seed layers) electrodeposition of platinum, silver, and pH-sensitive iridium oxide for the Si-based arrays. We demonstrated oxygen (O) detection in these adsorbed layers using pH sensing of the hydroxide ion due to O reduction. We also demonstrated impedance sensing of adsorbed water layers produced at moderate relative humidity. We acquired a scanning probe microscope (SPM) for conductive electrostatic-force microscopy for mapping of water layers distribution on these sensing arrays, and technique development is under way.

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Refereed

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34478

LIGA Microsystems Aging: Evaluation and Mitigation

C. H. Cadden, N. Y. C. Yang

The deployment of LIGA (the German term Lithographie, Galvanoformung, und Abformung, for lithography, electro-forming, and molding) structures in Defense Programs applications requires a thorough understanding of potential long-term physical and chemical changes that may occur during service. While these components are generally fabricated from simple metallic systems such as copper (Cu), nickel (Ni), and Ni alloys, the electroplating process used to form them creates microstructural features that differ from those found in conventional (e.g., ingot metallurgy) processing of such materials. Physical changes in nonequilibrium microstructures may occur due to long-term exposure to temperatures sufficient to permit atomic and vacancy mobility. Chemical changes, particularly at the surfaces of LIGA parts, may occur in the presence of gaseous chemical species (e.g., water vapor, off-gassing compounds) and contact with other metallic structures. During the past year, Sandia microstructurally characterized several electrodeposited Ni-based materials, including pure Ni (from a Ni sulfamate bath), Ni-cobalt (Co), and Ni-manganese (Mn). Additionally, a series of Ni LIGA parts are being thermally cycled in controlled atmospheres for various exposure times; we have examined initial sets of samples.

We focused on two areas: a detailed characterization of a “baseline” LIGA material and the establishment of a testing procedure and protocol to evaluate dormancy and aging effects of LIGA components in controlled environments.

Currently, the baseline material for LIGA components is defined as pure Ni deposited from a Ni sulfamate bath. We characterized grain structure, hardness, and texture using x-ray diffraction and electron microscopy. We found parts to be 100% dense, having columnar grains oriented with their major axis parallel to the plating direction. We found microstructure and hardness of microparts to be highly sensitive to minor variations in plating condition. The presence of residual (unintentional) levels of grain refiner in one of the plating tanks resulted in a dramatic hardness increase compared to the nominal values and a change in texture orientation from 110 to 001.

Characterization of an advanced electroplated Ni-Co alloy demonstrated both the difficulty in obtaining compositional

During the past year, Sandia microstructurally characterized several electrodeposited Ni-based materials, including pure Ni (from a Ni sulfamate bath), Ni-cobalt (Co), and Ni-manganese (Mn). Additionally, a series of Ni LIGA parts are being thermally cycled in controlled atmospheres for various exposure times; we have examined initial sets of samples. ...The presence of residual (unintentional) levels of grain refiner in one of the plating tanks resulted in a dramatic hardness increase compared to the nominal values and a change in texture orientation from 110 to 001.

uniformity and the strong effect that chemical variations have on local microstructural and hardness characteristics.

Additional results show that the aspect ratio of parts can have an effect on grain size, hardness, and chemical uniformity. An increase in aspect ratio tends to coarsen grains, resulting in a hardness reduction. The magnitude of this effect is highly material-dependent; Ni-Co deposits exhibited a dramatic effect, and Ni-1%Mn was affected very little.

Microparts consist of three unique types of surfaces: one formed by machining (lapping) to define the final part thickness, a “base” formed during the etching process used to remove parts from the plating substrate, and the sidewall surfaces defined by the confines of the mold walls. Each surface has its inherent features: scratches on the lapped surface, etch pits on the base, and sidewall linear features derived from cracks in the polymethylmethacrylate (PMMA) molds, which may serve as sites for metallurgical changes on the surface of microparts.

We examined external surfaces of baseline composition dormancy specimens and archived the images for post-testing comparison. We then assembled specimens in fixtures that maintain desired configurations for both electroplated/electroplated and electroplated/stainless-steel (SS) material couples. The fixtures were subsequently sealed in SS vessels, evacuated, and backfilled with nitrogen gas. Two gas compositions are being utilized, one having a dewpoint of -82°C , the other -29°C . Sets of vessels are thermally cycled between $+71^{\circ}\text{C}$ and -54°C twice daily. Individual vessels will be withdrawn and the contents analyzed at 3, 6, 12, and 24 months of exposure.

We removed the first set of specimens after a 3-month exposure to the conditions mentioned above. Preliminary results indicate only slight differences after exposure; we observed minor changes (using optical microscopes) in features seen on some of the parts. Most of the changes are related to handling, i.e., scratches produced during assembly/disassembly. However, we are conducting closer examination of contact areas, particularly on vertical surfaces (gear teeth, sidewalls of washers, etc.) using electron microscopy to investigate more subtle phenomena.

Additional results show that the aspect ratio of parts can have an effect on grain size, hardness, and chemical uniformity. An increase in aspect ratio tends to coarsen grains, resulting in a hardness reduction. The magnitude of this effect is highly material-dependent; Ni-Co deposits exhibited a dramatic effect, and Ni-1%Mn was affected very little.

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34485

Science-Based Processing of Field-Structured Composites

R. L. Williamson

Over the past few years, a new class of materials called field-structured composites (FSCs) has emerged that poses interesting and novel process control challenges. FSCs are anisotropic particle composites produced in electric or magnetic fields that exhibit highly anisotropic properties due to the chain or sheetlike structures that form as a result of the induced dipolar forces between particles. The field-structuring gives tremendous control of material properties, and the potential for practical applications is great if feedback can be used to tailor material properties to meet specific needs. Recent research at Sandia shows that these materials have colossal thermoresistance, piezoresistance, magnetoresistance, and chemiresistance, making FSCs very promising as sensors if reliably produced with a desired resistivity. These materials pose non-trivial feedback-control challenges due to strong history effects, diverging time scales, and nonlinear dynamics. We intend to meet these challenges by developing science-based process control using newly discovered methods of achieving feedback in these materials. This involves using a rotating “destructuring” magnetic field to disrupt previously established structures that give rise to strong hysteresis in the sample conductivity-field strength response curve. The goal is to precisely control conductivity in samples during polymerization, or during solvent evaporation from samples where metal particles have been introduced into a polymer matrix through swelling. These systems pose exceptionally challenging control problems because the particle dynamics occur on diverging time scales.

The goal is to precisely control conductivity in samples during polymerization, or during solvent evaporation from samples where metal particles have been introduced into a polymer matrix through swelling. These systems pose exceptionally challenging control problems because the particle dynamics occur on diverging time scales.

(1) We completed a field parameter study using the triaxial field apparatus designed and constructed previously.

(2) We successfully produced complex material structures in polymerizing host systems.

(3) We characterized conductivity degradation with time in chained composite structures as compared to sheet composite structures.

(4) We developed a technique to coat plastic microbeads with magnetic Ni(P) alloy.

(5) We developed a technique to coat nickel (Ni) microparticles with a passivating layer of gold (Au).

(6) We demonstrated “long-term” stability of Au-coated Ni particles toward conductivity degradation.

(7) We characterized the resistance of silicone-based FSCs as a function of temperature and strain.

(8) We developed a prototype chemical sensor.

Our milestones called for controlling resistance/conductance of a candidate FSC. However, when we discovered that a sample with stable resistance/conductance could not be produced due to oxidation, we decided that this problem had to be solved before control work could be initiated. We reprioritized the project and placed producing passivated particles at the top of the list. Also, because of the rich variety of structures produced in the tri-axial field that were unanticipated in the original proposal, we decided to perform a consistent parameter study to determine which field settings produced which structures and whether they could be produced in curing polymer systems. These two activities became our new milestones, and we accomplished both. Stable, passivated particles can now be routinely produced in the laboratory in relatively large quantities (1–2 grams), and we have completed a parameter study in a polymer system.

In addition to the coating development work and field parameter study, we produced prototype sensors. The first consists of two electrically isolated, Au-coated surfaces bridged by Au/Ni chains in a silicone polymer matrix. The Au/Ni chains consist of 4–7 μm -diameter Ni particles coated with $\sim 0.1 \mu\text{m}$ Au. We measured the room-temperature resistance of the FSC bridge to be 0.7 ohm. We designed a circuit to drive current through the bridge at constant voltage. Current could be varied from 0.5 A to $\sim 1 \text{ pA}$ simply by exposing the sensor to chemical vapors (acetone, toluene, and pentane were all successfully used) in a jar. We performed multiple tests with reproducible results, and the sensor recovered fully between tests. We made another sensor in a plastic cell of rectangular cross section with two copper (Cu) electrodes mounted along opposite sides. Again, resistance could be reproducibly varied over an extremely wide range by heating the sample above its cure temperature or by squeezing and stretching it, demonstrating high sensitivity to thermal or mechanically induced strain. These “sensors” are admittedly crude devices; however, they demonstrate that stable, reusable, extremely sensitive sensors can be constructed from FSCs.

Stable, passivated particles can now be routinely produced in the laboratory in relatively large quantities (1–2 grams), and we have completed a parameter study in a polymer system. ...we produced prototype sensors. ...stable, reusable, extremely sensitive sensors can be constructed from FSCs.

Refereed

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34699

Exploration of New Multivariate Spectral Calibration Algorithms

D. M. Haaland, C. M. Wehlburg, M. H. Van Benthem, D. K. Melgaard, M. R. Keenan

In related projects, Sandia developed a number of powerful new multivariate calibration algorithms that have been demonstrated to correct many of the outstanding limitations of traditional quantitative multivariate spectral calibrations and to greatly extend our ability to solve new problems. We developed a family of augmented classical least-squares (ACLS) multivariate algorithms and greatly improved multivariate-curve resolution (MCR) methods. The ACLS algorithms have the ability to be rapidly updated during prediction without recalibration while the MCR techniques allow us to perform multivariate calibrations without the use of standards. The rapid updating feature of the ACLS algorithms is a significant advantage over previous chemometric algorithms. We will continue to quantify the relative merits and predictive performance of these new multivariate algorithms relative to traditional multivariate calibration methods, and we will explore exciting new potential applications using the improved MCR algorithms. For example, the new ACLS algorithms can take advantage of weighted least-squares methods to accommodate nonuniform noise in spectral data. We will test the ability to better handle nonuniform spectral noise with simulation calibration data. We will use the improved MCR capabilities to test our hypothesis that they can be used to improve spectral calibrations that are currently limited by the reference methods required to build multivariate calibration methods. Since reference errors are often the limiting factor in multivariate spectral calibrations, reducing or eliminating this limitation would be a significant advance in chemometric data-analysis capabilities. If we can successfully reduce the impact of reference errors in spectral calibrations, we also have the opportunity to determine if the generally high precision of spectral measurements can be used to decrease errors in the primary reference methods. Success at this goal could have a very significant impact on all our instrumental analytical reference tools.

We implemented an improved factor-selection method for the ACLS algorithms and tested its effectiveness using infrared (IR) spectra for a system of acetone and isopropanol at parts-per-million (ppm) concentrations employing a sensor consisting of a thin hydrophobic coating of porous sol-gel on an IR

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waveguide. We demonstrated that the factor selection resulted in fewer factors being required and generated better prediction abilities for the isopropanol analyte.

We demonstrated the ability of ACLS methods coupled with MCR algorithms and repeat hyperspectral images (HSI) to greatly reduce the detrimental effects of systematic noise and spatial distortions in the analysis of our hyperspectral IR images. We also demonstrated that the MCR methods applied to spectra obtained from a system of dilute aqueous solutions can generate better estimates of the pure-component spectra than standard partial least-squares (PLS) methods.

We made comparisons of the calibration and prediction abilities of the four new ACLS methods among themselves and with the current standard PLS algorithm. We generated simulated datasets based on real data to test and compare the relative performance of the algorithms. The simulations include ideal random spectral noise, correlated spectral noise, nonuniform correlated errors, concentration errors, and different amounts of these various noise sources. Nonlinearities in the spectral responses were also simulated. We considered two nonlinearities: (1) a logarithmic damping of intensity similar to detector roll-off at high intensities, and (2) adding uniform noise in transmittance and converting back to intensity using absorbance = $\log(\text{transmittance})$ to emulate the actual noise characteristics of spectrometer data collection. We conducted a large number of trials with three different levels of concentration and spectral noise (50 samples of 10 separate distinct calibrations and 20 separate predictions) for each case to minimize the possibility of drawing conclusions based on statistical anomalies. We performed the statistical significance comparisons of the methods using the Wilcoxon-signed rank test. This method provides a greater sensitivity to differences than can be had using the standard errors of prediction (SEP), but while the differences may be statistically significant, the actual impact on SEPs is often limited by reference errors. A critical result of this investigation was that the ACLS methods did show significantly improved prediction ability over classical least-squares (CLS) when nonlinearities are present. In the noise-free case, the traditional PLS and ACLS methods are essentially equivalent, with PLS giving slightly better results for glucose but poorer results for ethanol. Increasing the magnitude of the nonlinearity was slightly more detrimental to PLS than ACLS. With the addition of random noise, the results for glucose were significantly better for PLS than the ACLS methods, but were equivalent for the other components. With correlated noise, the reverse was true—the ACLS methods

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showed superior prediction ability for glucose. Since correlated noise is almost always present in the spectral data in the IR frequencies, this result is particularly significant. Generally the concentration noise had a similar effect on all the methods, except for the case with relatively small correlated error and logarithmic nonlinearities where PLS was degraded much more than ACLS. This study proved valuable in establishing the importance of the ACLS methods by showing that they were capable of dealing as effectively as PLS with nonlinearities and handled correlated noise as well as or better than PLS. These results, and the advantages in the speed, capabilities, and efficiency of prediction augmentation, make ACLS the multivariate analysis method of choice.

This study proved valuable in establishing the importance of the ACLS methods by showing that they were capable of dealing as effectively as PLS with nonlinearities and handled correlated noise as well as or better than PLS.

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The Basics of Aqueous Nanofluidics: “Interphase” Structure and Surface Forces

P. J. Feibelman, K. Leung, D. L. Huber, B. C. Bunker, D. M. Teter

To understand flow through narrow pores, biomaterials properties, micromachine operation, and other key nanofluidic phenomena, we need to learn how the unexpectedly strong forces measured as far as tens of nanometers from water-solid interfaces are mediated by near-surface water structure. Using ab initio calculations and a suite of incisive experiments, Sandia will identify and characterize icelike, clathratelike, and possibly other arrangements of water molecules in the “interphase” adjacent to ice-nucleating, hydrophobic, and intermediate surfaces. The measurement techniques, including infrared (IR) spectroscopy, interfacial-force microscopy (IFM), and contact-angle studies, will illuminate the relations among interphase structure and energetics, mechanical properties, and hydration forces. Our theoretical efforts will target an explanation of how templates produced by strong short-range interactions nucleate near-surface ordering of water molecules. For this purpose, we will develop and deploy a computational scheme in which the near-surface transition region is described by a classical water potential, specifically designed to reproduce the ab initio phases and properties of bulk water, while an ab initio description of the immediate surface vicinity provides a boundary constraint amounting to a template. After initial work in which novel experimental and theoretical methods are developed and validated, we will apply theory and experiment concurrently to a set of representative cases, including a AgI surface (epitaxy with ice), a clean metal, and a self-assembled-monolayer (SAM)-covered (oily) surface. We will thus learn the microscopic underpinnings of the relation between hydration force strength, surface chemistry (e.g., hydrophilicity), and physics (e.g., epitaxial match).

We showed theoretically that water wets only the precious metal surface, Ru(0001) (ruthenium), because half the molecules in the first adlayer dissociate. This result is at variance with the conventional idea that the first adlayer is “icelike.” But the half-dissociated layer’s theoretical structure agrees with experiment, while an icelike layer’s does not. We extended our calculations to water on other d-band metal surfaces and computed vibration spectra and their consequences for “zero-point” contributions to water adsorption energetics. We computed the energies of several models of the second layer

Our theoretical efforts will target an explanation of how templates produced by strong short-range interactions nucleate near-surface ordering of water molecules.

of water on Ru(0001), preliminary to an extensive, classical molecular dynamics search for the optimal structure. We developed classical water-water and water-ion potentials by compiling and fitting to an extensive *ab initio* database of water cluster and solvated ion energetic, structural, and vibrational information. We used the new potentials to solve a significant problem in nuclear-waste transport (“Shipping Cask Weeping”).

We measured forces between tips and samples coated with a polymer that is swollen and hydrophilic at room temperature (RT), but collapses and becomes more hydrophobic above 35°C. In the RT phase, we observed a repulsive hydration force extending several nanometers from the surface. Approaching the phase transition collapses the repulsive force toward the sample.

We developed a humidity-control apparatus, linked to an attenuated total reflection (ATR) fluid-flow cell to collect IR spectra of ultrathin water layers. We learned to grow millimeter-sized hexagonal AgI single-crystal samples and obtained water on AgI ATR spectra qualitatively different from those of bulk water and water adsorbed on nonionic surfaces.

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38689

Design, Synthesis, and Characterization of Soft-Matter Nanolayer Superlattices

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Recently, birefringent polymer nanolayer superlattices that displayed enhanced reflectivities were reported in the literature. These superlattices consisted of alternating nanolayers of isotropic polymethylmethacrylate (PMMA) and either birefringent polyester or birefringent syndiotactic polystyrene. We determined the reflectivities of the *p*- (in plane) and *s*- (perpendicular) polarized light from the superlattices by the indices of refraction of the nanolayers. However, as reported, these superlattices are passive materials: once fabricated, the optical properties cannot be changed in response to the reflected light or to a trigger signal. This project seeks to modify by organic chemistry the composition of one of the nanolayers to include photochromic molecules that could change the indices of refraction of that set of nanolayers when triggered by an external signal. This change in refractive indices will change the overall reflectivity and the value of the Brewster angle enabling optical switching. Sandia is synthesizing photoswitchable polymers by appending azobenzene dyes to the PMMA nanolayers. The azobenzene functionality undergoes a *trans*-*cis* photoisomerization that changes the refractive index of the material. To help guide the synthetic effort, computations of optimum geometries and optical properties at the semiempirical level are currently under way for an initial set of diazo compounds. The results will be calibrated against available experimental data to determine if the semiempirical methods can reproduce trends in optical properties of substituted diazo compounds. We will perform superlattice fabrication with a modified coextruder. Ultimately, we will use these novel materials for fabricating optical microdevices such as stationary (*i.e.*, no mechanical moving parts) optical switches.

We focused our synthetic, modeling, and characterization efforts on photoswitchable azobenzene dye (ABD) chromophores as candidates for incorporation into PMMA nanolayers. We prepared two azobenzene polymers with different polar and electronic substituents. We prepared an azo polymer bearing no substituent in the azobenzene para position by reacting methacryloyl chloride with 4-(phenylazo)phenol followed by free-radical polymerization. Ultraviolet-violet (UV-V) in absorption spectra of a cast film of this polymer

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showed the expected photoswitching behavior. We prepared another azo polymer bearing a para nitro group by reacting methacryloyl chloride with 4-(4-nitrophenylazo)phenol followed by free-radical polymerization. Ultraviolet-visible (UV-vis) absorption characterization of this polymer is currently under way. Our modeling work focused on determining a reasonable model PMMA system for predicting condensed-phase index of refraction. The two model systems considered approximated the polymer backbone with methyl and isopropyl groups. We are currently investigating the effects of water and benzene solvation on the optical properties of the model PMMA systems. By comparing our solvation predictions with available data, we will choose a model PMMA system. For our initial work in superlattice fabrication, two microlayer superlattice structures (sixteen-layer structures with 0.8 mm-thick layers) were made on a coextruder at the University of Minnesota.

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38690

Photocontrol of Nanointeractions in Microsystems

N. S. Bell, D. R. Wheeler, D. A. Loy, G. M. Jamison, K. S. Potter, S. Y. Lin

The manipulation of physical interactions between structural moieties on the molecular scale is a fundamental hurdle in the realization and operation of nanostructured materials and high-surface-area microsystem architectures. These include such nanointeraction-based phenomena as self-assembly, fluid flow, and interfacial tribology. Sandia's research utilizes photo-sensitive molecular structures to tune such interactions reversibly. This new material strategy provides optical actuation of nanointeractions impacting behavior on both the nano- and macroscales and potentially impacting directed nanostructure formation, microfluidic rheology, and tribological control.

Our activities focused on the identification and examination of organic structures possessing known photophysical effects that have a high probability for influencing target interaction processes, e.g., physical entanglement, hydrophobicity/-philicity, local electrostatic charge, or pH changes. Their incorporation into polymeric chemistries will allow their application to inorganic colloids as photoactive surfactants. This will allow the photoactuated control of interparticle nanointeractions in self-assembled photonic bandgap (PBG) structures (artificial opals).

Extension of these fundamental findings can also provide optically tuned microfluidic rheology and tribological control useful in a range of microsystems with an impact on Department of Energy/Defense Programs (DOE/DP) technologies for stockpile safety and security.

We initiated an investigation of the properties of films of photosensitive organic moieties. The systems include derivatives of azobenzene, furyl fulgide, and benzospiropyran functionalized to covalently bond to silica surfaces. We chose these organic moieties because they are known to have reversible changes in conformation in response to specific photonic frequencies. We studied these films of photoactive organic moieties using spectroscopy and contact-angle measurements.

Another milestone involves the incorporation of these organic species into polymeric structures to act as photosensitive surfactants. Several publications are available where a conventional polymer is modified using a

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commercially available dye molecule. These polymers show photosensitive material properties including changes in solubility in nonaqueous solvents and changes in contact angle. Work to adapt knowledge from the literature is currently under way. In addition, the University of Arizona chemistry department is producing dendrimer structures with reactive groups for adhesion on silica-based substrates. We received four functionalities and are preparing them for testing.

Testing of a photosensitive colloidal system will proceed once we complete the synthesis and characterization of the various systems. We will demonstrate reversible photoactuated agglomeration of colloids using either mechanical or electrostatically based interaction mechanisms. There is one example of this behavior in the literature using spiropyran, and therefore we believe we can achieve this goal rapidly.

We successfully achieved synthesis of candidate photoactive organic structures and the demonstration of the targeted photophysical responses in these systems. Additional synthetic efforts to tailor aspects of these structures for covalent attachment to silica colloid surfaces are also completed or under way for the candidate systems. With these tasks confirmed, the project is on track to introduce these molecular substituents into a colloidal system to demonstrate photophysical control of rheological response.

The result of the established project was the formation of a colloidal crystal with a photocontrolled mechanical response. Studies of the literature show that photomechanical responses in polymers are virtually unknown. In fact, one source relies on an uptake of ambient water vapor to generate the response and concomitant humidity sensitivity. The response is also not rapid. In general, photocontrol of polymer properties utilizes secondary effects such as phase transitions or changes in nonlinear optical properties to manufacture device responses. There is a need to consider altering the demonstration element of this project (a photomodulated colloidal crystal) based on the potential device properties. A significant demonstration that also shares the goals of the project would be a method to control the domain size and defect structure in a colloidal crystal.

Production of a colloidal crystal without defects is a significant goal in the formation of devices using monodisperse particles to control the diffraction of light in photonic networks. We believe that addressing this problem will make use of the current activity of the project and is within the desired project objective of controlling macroscopic properties through nanointeractions. Methods to control the formation of colloidal crystal arrays require a transition in the volume fraction of

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particles within a kinetic processing window. Rapid coagulation and concentration of particles lead to an amorphous structure, and extremely slow coagulation promotes multiple crystal nucleation events and a high-defect density.

We propose to control the removal of defects in the fabrication of a colloidal crystal analogously to the phenomenon of zone refining of metals or zone growth of single crystals. By photonicallly sweeping the stability of the particles over the substrate, a single-crystal region should be possible to fabricate. Potentially, the growth of crystalline particles could be directed over a substrate to provide a waveguide between components.

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38691

Electrochemically Deposited Alloys with Tailored Nanostructures for LIGA Micromachines

D. C. Dibble, R. P. Janek, J. J. Kelly, S. K. Si

The performance of LIGA (the German term Lithographie, Galvanoformung, und Abformung, for lithography, electro-forming, and molding) micromachines is directly linked to the mechanical, magnetic, and tribological properties of the electrodeposited alloys used in component fabrication. Surface-active compounds are used in the electrodeposition process to control grain nanostructure, composition, and internal stress of the alloy. Additives dramatically alter these properties and can greatly enhance the mechanical strength of the component, or they may contribute to undesirable effects such as fracture embrittlement. Additives for electrodeposition processes are empirically developed. More importantly, there is little, if any, physico-chemical understanding of the relationship between additive structure and electrochemical action. Sandia seeks to develop the science base needed for the rational development of alloy-deposition processes in LIGA using additives and other advanced electrodeposition techniques (such as pulsed-current electrodeposition). To such effect we will develop nanoscale diagnostics that can be performed in situ electrodeposition. We will use these diagnostics to characterize in detail the electrodeposits at the nanometer scale. We will clearly focus the efforts of such an investigation on improving process conditions and facilitate them by a close collaborative effort between fundamental surface science and electrochemical engineering methods.

We completed the installation of two combination atomic-force microscopes (AFM)/scanning-tunneling microscopes (STMs) capable of *in situ* imaging of cathode surfaces with near atomic resolution for electrochemical experiments. Optimization of experimental hardware for nickel (Ni) electrodeposition included lithographically patterned electrodes, redesign of electrochemical cells, and other hardware improvements. We achieved imaging with STM and AFM during controlled electrodeposition and etching experiments on well-prepared gold (111) and polycrystalline surfaces in a standard Watts Ni electroplating solution. The goal of these initial experiments was to examine the epitaxy and grain evolution of the first several monolayers of the electrodeposit for the establishment of baseline experimental

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conditions prior to the introduction of additives and alterations of substrate and solution chemistry. We identified some additives of interest for this study, including saccharin, coumarin, sulfamate, iron, and manganese. We characterized experimental conditions within the electrochemical cell by cyclic voltammetry and optimized them with respect to pH, Ni concentration, and deposition potential.

38692

Nanostructured Materials for Directed Transport of Excitation Energy

M. B. Sinclair, D. Y. Sasaki, J. A. Floro, J. R. Wendt

One functionality that is extremely desirable for nanostructured materials is the ability to efficiently activate or interrogate structures within a nanomaterial using optical energy. However, given the packing densities obtainable with nanofabrication, direct focusing of incident optical energy onto individual nanostructures is impractical. Sandia's research will determine how the phenomenon of energy transfer can be harnessed to provide this functionality. Energy transfer is the process by which excitation energy resulting from absorption of photons can become delocalized and move from the site where the photon was absorbed. Energy transfer plays a prominent role in the photosynthetic process, where "light-harvesting antennas" efficiently absorb sunlight and deliver the excitation energy to the photosynthetic reaction center. The antennas comprise arrays of absorbing organic chromophores that are coupled via near-field electromagnetic (EM) interactions. We will use the tools of nanotechnology to control the structure, and, hence, the energy-transport properties of chromophore arrays. We will use nanolithography to pattern substrates in a manner that will allow us to measure the extent of delocalization in chromophore arrays. We will also use nanolithography to create site-energy and site-spacing gradients within chromophore arrays in an effort to drive excitation-energy transport in predetermined directions. We will also utilize self-assembly techniques such as self-assembled monolayers (SAMs) and Langmuir-Blodgett (LB) films to control the growth, structure, and energy-transport properties of chromophore arrays. Recent theoretical investigations led to the prediction that surface plasmon coupling between adjacent nanoparticles in metallic nanoparticle chains can lead to energy delocalization and transport. We will fabricate metallic nanoparticle chains using both nanolithography and self-assembly. Using a variety of optical microscopies, we will develop methods to couple EM energy into these structures and characterize their energy-transport properties.

We successfully fabricated a variety of metallic nanoparticle arrays using electron-beam nanolithography. These nanoparticle arrays include both circular and elliptical particles arranged in regular square lattices as well as rectangular lattices. Polarized light microscopy revealed interesting optical

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dichroism. We synthesized azobenzene-derivatized amphiphiles and used these to form LB films that exhibit strong intermolecular interactions. We also prepared LB films of a cyanine-based molecular species and are currently performing optical analysis of the degree of molecular aggregation. We began the synthesis of another organic chromophore that is known to exhibit profound intermolecular interactions in the solid state. We prepared nanoparticle island films of amorphous silicon that show pronounced optical effects that we believe are associated with interparticle interactions. We also initiated an effort to prepare highly terraced manganese-oxide (MgO) substrates for the production of metallic nanoparticle chains. We investigated the effect of annealing on both polished and cleaved MgO surfaces on the morphology. Cleaved surfaces appear to be most promising for the current application. We obtained terraced surfaces with step heights of order 50 nm, ideal for the growth of metallic nanoparticles. We also began to deposit discontinuous silver films on these substrates and to investigate the nucleation and coarsening of nanoparticles.

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Modeling Local Chemistry in the Presence of Collective Phenomena

N. A. Modine, M. E. Chandross

Many materials science problems are characterized by the interplay of two phenomena: chemical specificity (CS), controlled by the detailed behavior of chemical bonds, and collective phenomena (CP), where new behavior emerges from many body interactions. Sandia seeks to develop the world's first robust and efficient model bridging the length scales involved in these phenomena. To maintain a preeminent focus on materials science, we will apply our approach to obtain an unprecedented understanding of the interplay between chemistry and collective phenomena during the aging of a complex material system, Zeolite-3A-based desiccants. Such investigations require a coupling of quantum mechanical (QM) methods and classical methods into the same simulation since classical simulation techniques alone cannot model CS reliably, while QM methods alone are incapable of treating the extended length and time scales characteristic of CP. In typical situations, where the reactions responsible for CS are localized, while the weaker, longer-range interactions involved in CP can be classically represented, an efficient QM-to-classical coupling can be obtained by exploiting the natural spatial locality of electronic structure (Kohn's nearsightedness). Previous efforts along these lines used a simplified, empirical QM model and thus are limited to a narrow range of materials. In contrast, our first-principles approach has the potential to impact numerous mission-critical Sandia programs. In addition to the aging and reliability of desiccants, our model eventually could be applied to problems such as (1) science-based processing for ceramic/metal joints, e.g., in neutron tubes, where the relationship between chemical composition (CS) and interface integrity (CP) is poorly understood, and (2) proteomics, where active sites (CS) interact with a complex background consisting of the rest of the protein and its aqueous environment (CP).

Our first three milestones required the implementation of a Green's-function-based electronic structure (GFES) method implementing self-consistent density-functional theory (DFT) with the calculation of accurate forces. We verified that this approach provides a highly localized representation of the electronic structure of Zeolite-4A, and the resulting electronic energy is variational and exponentially convergent. Despite unexpected technical problems with Sandia's Computational

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Plant (CPlant) computer system, we made strong progress toward using the new capabilities that we are developing to study the structure of Zeolite-4A. Compaq reintroduced a previously resolved compiler bug that prevents compilation of our GFES software on the CPlant system. We isolated and reported the problem to Compaq, and they assured us that it will be fixed in the next release. Therefore, we believe that this represents a short-term setback in our plans. We achieved our goals by studying a smaller model system that captures many of the important features of Zeolite-4A. We investigated ion rearrangements, modifications to the cage structure, and the absorption of a single water molecule. Our main conclusion is that water, which is polar and forms hydrogen bonds, behaves in a new and different manner. Unlike previously studied molecules, water prefers to sit in the eight oxygen rings and, due to the limited space in these rings, crowding effects are important. We identified a promising approximation for the Green's function, but we have been unable to evaluate the accuracy of this approximation due to the limited system size that we can treat with the currently available computer resources. We also began architectural design of required software.

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The Effects of Varying Humidity on Copper-Sulfide Film Formation

J. P. Sullivan, N. A. Missert, T. M. Mayer, J. C. Barbour, M. J. Campin, R. G. Copeland

Atmospheric corrosion of electrical components has been linked to a significant number of materials-related significant finding investigations (SFIs) for the nuclear weapons stockpile. Further, the increasing use of copper (Cu) in commercial systems will require a long-term commitment to understand Cu corrosion mechanisms to reliably predict corrosion rates for commercial-off-the-shelf discrete components in the future stockpile. The complex interactions between a sulfidizing environment and an oxidized Cu surface are dependent on relative humidity (RH) and temperature. Small changes in the ambient temperature near room temperature may cause significant changes in the sulfidation mechanism that can lead to greatly differing morphology of the corrosion product layer. This corrosion product layer, primarily Cu_2S , can impede mechanical functions of connectors and switches and alter the performance of electrical components. This project will study the effects of varying RH in the initial stages of Cu sulfidation and in the resulting Cu_2S product layer. Kinetic studies revealed that the initial stages of sulfidation follow different reaction kinetics at high and low RH and may even be governed by different chemical reactions. High-resolution transmission electron microscopy (TEM) revealed significant differences in Cu_2S morphology at low and high RH with high-RH Cu_2S films showing small grain sizes and a high concentration of voids. X-ray reflectivity and ellipsometry showed important differences in how the Cu_2S film nucleates and in the effect of RH on the properties of the native Cu oxide surface on Cu. These measurements will ultimately lead to the development of quantitative, predictive models of Cu sulfidation, which will be an important contribution to the materials-aging program at Sandia.

We made several important discoveries regarding the role of RH in the environment during the very initial stages of Cu sulfidation. Unexpectedly, we found that the activation energy for the formation of Cu sulfide during the early stages of sulfidation is very dependent on RH, 0.34 eV at 0.5% RH and ~ 0.0 eV at 80% RH. While this result would not be surprising for latter stages of Cu sulfidation where the sulfidation rates are clearly different, at the early stages of sulfidation it was thought that the reaction rate was limited by mass transport of H_2S in

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the gas phase. Our new results show that this model is overly simplistic and that the rate-controlling mechanism itself is likely to be different at low and high RH at the initial stages of sulfidation. Through the use of ellipsometry, we also found that hydrogen dioxide (H_2O , water) or H_2O vapor produces noticeable changes in the properties of copper-dioxide (Cu_2O) films that naturally form on Cu, and this suggests one possible clue to the different surface reactions at low and high RH; namely, the reaction at high RH may proceed following chemical modification of the Cu surface by H_2O . We also discovered using x-ray reflectivity, atomic force microscopy, scanning electron microscopy (SEM), and TEM that the growth process of the sulfide and the grain structure and morphology of Cu_2S during early stages of sulfidation show a strong dependence on RH. The initial sulfide that forms at high RH nucleates as small, equiaxed grains that exhibit an initial coverage that is patchy. As the Cu_2S layer thickens, numerous small (~ 10 nm) voids appear in the Cu_2S that was formed at high RH, while the Cu_2S formed at low RH is apparently free of voids. It is thought that these voids either result from the low Cu mobility in high-RH-formed Cu_2S or lead to the low Cu mobility seen in this material. Taken together, these findings suggest important new directions for understanding the effect of humidity on Cu sulfidation, such as exploring the possibility that sulfidation at high RH levels might initiate from precipitation of Cu_2S from solution.

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39017

Solution-Based Nanoengineering of Materials

J. A. Voigt, R. T. Cygan, T. J. Boyle, L. J. Criscenti, J. Liu, E. N. Coker

Solution-based synthesis is a powerful approach for creating nanostructured materials. Although there have been significant recent successes in its application to fabricating nanomaterials, the general principles that control solution synthesis are not well understood. Sandia's purpose in this project is to develop the scientific principles required to design and build unique nanostructures in crystalline oxides and II–VI semiconductors using solution-based molecular self-assembly techniques. The ability to synthesize these materials in a range of different nanoarchitectures (from controlled morphology nanocrystals to surface-templated three-dimensional [3-D] structures) will provide new opportunities for the development of interactive interfaces for optics, electronics, and sensors. We used the homogeneous precipitation of zinc oxide (ZnO) in aqueous solution as the model system.

(1) *Molecular models of ZnO morphology, surfaces, and ligand adsorption.* We used interatomic potential models to evaluate surface energies and attachment energies of the stable surfaces of ZnO, then used them to derive equilibrium morphologies of ZnO. The resulting morphologies include two versions of the hexagonal prism and a dihexagonal prism, with the stabilization of basal, columnar, and pyramidal forms. Additional columnar forms include and are stabilized in one of the surface-energy models. These morphologies are consistent with the general results of the experimental growth processing of ZnO. The crystal structure for ZnO (zincite) suggests optimum oxygen-oxygen distances that are unique to each surface structure and that can be used to select candidate complexing compounds leading to surface inhibition or selective dissolution of the particular surface.

(2) *ZnO nucleation.* Our initial work on the nucleation of ZnO films by homogeneous precipitation in aqueous solution focused on reproducing the work of Vayssieres and coworkers [L. Vayssieres, *et al.*, *J. Phys. Chem B* 2001, 105 3350–3352]. Their process utilizes a temperature-driven thermal decomposition of a Zn-hexamethylenetetraamine (HMT) complex that produces a pH change. The pH shift, in turn, causes the hydrolysis and precipitation of ZnO. Using modifications of this process, we produced equivalent 3-D arrays of highly oriented ZnO microrods. We extended this work to show that these arrays can be grown in an HMT-free

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solution in which the substrate has been slurry-coated with a ZnO film.

(3) *ZnO growth and dissolution.* The ability to reproducibly prepare a variety of ZnO film structures was critical to beginning our exploration of how to influence ZnO growth and dissolution—they are used as the “substrates” for these experiments. As shown by the following examples, both growth modification and controlled dissolution are potentially powerful tools for controlling the structure of extended 3-D films. We demonstrated that the growth of ZnO microrods can be controlled by adding the appropriate growth modifier. We subjected an array of ZnO microrods to additional growth of ZnO in the presence of a low level of citrate anions. We capped the rods with plates of ZnO, and it can be seen that the plates grew on the ends of the rods. The change in ZnO growth in the presence of trace amounts of citrate is explained by the results of the adsorption modeling. The calculated binding energies show that citrate has a high affinity for the basal plane, and little or no affinity for the columnar faces, thus poisoning the basal plane growth. As a result, we grew large-faced, platelike ZnO crystallites.

In studying the ZnO system, it became readily apparent that dissolution as well as growth can be used as a “tool” to engineer film nanostructures. We prepared several examples of interesting ZnO structures using dissolution in combination with growth. Depending on which crystal faces are “protected” from dissolution, different ZnO morphologies evolve. It can be envisioned that with the combination of patterned nucleation and controlled growth (e.g., example above) and dissolution, a wide range of technologically important structures can be fabricated.

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Microsystems and Engineering Sciences Applications (MESA)

The Microsystems and Engineering Sciences Applications (MESA) investment area is working to create a delivery system comprising the facilities, infrastructure, and supporting network of capabilities needed to provide microsystems-based solutions, products, and services in support of critical national priorities. This MESA delivery system will include personnel and facilities from many different parts of Sandia, and will incorporate all of the elements needed to meet specifications, cost requirements, and schedules for the delivery of reliable, microsystems-based solutions for Sandia's customers. This research will involve supporting commercial and university relationships.

Tens of thousands of sites containing toxic-chemical spills, leaking underground-storage tanks, and chemical-waste dumps require accurate characterization and long-term monitoring to reduce health risks and ensure public safety. However, current methods are costly and time-intensive; also, limitations in sampling and analytical techniques exist. As much as 80 percent of the costs associated with site characterization and cleanup of a Superfund site can be attributed to laboratory analyses. “Microchemical

Sensors for Characterization and Monitoring of Volatile Contaminants” addresses the need for inexpensive, real-time, continuous, *in situ* sensing and characterization methods. We designed, fabricated, and tested a prototype sensor package and cable that satisfy these requirements. Two patent disclosures have been filed.

10756

New Architectures for Micro-Total-Analytical Systems

P. C. Galambos, S. Montague, M. Okandan, Y. Fintschenko, E. F. Hasselbrink, J. A. Irvin, B. J. Kirby, C. D. James

The goal of this project is to expand Sandia's unique capabilities in electrokinetic pumping (EKP) to new substrate materials. The two approaches are SUMMiT-VTM fabrication, which offers the advantages of complementary metallic-oxide semiconductor (CMOS)-compatible fabrication, and porous polymer monoliths, which can be polymerized in glass, silica, plastic, or silicon (Si) substrates, and hence offer some platform independence. Both approaches are high-risk with high-payoff potential, as they will greatly reduce the cost of EKP fabrication, which is presently labor-intensive.

The research focus of this project has been enhanced to reflect our growing understanding that EKP is a technology that may have applications in microactuation, microheat transfer, and a host of other technologies besides micro-total-analysis systems. In particular, microactuation is of interest because of Sandia's core capability in surface-micromachined (SMM) Si systems. Toward this end, our goal is not merely to achieve EKP in these systems, but also to demonstrate these novel capabilities in an integrated platform.

The thrust of this project was to test components and architectures developed in previous years for highly integrated microfluidic microsystems. Accomplishments include (1) demonstration of packaging of on-Si silicon-nitride (SiN) microfluidics with glass microfluidics using anodic bonding, (2) demonstration of operation of on-chip SiN EKPs, (3) demonstration of dielectrophoretic particle concentration in on-Si SiN channels containing built-in electrodes, and (4) characterization of additives for significantly improving EKP performance.

We developed a method for aligned anodic bonding of individual Si die to glass flow manifolds. We fabricated laminated borosilicate glass manifolds containing channels connecting larger, widely spaced holes with smaller, more tightly spaced holes. The smaller holes in the glass match those on the bottom of the Si die. Bosch-etched vias route fluid from the connection on the bottom of the die to the front of die channels. We accomplished the Si/glass attachment by developing a fixture allowing precise (1 mm) optical alignment of the vacuum-mounted Si die to the glass, and the application

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of high temperature (325°C) and voltage (1500 V) to the die/glass interface, thereby anodically bonding the die to the glass with aligned fluid connections. This die-attach method makes small-scale hybrid glass/Si integration feasible.

We demonstrated electroosmotic pumping of an aqueous solution in the glass manifold channel using the attached on-Si SiN EKP. At 20 V, we observed electrolytic bubble generation at the integrated electrodes in the SiN channels. Therefore, we used a direct-current (DC) voltage of 15 V to electroosmotically pump without gas bubbles. The electrodes were only 700 nm apart, so a high field of 21.4 kV/m was generated at 15 V. Since the electrodes are photolithographically defined and fabricated with the channels in a monolithic SMM process, it is relatively easy to fabricate electrodes that are 1 mm apart, allowing even higher fields at lower voltages. Upon applying 15 V to the in-channel electrodes, we observed the air/water meniscus in the connected glass flow manifold channel move at approximately 200 mm/min, indicating pumping. To our knowledge, this is the first on-Si EKP to be demonstrated and opens up the development of highly integrated, extremely small (down to 1 mm) microsystems containing microfluidics, electronics, and microelectromechanical systems (MEMS) on a monolithic, mass-producible Si substrate.

We investigated dielectrophoretic effects by loading the SiN channels with a 1 mm bead solution. We applied a 10 V AC signal at 1–30 MHz to one of the built-in poly-Si electrodes while a second electrode was grounded, resulting in dielectrophoretic bead motion. Since the electrodes are so close together—in some cases 2 μm apart—very high fields can be generated with small voltages (5 MV/m). One potentially useful phenomenon observed was the concentration of beads in regions of high (positive dielectrophoresis) and low (negative dielectrophoresis) field gradients. An on-chip dielectrophoretic particle concentrator could be used to collect and manipulate cells in a highly integrated microfluidic microsystem.

We developed additives for improved EKP performance. The addition of trimethylammonium propane sulfonate to a pumped fluid increased the flowrate by 20% and improved efficiency and pressure performance by a factor of 3. By tailoring fluid properties in sections of a microfluidic microsystem (in this case, the EKP section), significant performance benefits can be achieved (lower-voltage and/or higher-pressure operation).

We developed several potential components and architectures for the micro-total-analytical system (μTAS): (1) on-chip dielectrophoretic concentrators—useful in cellular

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sample pretreatment, on-Si EKP—allowing production of highly integrated monolithic microsystems in Si, (2) hybrid precisely aligned and sealed (anodic bond) glass/Si microfluidic microsystems—allowing Si microfluidics to be integrated with glass microfluidics in a compact package, and (3) EKP solution additives—allowing higher-performance (pressure, efficiency, flowrate) EKP.

Refereed

Galambos, P. C., M. Okandan, K. R. Pohl, G. L. Benavides, M. W. Jenkins, D. J. Bennett, and M. S. Stay. 2002. Packaging dissimilar materials for microfluidic applications. *Proc. ASME International Mechanical Engineering Congress and Exposition IMECE'02, Microfluidic V* (November, New Orleans, Louisiana): FE-7B.2002.

26553

Microchemical Sensors for Characterization and Monitoring of Volatile Contaminants

R. C. Hughes, C. E. Davis, M. L. Thomas, D. A. Rivera, L. K. McGrath, M. T. Itamura, J. L. Wright

Tens of thousands of sites containing toxic-chemical spills, leaking underground-storage tanks, and chemical-waste dumps require characterization and long-term monitoring to reduce health risks and ensure public safety. In addition, over two million underground-storage tanks containing hazardous (and often volatile) contaminants are being regulated by the Environmental Protection Agency, and some form of monitoring is required to detect leaks from the tanks and pipe network. However, current methods are costly and time-intensive, and limitations in sampling and analytical techniques exist. For example, the Department of Energy's Savannah River Site requires manual collection of nearly 40,000 groundwater samples per year, which can cost between \$100 and \$1,000 per sample for off-site analysis (not including the cost of collection). In addition, as much as 80% of the costs associated with site characterization of a Superfund site can be attributed to laboratory analyses. The integrity of these analyses can also be compromised during sample collection, transport, and storage. Finally, although commercial tools are available for chemical detection, e.g., gas chromatographs, few have been adapted for use in geologic environments for long-term monitoring or remediation applications. Therefore, a need exists for inexpensive, real-time, continuous, in situ sensing and characterization methods. In this project, Sandia is developing a real-time, continuous, volatile-organic-compound (VOC) sensor that can be deployed in soil, air, or water for long-term applications. This project investigates the use of chemiresistor-sensor arrays to detect VOCs in subsurface environments.

We made significant progress in the areas of chemiresistor-sensor development and testing. With regard to sensor development, we revised the waterproof package to improve the ruggedness and waterproof seal. We designed a new manifold that will position a preconcentrator above the existing chemiresistor package with only slight modification to the current waterproof housing. We also designed a new spiral chemiresistor that may improve the stability and performance of the sensor by providing a larger contact area between the carbon (C)-loaded polymer and traces.

Chemiresistor probe disassembled.

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We performed a number of laboratory experiments to test and evaluate the functionality of these sensors in subsurface environments. These experiments and analyses include polymer optimization, C comparisons, surfactant addition, sensitivity evaluation, preconcentrator testing, data analysis, pattern recognition, temperature control, and *in situ* contaminant characterization. We also initiated field tests at the Chemical Waste Landfill, Edwards Air Force Base, and at the Nevada Test Site to evaluate the robustness, longevity, and performance of the chemiresistor sensor package.

Field test at Edwards Air Force Base.

Refereed

Davis, C. E., R. C. Hughes, M. L. Thomas, and C. K. Ho. 2002. Data-analysis methods for real-time VOC chemiresistor sensor. Proc. *Sensors Expo and Conference Spring 2002* 1 (20–23 May, San Jose, California): 179–91.

Ho, C. K., and R. C. Hughes. 2002. *In situ* chemiresistor sensor package for real-time detection of volatile organic compounds in soil and groundwater. *Sensors* 2:23–34.

26573

Ultralow-Power Spread-Spectrum Receivers for Microtags to Improve Security During Critical Operations

R. W. Brocato, J. R. Wendt, D. D. Spencer, J. L. Schoeneman, E. J. Heller, K. W. Plummer, S. R. Smith, S. A. Jones, R. T. Mitchell, G. M. Schwartz

Sandia's goal in this project was to develop a programmable spread-spectrum receiver based on surface acoustic-wave (SAW) correlator technology. To reduce power requirements and size, the receiver architecture does not use standard frequency down-conversion, but directly demodulates the signal from the carrier frequency to the data frequency. The design is based on the technique of correlating the received radio-frequency (RF) signal with the preprogrammed spreading code. There were two principal areas of technical development during recent work. First, we refined development of fixed-code SAW correlators and their related interface circuitry. Second, we built, tested, and demonstrated an electrically programmable SAW correlator.

This project addresses a microsystem security need by developing an ultralow-power RF receiver architecture useful for microtag and zero-power receiver applications. There currently does not exist a commercial receiver capability to meet low-power requirements for microtags in security-related applications. Such receivers are not expected to become commercially available due to incompatible market demands.

This microsystem-based wireless RF communication receiver development differs from commercial offerings by having smaller size and much-reduced energy consumption. Primary project emphasis was on the realization of an ultraminiature, short-range (< 1 km), energy-efficient spread-spectrum receiver. The central concept behind the spread-spectrum receiver was the use of SAW correlators to directly and passively demodulate a broadband-coded radio signal into baseband data.

SAW correlators have been developed in the past and demonstrated to be useful for low-power, spread-spectrum radio receivers. What is unique about this project is the development of an electrically programmable SAW correlator. In the past, a different correlator had to be fabricated for each transmitter/receiver pair. If a receiver had to listen to several transmitters, it had to have a separate correlator for each device to which it had to listen. With the programmable correlator, a single SAW

Side view of PSAW test board.

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device is built for all transmitters and receivers in a system. The radio then electronically adjusts its correlator for the transmitter to which it must listen, or the receiver to which it must talk.

Early work focused on overcoming a long list of manufacturing- and fabrication-related obstacles. We overcame several technical problems, including developing electron-beam-based lithography for high-frequency operation, settling questions about manufacturing repeatability and temperature stability, getting adequate signal strength by optimizing substrate material type, developing microwave-matching networks, and resolving packaging problems. All of these issues were effectively dealt with and adequately resolved.

We developed the programmable SAW correlator and demonstrated it within the system context of a spread-spectrum radio receiver. We fabricated the programmable SAW correlator by flip-chip bonding a lithium niobate SAW correlator to a silicon programming chip and then packaging the entire assembly in a leadless chip carrier. We then tested the packaged device and demonstrated it on a printed-circuit test board. Electrical waveforms from testing with correct and orthogonal codes exhibited reasonable signal-to-noise levels. The basic spread-spectrum radio receiver demonstrates acceptable performance.

Top view of PSAW integrated circuit.

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26770

Interconnection Technology for Next Generation of Integrated Microsystems

R. Chanchani, T. A. Fischer, G. R. Sloan, D. J. Rieger, K. M. Norman, D. T. Bethke, R. B. Hurley

True microsystems of the future will require denser interconnect technologies that will facilitate both integration and miniaturization of electronics, optics, and microelectromechanical systems (MEMS) in a single package. Various high-density interconnect technologies that exist in the industry do not offer the level of flexibility and integration capability that would be required. To address this issue, Sandia developed a multilayer interconnect technology that is broadly applicable to numerous future Sandia microsystems. This interconnect technology consists of thin-film deposited benzocyclobutene (BCB) dielectric with copper (Cu) conductors on a variety of base substrate materials, namely silicon (Si), alumina, and low-temperature co-fired ceramics (LTCC). Also within this interconnect structure, we embedded passives like resistors, capacitors, and inductors. This technology will support the next generation of Sandia applications like synthetic-aperture radar (SAR) miniaturization, radar fuzes, advanced telemetry, and advanced intelligence applications.

Based on the feedback from our customers, we added several new tasks to the original goals of this project: 20 μm -thick BCB multilayer stack, deposition of BCB/Cu stack on LTCC, and the development of ultrahigh-density circuit for magnetic levitation.

We demonstrated the feasibility of fabricating high-density integrated substrate technology using BCB dielectric with Cu conductors in multilayer structure with embedded passives (resistors, capacitors, and inductors). Previously, we demonstrated the baseline high-density substrate technology consisting of multilayers of thin-film-deposited 5 μm -thick BCB dielectric with 2 μm -thick Cu conductors on 4 in. Si wafers. Recently, we enhanced this baseline technology in the following ways.

(1) We developed processes to deposit BCB/Cu layers on alumina and LTCC base substrates. The roughness of ceramic was critical in obtaining a good adhesion between BCB and ceramic. In the case of low-temperature co-fired multilayer ceramic substrates, we had to take into account a dimensional tolerance in ceramic when designing the substrate. A test vehicle (TV-1), which we designed in early work, was used for

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the development of BCB/Cu on alumina. We designed a separate test vehicle (TV-1a) to develop this technology on LTCC.

(2) We developed a process for 20 μm -thick nonphotodefinable BCB. We showed that the minimum via size that is feasible is 50 μm , as compared to 35 μm vias in 5 μm -thick photodefinable BCB.

(3) We demonstrated the feasibility of embedding passive components of thin-film TaN resistors with sheet resistivity of 100 ohms per square. We designed a special test vehicle (TV-2) with resistor values from 10 ohms to 10 K ohms for this development. TaN thickness has to be optimized to reduce “wrinkling” of BCB at TaN deposition sites.

(4) We demonstrated the feasibility of embedding Ta pentoxide capacitors in 5 μm BCB. We designed a special test vehicle (TV-3) with capacitor values from 50 pF to 100 nF for this development. The major issue was the shorting of large-area capacitors (100 nF capacitors). The quality of Cu and Ta metal deposition is critical to preventing the shorts.

(5) We demonstrated the feasibility of embedding inductors in 5 μm BCB. We designed a special test vehicle (TV-4) with inductance values from 1 nanohenry to 40 nanohenry for this development.

We are currently developing two application modules using this technology.

(a) We designed a module (TV-5) to characterize the transmission, cross-talk, low-pass filter characteristic of the technology. The architecture of this module involves a combination of 20 μm - and 5 μm -thick BCB with Cu lines and embedded TaN resistors. We are currently developing the processes to combine these different features in a single module.

(b) We designed a substrate of very high density circuitry of Cu wires on BCB for wideband magnetic actuator. This substrate requires a high density of Cu wires (120 μm wide with 20 μm spacing) in 60 mm x 60 mm area. We demonstrated that this technology could potentially make such a substrate, but the cleanroom quality in the Compound Semiconductor Research Laboratory (CSRL) was not adequate to yield good large-area substrate.

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41427

Predicting and Validating MEMS Interface Reliability

M. P. de Boer, F. B. Van Swol, M. B. Sinclair, R. A. Plass, W. R. Ashurst

Microelectromechanical systems (MEMS) show great promise for delivering systems solutions for Sandia applications. However, failure at contacting and sliding surfaces is of critical concern. The physics and chemistry of the interfaces created, and their evolution due to aging, are not well understood. Predicting and validating MEMS interface reliability require applying knowledge of molecular-scale behavior of hydrophobic and hydrophilic surfaces to model characteristics of real MEMS devices. A crucial factor is the nanometer-scale roughness of the real interfaces. In this project, we shall employ a joint experimental and modeling approach that links length scales from Ångstrom to millimeter to elucidate the mechanisms that cause change in performance of test structures sensitive to adhesion under accelerated aging conditions. Capillary forces are one major mechanism for large adhesion increase in MEMS. A simple Laplace-Kelvin approach is limited at the nanometer scale. Density-functional theory (DFT) has been developed to accurately describe solvation forces in polydisperse nanopore networks and will be applied to model the rough interfaces we will investigate. We shall also construct a test system that enables measurement of interfacial properties under controlled conditions such as temperature and humidity. This will enable us to explore the interactive effects of these factors with the coating and surface roughness. By measuring and modeling the evolving interface as a function of aging conditions, we will develop validated lifetime models. This project will result in the development of reliable interfacial models at the molecular scale for MEMS performance and service life.

We initiated work on all fronts to develop an integrated experimental/modeling program to achieve predictive capability of MEMS adhesion in various ambients. We applied our modeling approach using DFT to MEMS problems. We also made progress on an analytical approach to modeling adhesion between our rough surfaces by modifying a well-known adhesion theory for the case of capillary condensation. Experimentally, obtaining self-consistent results has proven difficult. Namely, we are not seeing expected adhesion versus relative humidity (RH) trends as predicted by our theory or in agreement with an earlier experimental result. The likely

By measuring and modeling the evolving interface as a function of aging conditions, we will develop validated lifetime models. This project will result in the development of reliable interfacial models at the molecular scale for MEMS performance and service life.

reasons are either (1) surface contamination or (2) higher surface roughness. To address surface contamination, we are placing emphasis on constructing the first ultraclean MEMS test chamber that will allow simultaneous control of temperature and vapor pressure while viewing samples by interferometry. We obtained interferometry through our window, electrical probing with four independent probes, a base pressure of 1×10^{-8} Torr after bakeout, and stable O_2 and H_2O plasmas and thermal heating for sample cleaning. Also, we constructed a vapor-delivery system and installed a residual-gas analyzer allowing moderate analytical capability. Chamber “shakeout” is under way, including establishment protocols for testing procedures. To address higher surface roughness, we are processing a lot through our fabrication facility in which the poly O received a chemical mechanical polishing procedure. Preliminary measurements indicate that a roughness of less than 2 nm root-mean-square (RMS) will be achieved. This presently compares with greater than 3 nm RMS on our smoothest lots. Although the difference may not seem large, the Kelvin radius, which controls system response, is only 1.5 nm at 50% RH. The earlier result mentioned above had a 1.5 nm RMS roughness for poly O.

Preliminary measurements indicate that a roughness of less than 2 nm root-mean-square (RMS) will be achieved. This presently compares with greater than 3 nm RMS on our smoothest lots. Although the difference may not seem large, the Kelvin radius, which controls system response, is only 1.5 nm at 50% RH.

Nonproliferation and Materials Control

The Nonproliferation and Materials Control investment area seeks innovative ideas for reducing the nation's vulnerability to threats from the use of weapons of mass destruction—including nuclear, biological, or chemical weapons. Innovative research will promote a collective of capabilities and products that will enable development of organized system-level responses to national security challenges. This research focuses on (1) technologies for materials management and international cooperation, (2) security systems and technologies, (3) response to biological and chemical threats, (4) technologies for intelligence, and (5) global virtual presence.

Neutron radiography is an important nondestructive evaluation method that provides unique information valuable to Sandia's mission in nonproliferation and materials control. Neutron radiography also has important applications in airport security, protein structure, corrosion detection, and medicine. "Advanced Digital Detectors for Neutron Imaging" applies Sandia's recent advances in semiconductor radiation-detection materials to develop the first direct digital-imaging detectors for neutron radiography. The focus is to address fabrication issues in the candidate

materials. Detailed evaluation of application-specific integrated-circuit (ASIC) compatibility is being performed. Extremely low noise performance is achievable, and compatibility with existing ASIC technology is expected. Three patent disclosures and two patent applications have been filed; one patent has been granted.

10724

High-Speed 2-D Hadamard Transform Spectral Imager for IR Applications

J. C. Wehlburg, S. M. Gentry, J. L. Smith, C. M. Wehlburg, D. A. Smith, M. W. Smith

There exists the need for staring systems capable of real-time high-speed imagery in a large number of spectral bands. Existing spectral-imaging technologies do not support these rates where mechanical scanning mechanisms are too slow. Techniques that employ electronic scanning methods and two-dimensional (2-D) focal planes are required. In addition, techniques that support changing spectral sampling on the fly are able to match changing target and background conditions, particularly when optimization of signal-to-noise ratio (SNR) is desired. Finally, under certain noise conditions, spectral multiplexing techniques have the potential of increasing the SNR and decreasing the sample rate for a given measurement.

Two-dimensional Hadamard transform spectral-imaging approaches have the potential to achieve all of the above requirements. Recent advances in micromirror-array technology allow the possibility of realizing these designs. The micromirrors allow electronic switching of light between optical systems necessary to realize the Hadamard encoding matrices without significant loss of light. Since these devices are electronically programmable, they allow the system to be spectrally reconfigured in microseconds. Under nonphoton noise-limited conditions, Hadamard techniques achieve a ($N^{0.5}$) SNR advantage over nonmultiplexed approaches, where N is the number of spectral samples.

In this project, Sandia will develop a prototype staring Hadamard Transform Spectral Imager (HTSI) using commercially available micromirror arrays. Successful completion of the project would require demonstration of the technique at high scan rates and the necessary electronically tunable features.

The project started out with a design that used spectral encoding to construct the HTSI in the 0.5–2.5 μm range. Optical design issues made that option not viable. We then evaluated a 0.4–0.9 μm visible HTSI system using spectral encoding. We completed an optical design for this system. At the same time that we developed the concept for a spatial encoding system and after completing the system analysis, we determined that the HTSI system should use the spatial system and created an optical design and system model. We then filed a patent for both the spectral and the spatial 2-D encoding

Two-dimensional Hadamard transform spectral-imaging approaches have the potential to achieve all of the above requirements. Recent advances in micromirror-array technology allow the possibility of realizing these designs.

methods. The Texas Instruments (TI) Digital Micromirror Device (DMD) was designed for projectors, so it was not optimized for the HTSI. Sandia currently produces custom micromirror arrays for other applications, and we investigated the microelectromechanical systems (MEMS) technology-created micromirror design.

We developed two designs for a 2-D HTSI. One is a spectral encoding method and the other is a spatial encoding method. We also created two simulations to allow engineering options for both designs to be evaluated and completed optical designs for both techniques. We tolerated the spatial encoding method optical design and completed a mechanical design. To evaluate possible improvements to the HTSI, we investigated Sandia MEMS micromirror technology. The MEMS technology showed that it could create a part with the desired specifications, but the timetable and budget were outside the scope of this project. We purchased and assembled the data-acquisition system and submitted a patent application (SD6617) for both methods of Hadamard spectral image.

We developed two designs for a 2-D HTSI. One is a spectral encoding method and the other is a spatial encoding method.

Refereed

Smith, M. W., J. L. Smith, G. K. Torrington, C. M. Wehlburg, and J. C. Wehlburg. 2002. Theoretical description and numerical simulations of a simplified Hadamard transform imaging spectrometer. *Proc. SPIE* 4816 (July, Seattle, Washington).

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10762

Self-Assembled Tamper-Detection Seals

E. B. Cummings, I. G. Waddoups, P. M. Dentinger, B. A. Simmons, C. A. Lajeunesse

The modernization of tamper-evident tags and seals largely stopped in the 1970s, when the technology was considered “mature” and unbreakable. After 30 years of technological innovations in printing, reproduction, computers, and robotics, experts raise serious concerns about the security of existing tags. Research into ultrasecure tags and seals has produced several promising technologies (e.g., glitter and fiber-optic tags) that are supremely difficult to counterfeit but that require meticulous arrangement of evaluation apparatus, making the technology inapplicable for walk-through inspections.

This project developed a tag-and-seal methodology that simultaneously addresses issues of security and walk-through inspections. The tags and seals have a layered architecture, in which each layer contributes a unique and difficult-to-counterfeit stochastic signature. The security of these tags can be scaled to fit the application by adjusting the number of layers. An important and novel feature is that at least some of the layers in these tags can be re-randomized or “reset” in the field, allowing inspectors to foil time-consuming counterfeit efforts to reproduce or restore a signature by periodically resetting the signature.

Walk-through inspections require minimal apparatus and alignment. Sandia developed a novel barcoding methodology to provide tags with both high-resolution image fiducials for automated image comparison and an integral capacity for secure data storage. This methodology works with minimal alignment requirements and supports detailed automated image comparison for tamper detection using images taken by handheld stock or digital cameras.

In this project, we developed and tested the novel barcode methodology, implementation software and hardware system, tag and seal architecture, and resettable element composition, including age testing to 6 months. Each element of this system is Sandia commercially sensitive intellectual property. We filed a patent, now pending, for the barcode methodology “A Self-Registering Spread-Spectrum Barcode,” U.S. 09/870391. We will file a continuation-in-part of this patent that covers the details of the tamper-indicating layers and tag architecture.

We previously developed a novel spread-spectrum barcode methodology to support automated tag evaluation, implemented

Sandia developed a novel barcoding methodology to provide tags with both high-resolution image fiducials for automated image comparison and an integral capacity for secure data storage. This methodology works with minimal alignment requirements and supports detailed automated image comparison for tamper detection using images taken by handheld stock or digital cameras. ...Each element of this system is Sandia commercially sensitive intellectual property.

this methodology in the Barcode software, devised a tag architecture, and selected candidate materials for the secure tags. Recently, we refined the Barcode software, incorporating accurate and robust image-registration algorithms and numerous other improvements, tested the selected materials, and tested the ability of the system to resolve shifts in the locations of particles to detect tampering. Specifically, we did the following:

- Prepared continuation-in-part of the previous spread-spectrum barcode patent (U.S. 09/870391) that covers the application to secure tags and seals and details of the tamper-indicating layers and tag architecture.
- Filed *Commerce Business Daily* release and press release on the spread-spectrum barcode technology.
- Presented the technology on the cable TV network program *Sandia Now*.
- Attracted several potential commercial partners for the secure tag and barcoding systems.
- Successfully completed 6-month aging studies of the tag components.
- Demonstrated subpixel sensitivity to single-particle displacements in automated comparisons of actual tag images.
- Demonstrated a proprietary tag component that holds particles stably, even when mounted vertically for 6 months and left untouched, but that can be completely reset and re-randomized manually or with a roller in seconds.
- Extended the spread-spectrum barcode program, Barcode, to support automated image comparison for tamper detection, improved image registration and data recovery, multiple dataset overlays, and automatic real-time analysis of images taken by a camera connected by universal serial bus (USB) and Firewire to a laptop computer.
- Wrote a user's manual and programmer's guide for the Barcode software.

Many of the details of the tag are proprietary and sensitive to public release while in negotiations with commercial partners or licensors; however, our public disclosure of the spread-spectrum barcode technology attracted several potential partners and both print and television media coverage.

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26538

Threat-Assessment Study for Short-Pulse Laser Technologies in Directed-Energy and Countersensor Applications

S. M. Cameron, L. A. Boye, P. J. Federico, S. B. Dron, M. M. Hoffman

Recent developments in the area of short-pulse, high-energy laser research present new potential vulnerabilities for optical detectors, threat-warning sensors, and self-protection technologies. Owing to the unprecedented power density, unique temporal-spatial coherence signatures, and broad spectral self-phase modulation associated with propagation of self-focused ultrashort optical pulses in atmosphere and optical media, new interaction mechanisms for laser-based directed energy are possible using this emerging capability. The combination of commercially available short-pulse laser technology with the global proliferation of advanced optical technologies will likely create opportunities for operational exploitation and military use by adversaries over the next 5–10 years. In this project, Sandia assessed the evolving threat-development cycle of foreign femtosecond-laser capability for military application and implication from a technology perspective.

We compiled classified and unclassified database searches and correlations for specified keyword suites and contextual technical content. We evaluated proliferation paths, threat metrics, and activity indicators for significance to the development of adversarial capability. We communicated the results and recommendations for further study in a report and numerous briefings to the cognizant national threat-assessment community. As part of the work, we improved automated software tools for natural language processing and created several new databases for future follow-on parametric analysis and review. The analysis methodology implemented in our approach allowed us to explore new insights and linkages in an interdisciplinary environment combining technical and intelligence expertise. We expect that the lessons learned in this process may have broad application for similar studies in the future. The findings may impact future technology investment strategies for combating laser threats and increase awareness of the impact of new technology frontiers that are significantly different from historical precepts on the tactical and strategic battlespace of the future.

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26559

Development of a Microoptic Gyroscope

R. D. Kinney, G. A. Vawter, W. J. Zubrzycki, J. J. Hudgens

Rotation sensors (gyroscopes) and accelerometers are essential components for all precision-guided weapons and autonomous mobile surveillance platforms. Microelectromechanical systems (MEMS) gyroscope (gyro) development has been based primarily on the properties of moving mass to sense rotation and failed to keep pace with the concurrent development of MEMS accelerometers because the reduction of size, and therefore mass, is substantially more detrimental to the performance of gyros than to accelerometers.

A small (~ 0.2 cu in.), robust (~ 20,000 g), inexpensive (~ \$500), tactical-grade performance (~ 10–20 deg/hr) gyro is vital for the successful implementation of the next generation of smart weapons and surveillance apparatus. The range of applications (relevant to Sandia's mission) that are substantially enhanced in capability or enabled by the availability of a gyro possessing the above attributes includes weapon guidance, fuzing and safing; synthetic-aperture radar (SAR) motion compensation; autonomous air and ground vehicles; gun-launched munitions; satellite control; and personnel tracking. For example, a gyro of this capability would open for consideration more fuzing options for earth-penetration weapons.

The MEMS gyros currently available are lacking in one or more of the attributes listed above. An integrated optical gyro has the potential of achieving all the desired attributes. Optical gyros use the properties of light to sense rotation and require no moving mass. Only the individual optical elements required for the generation, detection, and control of light are susceptible to shock. Integrating these elements greatly enhances the gyro's robustness while achieving size and cost reduction.

The project goal is to demonstrate a resonant microoptic gyro (RMOG) produced from a monolithic photonic integrated circuit coupled with a SiON waveguide resonator. During this project, Sandia developed the photonic elements necessary for a RMOG. We individually designed an aluminum gallium arsenide (AlGaAs) distributed Bragg reflector (DBR) laser, GaAs phase modulator, and GaAs photodiode detector. Furthermore, we fabricated a breadboard gyroscope that we used to confirm modeling and evaluate feedback circuits.

We designed and manufactured a polarization-maintaining silicon (Si) waveguide resonator. We derived optimal resonator designs from loss data and simulations utilizing modeling

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software developed and refined in this project. The resulting design was an 8 m-long, 20 mm outside-diameter silica waveguide spiral. The unique spiral design should result in < 20 degrees/hr performance in a small area. We fabricated the silica planar lightweight circuit (PLC) resonator by leveraging our experience in fabrication of silicon nitride (SiN)/SiON waveguides. Waveguides used form birefringence for polarization control.

We fabricated waveguide modulators. Sandia's world-leading active/passive integration technology based on selective-area disordering of the quantum-well (QW) active layer was used to make a selected length of the GaAs waveguide passive at the wavelength of interest. Electrodes were incorporated and, when biased, resulted in a phase shift of the light in the passive region.

We fabricated waveguide-based photodetectors and fabricated photodiodes in a GaAs waveguide.

We designed and fabricated an AlGaAs DBR laser. We fabricated this new laser by selective dry etching of gratings in AlGaAs with an indium gallium phosphate (InGaP) chemical stop-layer coupled with AlGaAs epitaxial regrowth to form the low-index-contrast grating needed by high-quality narrow-optical-spectrum lasers. Our preliminary investigations suggest that epitaxial regrowth on InGaP surfaces over thick AlGaAs layers was successful. The regrown grating will permit current injection through the grating region for either uniform gain or for wavelength-tuning to assist in locating the gyro resonance.

We fabricated a breadboard system and evaluated an analog serrodyne feedback circuit. Utilizing commercial-off-the-shelf (COTs) components, we fabricated a breadboard resonant fiber-optic gyroscope. By modulating the laser-diode current and monitoring the output of the resonator, we confirmed our gyroscope model. We evaluated analog serrodyne modulation by utilizing a 60 MHz serrodyne waveform generated by a 1 GHz arbitrary waveform generator. We then amplified the serrodyne signal by a high-bandwidth radio-frequency (RF) amplifier to achieve a 2π phase shift in the phase modulators. By adjusting the frequency of the serrodyne modulation, we shifted the laser frequency to locate the resonant frequency of the gyroscope. Due to the narrow linewidth of the resonator and difficulties producing a 12 Vpp (peak-to-peak voltage), 60 MHz analog serrodyne waveform, we could not lock onto the resonance. We decided to not continue work on analog serrodyne modulation, but instead will develop a digital serrodyne modulation scheme that circumvents the issues detailed above.

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26560

Synergistic Merging of Multispectral Transient Radiometry and Multispectral Imaging Technology for Enhanced Global Situational Awareness Through Accurate Geolocation

D. S. Strong, R. L. Schmidt, R. D. Wickstrom, J. L. Smith, D. E. Bodette, O. M. Solomon, Jr., E. N. Reckase, R. E. Pepping

Accurate characterization of strategic intelligence sites is a critical and difficult problem. Sandia will explore the synergistic exploitation of multispectral transient radiometry (MSTR) and multispectral imaging (MSI) data to attain absolute geolocation to subpixel accuracies (potential improvement by more than 2 orders of magnitude). We will develop registration techniques that exploit emissive multispectral signatures coupled with reflective signatures and perform spectral feature correlation (SFC) based on a number of simultaneous spectral bands. These techniques have the potential to significantly outperform traditional techniques for scenes with low-intensity signatures for which operations on a single spectral band are insufficient. Data fusion of this nature addresses critical national security challenges, including nonproliferation, surveillance, and global situational awareness.

A dwelling MSTR affords an impressive broad-area search and surveillance capability for important targets of interest and an ability to characterize transient events, but with limited spatial resolution. An MSI affords orders-of-magnitude improvement in spatial resolution, in addition to high-fidelity spectral signatures. However, it cannot dwell and has a comparatively small field of view (FOV). For global virtual presence, an innovative combination of the two could yield information necessary for very accurate geolocation coupled with scene/site characterization, e.g., battle-damage assessment (BDA).

With ready access to MSTR and MSI systems, Sandia is uniquely positioned to exploit their combined phenomenology. For enhancing geolocation, an MSTR could detect the site of interest, e.g., smoke stack, exploding bomb, or fire, and cue the MSI, which would then, through thermal and spectral signatures, pinpoint the location with high accuracy, resulting in orders-of-magnitude improvement in target geolocation. A proof-of-principle demonstration could be in BDA.

The basis for any image registration effort is some rich realistic examples from real-life systems. We were successful in developing and executing a number of common data collections from both the MSI and the MSTR systems. The collection

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planning was quite complex, with the ultimate goal of finding a time and earth location that allowed the two sensor systems to look through the same “air” at the same location and still be within the operational limits of each sensor’s field of regard. Once we collected the data, we successfully calibrated and corrected each dataset for various sensor artifacts and developed algorithms and software to orthonormalize the data to facilitate down-stream processing.

The research led to three candidate multispectral registration techniques that we adapted and applied to the MSI and MSTR datasets. The registration techniques that were successfully applied to the datasets were multispectral normalized correlation (MSNC) and multispectral principal components (MSPC). These showed good promise. In addition, we performed some limited work using multispectral feature registration (MSFR), but it was not thorough enough to provide any confidence in its general efficacy.

We explored the possibility of using MSI daylight scenes as a reference and performing registration against the same scene imaged at night. In this case, we utilized MSPC-based registration and demonstrated, for the limited datasets available, that this was indeed possible when utilizing the midwave infrared (MWIR) and longwave infrared (LWIR) spectral bands of the MSI system. We performed a principal components transform on the spectral signatures in the images to extract the dominant spectral-spatial features in the scenes. The resulting images have significant intensity disparities among the spatial features from day to night. The application of an absolute-difference edge operator followed by scaling to a common intensity range generated images that we successfully registered using a normalized cross-correlation routine.

Through the MSNC registration technique developed under this project, we performed a vicarious calibration between the MSI and the MSTR systems. Previously, without this research, vicarious calibration between these systems was not possible because one could not register the datasets to perform the in-scene radiometric comparisons. The vicarious calibration identified certain spectral bands of the MSTR system that had inconsistent calibration. Based on these results, the developers of the MSTR system performed an independent verification of the calibration and confirmed that calibration was indeed incorrect for the identified bands.

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26561

New Glass Technology for Enhanced Architectural Surety

S. J. Glass, E. K. Beauchamp, S. S. Kamat, C. S. Newton, R. G. Stone, M. G. Vigil, R. Tandon, J. E. Kooi, E. Hoover

The objective of this project is to understand the behavior of engineered stress profile (ESP) glass in architectural surety and other applications in which glass strength, reliability, and fragmentation are critical.

Better protection of building occupants from glass-related injuries that occur due to terrorist acts and natural disasters is needed. Rush modifications are being made to buildings to protect occupants from flying glass due to explosions. This project will provide a glass whose behavior under different loading is less lethal and better understood. The long-term impacts of the project are a new generic approach for improving glass reliability and enhanced design criteria for glass for use by engineers and architects in critical structures.

Regular annealed glass is extremely sensitive to the presence of any defect that produces a stress concentration. Its strength is normally controlled by the size of the worst defect, which varies considerably from sample to sample. The implications of this behavior are that glass fractures catastrophically at stresses considerably below its theoretical strength, and the failure stress variability is unacceptably high ($\pm 25\%$).

Sandia studied a two-step ion-exchange process that results in glass with a high compressive stress just below the surface to overcome these problems. Cracks initiate only at very high stresses, and they subsequently arrest. The glass-failure stress distribution is very narrow, and the glass fragments are very small (< 2 mm). The process was initially developed for a specialty-glass composition, but was also successfully implemented for glass compositions that are used for window glazing and automobile applications.

We studied the mechanical properties, multiple cracking behavior, effects of normal surface damage on strength and crack propagation, and the glass strength and fragmentation behavior under a variety of loading conditions.

We used ion-exchange processing to create ESPs in sodium aluminosilicate (SAS) and soda lime silicate (SLS) glass. We used treatments that gave multiple cracking prior to complete failure of the glass and a high Weibull modulus (low strength variability) to fabricate samples to test at various stressing rates. Unlike regular annealed glass, which is stronger at higher

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stressing rates, the SAS glass showed the opposite behavior with the slowest stressing rates giving the strongest samples. The SLS strength was almost insensitive to the stressing rate, but different from single-ion-exchanged behavior. This anomalous behavior for both glasses was tied to the number and depth of the noncatastrophic multiple cracks. The presence of the multiple cracks results in shielding of each of the subsequent cracks that form. As a result, higher and higher values of the applied stress are required to propagate the next crack to form. We found the highest crack densities for the slowest stressing rates. The depth and magnitude of the compressive stresses in the SAS glass were also sufficient to cause the crack to deviate significantly from its original trajectory, resulting in an even higher degree of crack shielding.

We also used ion-exchange processing to create compressive residual stress profiles in the surface of SLS glass. We chose one of these processes, which led to strengthening and multiple cracking behavior, for stress profile analysis and further testing. We used analysis of the residual stress profile by optical stress birefringence to calculate apparent fracture toughness curves. These curves predicted stable crack growth and multiple cracking behavior, with a final fracture stress of ~ 350 MPa, including shielding effects. Fracture strength measurements in 4-point-bend configuration showed progressive multiple-cracking behavior, with a characteristic strength of 275 MPa and a Weibull modulus of 38. The discrepancy between predicted and experimental strength values was linked to the presence of flaws larger than those expected to grow in a stable fashion. Strength measurements after Vickers indentation showed a nonlinear relationship between fracture stress and indentation load, with fracture strength insensitive to indent forces of up to 5 N. For larger indentation forces, fracture strength decreases, though strengths are still higher than for untreated glass.

We conducted blast-loading tests on ESP SAS glass to compare its failure pressure to that for annealed SAS glass. The ESP SAS was significantly stronger and exhibited extensive fragmentation. We conducted blast tests for different stand-off distances and charge sizes to determine the glass-failure pressure-scaling behavior.

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26562

Compact UV Laser Source for Chemical and Biological Sensing

D. A. V. Kliner

Sandia is developing a compact source of tunable ultraviolet (UV) radiation for high-sensitivity detection of trace species, with emphasis on biological warfare (BW) agents. This research exploits recent advances in fiber lasers (originally developed for telecommunications) to make possible instrumentation that is significantly smaller, more efficient (less power-consumptive), and less expensive than is allowed by current technology. Specifically, we are developing a pulsed, near-infrared (NIR) (~ 1020–1120 nm), ytterbium (Yb)-doped fiber laser, which will be frequency-quadrupled to the UV (~ 255–280 nm) spectral region. Based on a pilot study, UV powers of several milliwatts are attainable.

The proposed laser is well suited to detection of BW agents via laser-induced fluorescence (LiF) of tryptophan, for which 266 nm radiation (frequency-quadrupled neodymium:yttrium aluminum garnet [Nd:YAG] laser) is often employed. The proposed system offers several advantages: (1) access to the peak of the ~ 280 nm tryptophan-absorption band, (2) tunability, for avoiding interferences, and (3) external triggering, allowing the repetition rate and timing of the optical pulses to be synchronized to external sources, e.g., for detection of individual bio-aerosols. Furthermore, the fiber laser may be frequency-quintupled to access the 220 nm absorption band of tryptophan (a factor of ~ 8 larger than the 266 nm absorption), as well as absorption bands of the amino acids tyrosine and phenylalanine.

This research will position us to apply this fiber-based sulfur-dioxide (SO₂) technology to BW-agent detection. Moreover, the unique combination of physical and spectral characteristics of the fiber-based laser system will enable development of a new generation of lightweight, rugged, fast-response (real-time) chemical sensors for a wide variety of applications.

We quantitatively analyzed frequency-doubling, -tripling, -quadrupling, and -quintupling schemes for a rare-earth (RE)-doped fiber laser operating at ~ 1080 nm. We selected the optimum conversion scheme and calculated the dependence of the conversion efficiency on crystal length, spot size, peak power, and spatial beam overlap. We performed this analysis using the computer program SNLO. We purchased the

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appropriate nonlinear crystals and other optics to implement the conversion scheme.

We generated the second, third, fourth, and fifth harmonics of a Yb-doped fiber amplifier seeded by a passively Q-switched Nd:YAG microchip laser. We obtained very efficient nonlinear frequency conversion, e.g., 50% efficiency for both the doubling and the quadrupling stages. We compared the results to the SNLO calculations, and we found excellent agreement (typically within 5%) over a wide range of input powers.

The frequency-conversion experiments employed a fiber-amplified microchip laser rather than the Q-switched fiber laser for practical reasons. Most importantly, this source provided a higher peak power by use of a multimode gain fiber and a technique that we developed to enable single-mode operation of a multimode fiber amplifier. In addition, this source provided transform-limited pulses with smooth spectral and temporal profiles appropriate for a variety of chemical and biological sensing applications. These experiments provided the required proof-of-concept data with no reduction in generality because the chosen nonlinear conversion scheme has sufficient spectral coverage to be used with the tunable, Q-switched fiber laser. Moreover, the multimode technique is compatible with the design of the Q-switched fiber laser, and we plan to construct such a system in the future.

In designing the frequency-conversion scheme, we emphasized simplicity, compactness, reliability, and generality. We used critically phase-matched (angle-tuned) crystals operating at room temperature and a single lens to gently focus the output of the fiber amplifier prior to the train of crystals. Nonetheless, starting with only 320 mW of average power at 1064 nm (0.086 mJ per pulse at a 3.7 kHz repetition rate), we generated 160 mW at 532 nm, 38 mW at 355 nm, 69 mW at 266 nm, and 18 mW at 213 nm. One can also achieve high conversion efficiencies by using noncritically phase-matched (temperature-tuned) or quasiphase-matched crystals or by housing the crystals in resonant cavities, but these approaches increase the complexity and limit the tuning range of the system. The ability to use ambient-temperature critically phase-matched crystals, single-pass mixing, and a simple optical setup (one lens) provides a compact, rugged approach to generation of radiation throughout the visible and UV spectral regions. The present results do not represent the maximum visible and UV powers attainable with fiber sources. By operating the laser system at higher repetition rates and pulse energies and by further optimizing the nonlinear conversion scheme, visible and UV powers of > 1 W are possible.

We generated the second, third, fourth, and fifth harmonics of a Yb-doped fiber amplifier seeded by a passively Q-switched Nd:YAG microchip laser. We obtained very efficient nonlinear frequency conversion, e.g., 50% efficiency for both the doubling and the quadrupling stages. We compared the results to the SNLO calculations, and we found excellent agreement (typically within 5%) over a wide range of input powers.

The frequency-conversion studies exceeded the original goals, which specified only frequency-doubling and –quadrupling, with frequency-quintupling being attempted if time permitted. We also demonstrated frequency-tripling, and we evaluated two different frequency-quadrupling crystals.

Refereed

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26563

Advanced Digital Detectors for Neutron Imaging

F. P. Doty, D. H. Morse, D. A. Chinn, C. M. Cuppoletti, A. J. Antolak

Neutron radiography is an important nondestructive evaluation (NDE) method that provides unique information valuable to Sandia's mission in nonproliferation and materials control and many other important applications, including medicine, airport security, protein crystallography, and corrosion detection. Neutrons probe deep inside massive objects to detect small defects and chemical composition, even through high atomic number materials such as lead (Pb). Solid-state neutron-detection technology was made a high priority in a recent Department of Energy roadmap for radiation-detector development.

This project applies Sandia's recent advances in semiconductor radiation-detection materials to develop the first direct digital-imaging detectors for neutron radiography. Current approaches are limited to scintillator-based systems relying on externally coupled photon-detection schemes that seriously limit the performance. Our approach relies on new solid-state sensor materials, which convert neutrons directly to electronic signals via reactions $B_{10}(n,\alpha)Li_7$ and $Li_6(n,\alpha)T$. Charges generated in the conversion process are sensed directly in the conversion material, eliminating the losses associated with scintillators and resulting in potential improvements in both quantum efficiency and spatial resolution. In addition, charge collection in a solid can produce fast (nanoseconds) signal pulses, enabling timing and count rates superior to those of scintillation or gas-detection approaches.

A patent was granted on the use of lithium tetraborate (LBO) for neutron detection. We previously demonstrated bulk crystal counters and are investigating in-house synthesis of LBO films by a spin-on gel-casting. To date, no neutron-sensitive films have been tested. The focus for future work will be to investigate effects of gel stoichiometry and dopants on charge-collection efficiency.

Our focus was to fabricate and demonstrate operation of linear arrays. We used bulk samples of LBO and pyrolytic boron nitride (pBN) from commercial vendors and noted difficulties with pBN, including poor reproducibility and count-rate polarization. Therefore, LBO received more attention in current work.

We fabricated and tested bulk LBO devices using a proton beam to evaluate charge-collection properties. The estimated

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mobility-lifetime products for bulk LBO from this analysis are on the order of $1\text{E-}10\text{ cm}^2/\text{V}$. Based on these results, we quantitatively determined the performance expected from LBO pixels with an existing readout chip, developed by Oak Ridge National Laboratory for a high-energy physics application. The model evaluates leakage current, capacitance, and charge-collection efficiency versus pixel geometry and bias. Signal-to-noise ratios (SNRs) in the range of 2 to 20 are predicted for 256 to 32 μm spatial resolution arrays.

In addition to the bulk commercial crystals, we are pursuing in-house synthesis of LBO films. Preparation of thick films from aqueous gel solution has been reported. The gel-cast films have high resistivity and appear stable under high electric fields. However, none of the films made to date has been sensitive to radiation.

A patent application for borate crystal detectors was granted, and work on purchased bulk crystals will continue.

*A patent application for borate
crystal detectors was
granted, ...*

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Microfabricated Acoustic Spectrum Analyzer*E. J. Heller, L. F. Anderson, T. A. Friedmann, D. R. Adkins, R. J. Shul, D. C. Graf, H. L. Stalford*

This project is developing a microfabricated acoustic spectrum-analysis (MASA) chip for covert and remote acoustic monitoring. Full acoustic spectrum analysis and even voice recognition can be accomplished using a small microphone and extensive post-acquisition data processing. However, this is a slow, power-hungry process that is difficult to miniaturize and implement in limited-access, hostile, or covert-environment situations. This project will develop a similar technology to detect and recognize audible sound using an array of mechanical microresonators on a single chip. The envisioned MASA chip comprises a miniature microphone for pick-up, a frequency-mixing system to shift the signal to higher frequencies, and an integrated array of passive resonant elements used to separate the modified signal into component frequency bands. Each resonant element in the array will be tuned to detect sounds in a particular narrow-frequency band. It should be possible to identify preselected target sounds that have characteristic spectral features in the chosen frequency ranges. Pattern-recognition methods could be used to discriminate between various sounds and to trigger an appropriate reaction, eliminating the extensive computational needs required by complete spectrum analysis. With an adequate number of array elements, speech recognition should even be obtainable. As few as 20 bands are used in some telecommunications technology. The particular challenge in this application is to achieve adequate sensitivity at audio frequencies with resonators small enough to facilitate an array on a single chip. Arrays of this kind may provide the basic building blocks for miniature acoustic sensor systems capable of both covert and remote acoustic monitoring. Sandia is developing several acoustic devices as microsensors for an MASA array. A magnetically actuated flexural plate-wave (mag-FPW) array device is currently being tested under laboratory conditions. We are also fabricating a magnetically actuated micro-teeter-totter, consisting of small rocking paddles. In addition, we are fabricating resonant devices using the SUMMIT-V™ (Sandia Ultraplanar Multilevel MEMS Technology) microelectromechanical systems (MEMS) process. A prototype MASA device is nearing completion.

We demonstrated the ability to design and fabricate an array of mag-FPW microresonators. These resonators consist of a 1

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μm -thick, round silicon nitride (SiN) or diamondlike carbon (C) film supported around the perimeter by a Si substrate “frame.” These die are fabricated by bulk etching through a Si substrate using a highly anisotropic reactive-ion Si etching process. Presently, the arrays of FPWs consist of four elements per substrate, each having a unique resonant frequency. The typical resonant frequencies of the mag-FPW acoustic devices presently being fabricated are approximately 50 KHz. Although the typical frequency separation between array elements is designed to be approximately 200 Hz, several processing difficulties are resulting in poor control of some of the resonances. Specifically, chemical etching processes used to pattern and etch the Si wafer substrate cause some of these devices to be distorted, which results in a higher or lower frequency than designed. Nonuniformities in the stress of the SiN and diamondlike C films used to make these devices can also cause discrepancies in resonant frequency. In the future, the actual resonant frequencies and bandwidths for any given array will be application-specific. We have not yet chosen a specific application for the resonant arrays. The fabrication of arrays of resonant devices to specific frequency requirements will ultimately require a thorough understanding of the design principles for mag-FPWs and well-characterized and -controlled fabrication, as well as post-fabrication testing and tuning methods. We developed a printed circuit board to support testing the FPW arrays. The printed circuit board includes the input microphone and all drive and readout electronics. In the future, we will incorporate the FPW arrays into a hybrid surface-mount electronics version of a 4-channel MASA system.

We are demonstrating the MASA system with the mag-FPW microresonator because the mag-FPW currently shows the most promise for performance and miniaturization. We also fabricated a micro-teeter-totter device that consists of two membranes supported by small legs on two ends. The micro-teeter-totter is a Lorentz-driven device that has two differential paddles and uses impedance detection similar to the mag-FPW, but requires much less of the wafer area than mag-FPWs in a similar frequency range. Initial fabrication attempts produced prototype micro-teeter-totter devices. Several of the micro-teeter-totter devices have already undergone initial testing; we are designing an updated version. We are modifying the drive electronics used for the mag-FPWs to operate the micro-teeter-totter.

We are also fabricating several microresonator structures in the SUMMiT-VTM process and recently completed some of these resonator structures. We intend for these devices to

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develop and improve array sensitivity and reduce the response to external effects, such as temperature fluctuations. We are investigating several readout mechanisms for a variety of beam types that include microxylophone bars (free-standing bar supported at fundamental mode nodes), cantilever beams, and micro-teeter-totters. We are investigating the readout sensing methods for improved readout sensitivity, including comb-capacitance, piezoresistance, and impedance-based sensing (similar to the method used for FPWs). We are also considering a number of actuation methods, including Lorentz-based, electrostatic, piezoelectric, and acoustic actuation. Each of these resonators will have to be accurately designed for a specific application of interest.

Other MASA configurations designed for fabrication include clamped-clamped beams, driven directly by acoustic energy, with piezoresistive readout. These devices are intended to be driven directly by sound-wave energy without a microphone. We designed an array of 27 low-energy microresonators for fabrication in SwiFT™/SUMMiT™ process that is directly driven by acoustic energy.

By the end of this project, we plan to have designed, fabricated, and begun preliminary testing of a MASA system designed for a particular application of interest. Several different types of microresonator structures may be available to accommodate a variety of applications.

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Enabling Analytical and Modeling Tools for Enhanced Disease Surveillance

D. E. Kataoka, A. P. Zelicoff, M. W. Koch, E. L. Hoffman, M. M. Johnson, S. A. McKenna, T. J. Sa, P. C. Gray, R. L. Bilisoly, M. W. Trahan, H. R. Ammerlahn, D. D. Djordjevich, W. B. Wilcox, M. E. Goldsby, T. Nguyen, A. S. Yoshimura, M. F. Hawley

Early detection, identification, and warning are essential to minimize casualties from a biological attack. For covert attacks, sick people are likely to provide the first indication of an attack. An enhanced medical surveillance system that synthesizes distributed health-indicator information and rapidly analyzes the information can dramatically increase the number of lives saved.

Current surveillance methods to detect both biological attacks and natural outbreaks are hindered by factors such as distributed ownership of information, incompatible data-storage and -analysis programs, and patient privacy concerns. Moreover, because data are not widely shared, few data-mining algorithms have been tested on and applied to diverse health-indicator data.

This project addressed both integration of multiple data sources and development and integration of analytical tools for rapid detection of disease outbreaks. Sandia developed and tested two different algorithms for outbreak recognition. The first is a pattern-recognition (PR) technique that searches for space-time data clusters that may signal a disease outbreak. The second is a genetic algorithm to design and train neural networks (GANN) that we applied toward disease forecasting. We tested these algorithms against influenza, respiratory illness, and dengue fever data. Through this project, in combination with other internal funding, we delivered a distributed simulation capability to synthesize disparate information and models for earlier recognition and improved decision making in the event of a biological attack. The architecture incorporates user feedback and control so that a user's decision inputs can impact the scenario outcome as well as integrated security and role-based access control for communicating between distributed data and analytical tools. This work included construction of interfaces to various commercial database products and to one of the data-analysis algorithms developed through this project.

We obtained several health-indicator databases for testing, some through partnerships with health and military agencies.

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We developed two data-mining techniques. First, we examined whether the temporal incidence of disease is amenable to modeling with simple statistical distributions and determined that commonly applied distributions with well-behaved moments, such as the Gaussian distribution, do not accurately describe the incidence of many diseases. We then extended a mechanism for finding clusters in aggregated time-series data to detection in space and time. Unlike previous techniques that look for correlations between cases in space and cases in time, we took a more direct approach: For each date and region, the algorithm searches back in time and over nearby regions for all possible clusters. The user sets the maximum cluster size in time and space, and a binomial sequential probability ratio test (SPRT) determines the cluster's significance. Our approach not only indicates the presence of a cluster, but also its location and size. This technique detected influenza epidemics and respiratory illness with high sensitivity and specificity up to 4 weeks earlier than conventional approaches when applied to the flu and respiratory illness data, respectively.

The second approach is a GANN. The GANN is trained on a subset of data and then predicts the incidence of disease and epidemics. We examined monthly values for temperature, saturation deficit, precipitation, relative humidity, and cases of dengue fever. We had population data and forecasted the disease incidence. We had average sea surface-temperature data and forecasted epidemics. This technique predicted the disease incidence 30, 60, and 90 days in advance and epidemics 30 and 90 days in advance. We also applied GANN to forecast respiratory disease in the San Francisco Bay Area. We examined patient fields, including gender, county of residence, diagnostic code, admission date, and age category. Unlike dengue fever, which is a noncontagious, vector-borne disease, respiratory illnesses have multiple causes and may or may not be contagious. We demonstrated that the prevalence of dengue fever can be estimated by measuring environmental conditions that affect the vector, but estimating the prevalence of respiratory illness was much less straightforward. The GANN was unable to learn any correspondences for respiratory-illness incidence.

We delivered a distributed simulation capability, the Weapons of Mass Destruction Decision Analysis Center (WMDDAC), to synthesize distributed information and models for earlier recognition and improved decision making in bioterrorism events. The architecture includes user feedback and control so that decision inputs can impact the simulated

The user sets the maximum cluster size in time and space, and a binomial sequential probability ratio test (SPRT) determines the cluster's significance. Our approach not only indicates the presence of a cluster, but also its location and size. This technique detected influenza epidemics and respiratory illness with high sensitivity and specificity up to 4 weeks earlier than conventional approaches when applied to the flu and respiratory illness data, ...

scenario as well as integrated security and role-based access control.

WMDDAC simulates an anthrax release in the San Francisco Bay Area. The user plays the role of a public health officer and is able to make decisions during the simulation based on information representative of that which a real public health officer would access during an epidemic. The user can conduct a simple epidemiological investigation by examining various public health reports such as morbidity and death reports, as well as implement a prophylaxis strategy by activating a simulated national pharmaceutical stockpile and prophylaxis distribution centers and by directing people to seek treatment. A common request during early demonstrations was for analytical tools to understand whether the reported health data were normal or indicative of an epidemic. We therefore integrated the space-time clustering algorithm into the simulation. This work included construction of user interfaces and module development to enable the algorithm to communicate in the simulation framework.

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26566

Microtransmitter for Tag, Beacon, and Data-Exfiltration Applications

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This project is classified.

26567

Extensibility of Knowledge-Based Human-Agent Simulation

J. C. Forsythe, M. K. Snell, J. W. Wirsbinski, C. A. Wenner, A. E. Speed

The objective of this project is to develop methods to facilitate the development and application of cognitive models for simulation and intelligent systems applications. In previous work, Sandia developed and demonstrated an initial methodology with a simulation of close-quarters battle. In recent work, we refined and demonstrated the methodology for an application referred to as a cognitive collective. This application uses expert cognitive models as a basis for detecting patterns of behavior consistent with an insider threat.

We developed a computational cognitive model that simulates the processes by which expert decision makers apply their knowledge to recognize situations. The model consists of three primary components: (1) a collection of situations, (2) cues modeled using an associative network with spreading activation between related nodes in the network, and (3) a pattern recognizer that uses an evidence-accumulation approach to recognize situations based on activation of nodes in the associative network.

A significant issue motivating the current project concerns the methods employed to acquire knowledge from subject-matter experts (SMEs) that is essential to populate models. We refined techniques developed previously to create a comprehensive approach for acquiring knowledge. This involved the identification of situations and cues through semistructured interviews. Afterward, we collected related data to allow determination of the quantitative relationships between cue-cue pairs and situations and cues. With this knowledge, a computational model may be constructed for a specific SME.

Activities focused on the detection of an insider threat. We developed cognitive models for four SMEs (counterintelligence officer, investigative agent, security officer, and forensic psychologist). We combined these models to create what we referred to as a *cognitive collective*. Here, when presented with data concerning a potential threat, any individual model may recognize a suspicious pattern. However, models are able to interact and, in some cases, recognize patterns when no single model was able to do so. This latter feature represents the “collective.”

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We conducted a validation study wherein the actual experts were presented hypothetical cases individually and asked to indicate if they believed there was reason for suspicion. The response of models to the test cases was consistent with the corresponding expert for 93% of the cases (N=120).

Afterward, we allowed experts to discuss the cases as a group and then collectively decide if there was reason for suspicion. In this condition, the model responded in a manner consistent with the collective decision of the experts in 86% of the cases (N=30).

These findings are interpreted as a proof-of-principle that the basic approach to cognitive modeling, including knowledge elicitation methods, is reasonably sound.

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26568

Secure Authenticated Sensor Packs*T. J. Draelos, R. D. Miller, R. C. Schroepel, C. L. Beaver, R. A. Gonzales*

Sandia presents a VHSIC (very high speed integrated circuit) Hardware Description Language (VHDL) design that incorporates optimizations intended to provide digital-signature generation with as little power, space, and time as possible. These three primary objectives of power, size, and speed must be balanced along with other important goals, including flexibility of the hardware and ease of use. The highest-level function offered by our hardware design is Elliptic Curve Optimal El Gamal digital-signature generation. Our parameters are defined over the finite field Galois ($GF[2]$), which gives security that is roughly equivalent to that provided by 1500-bit RSA (Rivest, Shamir & Adelman) signatures.

Our optimizations include using the point-halving algorithm for elliptic curves (ECs), field towers to speed up the finite-field arithmetic in general, and further enhancements of basic finite-field arithmetic operations. The result is a synthesized VHDL digital-signature design (using a complementary metallic-oxide semiconductor [CMOS] $0.5\ \mu\text{m}$, 5 V, 25°C library) of 191,000 gates that generates a signature in 4.4 ms at 20 MHz.

One goal was to produce hardware for our low-power digital-signature design. Because of the expense in time and money of producing hardware, we chose instead to spend our time enhancing our VHDL design, the ultimate product of our work. We selected an El Gamal digital-signature variant that minimizes the number of operations necessary for signature generation. We developed and implemented several algorithmic optimizations of the computational elements necessary to compute a digital signature. Many of these elements can be applied to other EC algorithms over $GF(2^m)$.

We use the field $GF(2^{178})$ because optimizations can be derived from the fact that it can be realized as a field tower: $GF(2^{178}) = GF((2^{89})^2)$. In the case of characteristic two fields, the equation for the EC can be given by $E: y^2 + xy = x^3 + ax^2 + b$. For simplicity and saving on storage, we assume that $a = (1, 0)$. Further, we exploit properties of $GF(2^{89})$ to reduce some of the basic arithmetic operations (e.g., squaring, square root) to simple XOR (exclusive or logical operation) gates that are very fast in hardware. The “almost-inverse” algorithm is especially

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fast for smaller degree fields. Finally, we modify our EC multiplication algorithm to use point-halving, which offers a savings over the usual point-doubling.

We used several design optimizations to improve the area and performance of the hardware design. For multiplication in a finite field, which operates with a simple shift and add, we increased the radix of the multiply to 16. This allowed us to perform the multiply in 4-bit fragments, which provided a dramatic speed increase with a slight area penalty.

We implemented three optimizations in the almost-inverse algorithm. The first was a parallel degree-comparator circuit, which we optimized for both area and speed. The second optimized the search for a 1 in the least significant bit (LSB) of a variable by using a “look-ahead” technique with 4-bit blocks before defaulting to operating on the data 1 bit at a time. This increased speed with a very small area penalty. In a similar manner, we applied the third optimization to the last step in the algorithm, which divided and shifted the result a variable number of times. This, too, performed a “look-ahead” using 8-bit data blocks before defaulting to the single-bit implementation.

We parallelized the Qsolve algorithm and reduced the depth of the XOR tree to increase the speed. We optimized the implementation of the secure hash algorithm (SHA-1) to use a shift register for the main data storage, which reduced the area used with a corresponding increase in speed.

The deliverable for this project is a VHDL hardware design of the Optimal El Gamal digital-signature algorithm and EC arithmetic operations. We synthesized the design to a target CMOS 0.5 μm , 5 V library. It also underwent static timing analysis, timing simulations, and power analysis. The following is a summary of results for this target library using a 20 MHz system clock:

- *Initialization*: 0.25 ms (necessary any time the generating point is initialized and/or changed)
- *Signature generation*: 4.4 ms
- *Dynamic power-consumption estimation*: 150 mW (19 mW using a 1.8 V power supply)
- *Static (idle) power-consumption estimation*: 6 μW .

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26569

Remote Monitoring of Difficult, Real-Time Targets Using Video SAR Technique

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Monitoring and interpreting real-time activities at sites where access is difficult, remote, or denied is a primary issue for addressing both emerging threats and nonproliferation situations. Synthetic-aperture radar (SAR) has proven to be an effective means of remotely monitoring such sites due to its day/night, adverse-weather capabilities. Traditional SARs do not form images at a rate greater than that required to fly the length of the synthetic aperture. This rate is a function of range and radar wavelength and is often many tens of seconds at long ranges, causing SARs to miss changes that are occurring. Thus, SAR does not provide the situational awareness needed against scenes with dynamic content, such as moving targets, usually missing them completely. This limits the usefulness of SAR on a battlefield. An ideal sensor would not only be day/night, all-weather, as is SAR, but would also provide the continuous situational awareness needed against stationary as well as moving targets.

This project investigates a new technique invented at Sandia called VideoSAR, which will enable the forming of high-resolution SAR images at video rates many times a second (about 100 times higher rate than traditional SAR). This technique exploits the human eye's sensitivity to motion and provides users with improved awareness and measurement and signatures intelligence (MASINT) signatures of scene dynamics. This project includes investigations that optimize and benchmark the image-processing algorithms on three different hardware platforms: Mercury brand digital-signal processors (DSPs), LINUX personal computers (PCs), and custom hardware using reconfigurable logic. We also investigated the operations space to determine the conditions under which VideoSAR will produce visible target shadows.

We completed a study of the overlapped subaperture (OSA) SAR processing algorithm investigating the possibility of optimizing the algorithm for the highly overlapped VideoSAR data. The results of this study indicate that speed improvements are possible through reusing the partial results at each stage of the OSA processing, but that the tradeoff in image quality

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mandates that a real system reuse no more than the coarse azimuth processed data.

We completed a preliminary benchmark study that indicated the hardware necessary to process VideoSAR data in real time. This study compared an implementation like the real-time processors of Sandia's current SARs on Mercury brand DSP boards, an implementation running on rack-mounted LINUX PCs, and an implementation in reconfigurable logic. The results of this comparison indicate that the reconfigurable logic option is best in terms of total hardware cost and size, but would require a much greater development effort. The PC option appears significantly better than the Mercury option in cost, but significantly worse in size.

We performed several flight tests and preliminary analysis to characterize the shadow-finding performance of a VideoSAR system. From these data, we estimate that with sufficient signal-to-noise ratio (SNR) and with all radar and geometry parameter optimized, we should be able to see a vehicle the size of a pickup truck up to 15 nautical miles away or farther, moving on an asphalt road with speed from 0 to 40 mph. Vehicles on brighter clutter backgrounds or larger vehicles can be seen to farther ranges.

We investigated the use of automatic target tracking algorithms for shadow tracking in VideoSAR images. We showed the ability to automatically detect and track individual vehicles as they moved through a VideoSAR sequence.

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26572

Coating Chemical Preconcentrators to Improve Chemical-Agent Collection

C. L. Rhykerd, Jr., R. J. Kottenstette, M. A. Mitchell

Many Sandia customers, including the Department of Energy (DOE), Department of Defense (DoD), and the National Emergency Search Teams (NEST), as well as law enforcers and first responders, have an interest in trace-chemical-agent detection in the parts-per-billion (ppb), parts-per-trillion (ppt), and parts-per-quadrillion (ppq) ranges. Field-ready prototypes in this sensitivity range require that a sampler and preconcentrator be integrated into a detection system (probably using microsensors). The preconcentrator manages the mismatch between the sampler flow (L/s) and the low detector flow (mL/s). Sandia has developed, patented, and licensed a stainless-steel screen preconcentrator for explosives; this preconcentrator improves system sensitivity by 10,000 times. However, preliminary data with a chemical weapons simulant show that this metal surface is inappropriate for chemical agents because of low efficiency of adsorption and decomposition during thermal desorption.

We propose developing a preconcentrator subsystem to enhance chemical-agent detection and to do so within acceptable constraints. Coating the screen—to improve collection and reduce decomposition—is a logical engineering solution to this problem. Potential coating candidates include sol-gels (including silsesquioxanes), polymers (Navy Research Laboratory [NRL]), and carbon nanotubes (CNTs). Successful coatings must be robust during temperature cycling to 200°C to 300°C and must adhere well to the substrate. A detection system is available for these evaluations, and we will continue our effort to leverage newly developed materials. We evaluated uncoated screens and sol-gel- and nanocarbon (NC)-coated screens.

Capitalizing on Sandia's strengths in sample collection, preconcentration, and materials, our success will lead to improved chemical-detection systems with enhanced capabilities (including sensitivity, portability, cost, and speed). This impacts applications in chemical-agent detection, explosives detection, drug detection, and environmental monitoring.

We obtained Carboxin-coated screens from Lawrence Livermore National Laboratory (LLNL). Carboxin is a highly retentive material available through Suppelco. LLNL experienced difficulty coating the small 0.5 in. screens and consequently obtained larger, 2.5 in. screens instead. We

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prepared cetyl tetra ammonium bromide (CTAB) sol-gel- and Cyclo Dextrin-coated screens and obtained NC coatings.

During the review of methods and results in our previous work, we made the decision to place more emphasis on temperature control and reliable desorption. We used 0.5 in. screen preconcentrator in combination with a PCP, Inc., ion-mobility spectrometer (IMS) for these tests. We controlled screen temperature by screen heat time (typically, 1.4 s at 1.5 V yields about 200°C), but it depends on the conductivity and heat capacity of the screen. Thermocouples spot-welded to the screen monitor the temperature. The earlier dimethylmethylphosphonate (DMMP) detection limit for a sol-gel-coated screen was above 1 µg, an unexpectedly high mass. Speculation about the cause included improper screen heating and evaporation of the analyte. As a result of this review, we carried out desorption experiments with liquid transfer of the analyte in ethanol onto the coatings using both DMMP and nitroglycerin (NG). We expected NG to be much less volatile because it has a much lower vapor pressure than DMMP. The NG was detected reliably on a nanoporous C coating, with detection limits below 5 ng. The focus of our work turned to the screen heating for desorption.

We completed collection of data for the uncoated screens (stainless-steel Bekipor ST60AL3, 60 µm pores), the new CTAB sol-gel coating (DMMP analyte), and the NC (NG analyte). The investment of time with NG detection (< 5 ng limit of detection) was rewarded with reliable DMMP detection from the CTAB screens with limits of detection well below 20 ng. The advantage of working with NG was its lower volatility. This improved sensitivity represents more than 50 times improvement in detection compared to earlier results, primarily due to the improved temperature control during desorption. Adsorption efficiency remains poorly characterized, but a desorption temperature of 200°C seems to drive all the DMMP off in three to five heat cycles, with predictable exponential decay of the mass desorbed. Uncoated screens show negligible retention after one heat cycle, compared to 3–5 cycles for the CTAB sol-gel-coated screens. This result shows that the coatings are enhancing analyte retention as desired. Flashing the screen to 300°C cleans it off completely.

Electron micrographs of the CTAB sol-gel and Cyclo Dextrin coatings show islands of coating for drop coatings, but uniform results for spray-coated screens.

Based on internal review of the progress to date, we will emphasize adsorption experiments in upcoming work now that desorption properties for these coatings look promising.

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26574

Detection and Exploitation of Spread-Spectrum Waveforms

J. T. Cordaro, R. C. Ormesher, J. J. Mason, T. D. Atwood, D. D. Cox

Sandia seeks to develop and demonstrate critical portions of a system concept for collection, detection, and exploitation of spread-spectrum signals for tactical military missions. The developed concept includes all required aspects of an operational system, including the sensor platform and its auxiliary systems (power, control, and navigation), sensor electronics (antennas, receivers, digitizers, processors, and transmitters), required communications systems, and signal-detection and -exploitation algorithms.

In early work, we focused on developing algorithms to detect and exploit spread-spectrum signals originating at an adversary's transmitter. We have broadened the scope of our work to include a total system concept to provide more value to our country's national security.

In collaboration with the Physical Sciences Laboratory (PSL) at New Mexico State University (NMSU), we are developing a tactical signals intelligence (SIGINT) concept that employs high-altitude, free-flying balloons as the sensor platform, and tethered balloons, anchored in protected territory, as relays to a tactical ground station. We are continuing the algorithm work but are shifting the focus from discovery of previously uncharacterized spread-spectrum signals to detection and recognition of previously catalogued waveforms.

Technology challenges include design of lightweight sensors and signal processors, development of efficient SIGINT algorithms, and development of novel station-keeping methods for balloon or balloon-like platforms.

With PSL, we developed a preliminary concept for a balloon-mounted tactical SIGINT system.

We reviewed open-source intelligence to identify the most capable commercial spread-spectrum communications systems currently available. PSL is in the process of creating time-series waveform snapshots for these systems for use in an upcoming demonstration.

We identified the existing standard software toolsets currently being used by SIGINT analysts, and PSL provided us with a suitably configured workstation and training in the software toolsets. With PSL, we identified a champion for our concept within the SIGINT community.

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26575

Small-Power Direct-Conversion Microfluid Systems Using Logistical Fuels

K. Wally, S. F. Rice, B. C. Wu, M. F. Wright, T. N. Raber

Sandia's objective in this project was to investigate the conversion of liquid hydrocarbon (HC) fuel into hydrogen (H) in a process suitable for implementation in microfluidic systems to feed polymer electrolyte membrane (PEM) fuel cells or other small direct-conversion power converters (e.g., thermoelectric converters). Toward that end, the project pursued development along three paths: (1) experimental study of fuel reforming in a compact supercritical water reformer (SCWR), (2) development of a system design suitable for implementation in small, miniature, meso- and microscale fluidic systems, and (3) development of working prototypes of key components needed for implementation of such systems.

We conducted experiments to investigate reforming of organic compounds in supercritical water. We fed an aqueous organic solution to a high-pressure, positive-displacement pump. The reactor was coiled Inconel 625 tubing. An 800 W tube furnace heated the reactor to temperatures of 500°–700°C. System pressure was controlled by a back-pressure regulator operating at 27.6 MPa (4000 psig). We analyzed gas composition via gas chromatography (GC). Based on measured gas composition, we used global stoichiometry to determine the amount of water consumed relative to methanol.

We prepared aqueous solutions of methanol at differing concentrations (15%–45%) by weight to determine the effect of methanol concentration on both conversion and composition of product gas with the reactor at 700°C. In a second set of experiments, we fed 15% methanol solution to the reactor at different furnace temperatures (550°–700°C) to determine the effect of temperature on conversion and product gas composition. Additionally, we conducted several experiments with ethanol, ethylene glycol, acetone, and diesel fuel to investigate SCWR reforming of different fuels.

- *Methanol experiments.* In conversion of methanol at 700°C, the methanol is completely reacted (> 99%) for feeds of 15% and 25%, and at 35% for slower flowrate. The conversion is slightly less (98%–99%) for 35% methanol, and incomplete for 45% methanol feed. CO and CH₄ increase with feed concentration of methanol, whereas H₂ and CO₂ decrease. It is also valuable to compare the effect of residence time. For 15% methanol feed, the composition of the product gas is essentially

Miniature supercritical water reformer with integral counterflow heat exchanger. In this demonstration prototype, an electric heater rod is used to provide start-up heat and endothermic process heat.

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unchanged with residence time. For all other feed compositions, H_2 , CO_2 , and CH_4 increase with longer residence time, while CO decreases.

Complete conversion is observed with the reactor at $700^\circ C$ and nominal residence time of 3 s. Conversion of methanol drops steadily with decreasing temperature, reaching only 27% at $550^\circ C$. In this case, H_2 , CO_2 , and CH_4 increase while CO decreases with increasing temperature.

- *Other fuels.* At $700^\circ C$, both ethanol and ethylene glycol were completely converted ($> 99.5\%$). Ethanol reforming yields greater than 25% CH_4 . The product gas from ethylene glycol reforming had higher concentrations of CO (11%) and CH_4 (6%) relative to similar experiments with methanol. Changing the flowrate (residence time) did not significantly change product gas composition for either ethanol or ethylene glycol.

Acetone and diesel fuel both resulted in plugging of the SCWR. The fact that the reactor became plugged when feeding acetone is especially puzzling, and we have no explanation at this time.

Relevant reaction pathways include direct methanol decomposition, methanol hydrolysis, water-gas shift, and CO methanation.

The result of higher methanol concentration in the feed on the reformat gas composition is that more CO and less CO_2 are produced. The experimental results show that CO is produced at shorter residence times and is subsequently converted to CO_2 (and H_2) at longer residence times.

The conversion of methanol in supercritical water decreases significantly at lower temperatures. CH_4 is produced only at or above $650^\circ C$, consistent with this step being kinetically limited. At lower temperatures, CO is produced at concentrations higher than CO_2 .

- *Prototype systems.* We built the miniature SCWR to investigate SCWR operation with a thermodynamic cycle suitable for scaledown from miniature through microminiature.

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26576

High-Bandwidth Optical-Data Interconnects for Satellite Applications

D. K. Serkland, K. M. Geib, J. L. Rienstra, K. R. Lanes, G. M. Peake, E. L. Blansett

The aim of this project is to address the future needs of focal-plane-array (FPA) sensors by exploring the use of high-bandwidth fiber-optic interconnects to transmit FPA signals within a satellite. Sandia focused primarily on vertical-cavity surface-emitting laser (VCSEL)–based transmitters because of the previously demonstrated immunity of VCSELs to total radiation doses up to 1 Mrad. In addition, VCSELs offer high modulation bandwidth (roughly 10 GHz), low power consumption (roughly 5 mW), and high coupling efficiency (greater than –3 dB) to optical fibers.

We investigated low-power-dissipation cryogenic VCSELs designed to be driven directly by the output stages of low-power complementary metallic-oxide semiconductor (CMOS) analog-to-digital (A/D) converters situated next to a cooled FPA. We designed the VCSELs for operation below 200 K. At 200 K we measured a threshold current of 0.67 mA and a threshold voltage of 2.16 V, which translates into a threshold power dissipation of 1.45 mW. We expect that with further optimization, the threshold power dissipation of a cryogenic VCSEL could be reduced below 1 mW. We also observed that differential quantum efficiency increased as the temperature was lowered and eventually saturated near 100%. Importantly, the voltage drop across the VCSEL did not start to rise dramatically until the temperature was lowered below 100 K, which implies that conventional doping concentrations can be used for VCSELs operating down to about 100 K.

We decided early on to partner with Peregrine Semiconductor, Inc., to benefit from their expertise in radiation-hard silicon-on-sapphire electronic circuitry and their expertise in VCSEL transceiver manufacturing. Their existing VCSEL transceivers are being modified to meet the needs of data transmission from FPAs on satellites. Since Peregrine does not make the optoelectronic devices used in their transceivers, our group at Sandia provides a complementary strength in customized design and fabrication of VCSELs and photodiodes.

We focused on optimizing our VCSEL fabrication process to achieve high-speed linear arrays of VCSELs that are compatible with wire-bonding and flip-chip-bonding technologies. We developed a new “linear array” mask set and

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optimized our fabrication process to produce arrays of bondable VCSELs with high yield. Our method to produce VCSELs with bondpads relies on an etched two-tier mesa structure that rises up from a semi-insulating gallium arsenide (GaAs) substrate. A metal bridge is formed to connect the anode *p*-type contact on the top mesa to a bondpad on the semi-insulating substrate. Simultaneously, we form a similar metal bridge to connect the cathode *n*-type contact on the top of the lower mesa to another bondpad on the semi-insulating substrate. This arrangement yields electrically isolated anode and cathode bondpads with a capacitance between them of less than 1 pF. We measured the 3 dB bandwidth of these VCSELs to be roughly 10 GHz, which is suitable for non-return-to-zero digital modulation at rates up to about 10 Gb/s. One of the key microfabrication challenges that we faced was that the selective oxidation process used to create the current-confining oxide apertures also oxidized high-aluminum-composition aluminum gallium arsenide (AlGaAs) layers of the distributed Bragg reflector (DBR) that were exposed after etching the top mesa. These unintended oxide layers proved to be impervious to our reactive-ion etch process used to define the lower mesas, which reduced our yield to roughly 50%. We remedied this problem by etching both mesas before doing the selective oxidation process step. Additionally, we found that a 5 s wet etch in 1% hydrogen fluoride (HF) following the top mesa etch-step selectively removed the high-aluminum-composition layers that were most susceptible to unwanted oxide formation.

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26577

Robust Chemometrics for Remote Spectral Sensing

M. M. Moya, E. V. Thomas, C. M. Boney, M. R. Keenan, D. M. Haaland, M. H. Van Benthem, M. W. Smith

Sandia chemometrics researchers have developed new techniques that promise to improve the robustness, performance, and utility of satellite-based hyperspectral imaging (HSI) for applications in nuclear nonproliferation, chemical and biological weapons (CW/BW) detection, and national intelligence. These applications require reliable identification, characterization, and quantification of target chemicals and materials. The performance of current spectral analysis algorithms suffers in the presence of background and sensor noise, residual pixel calibration errors, sensor artifacts and drift, and atmospheric correction errors. Spectral shape changes are complex, nonlinear, and time-varying. Sandia has 20 years of experience in developing multivariate algorithms for quantitative and qualitative spectral analyses in the presence of similar errors in the laboratory. The techniques augment the target model with spectra that correspond to these spectral shape deviations. Chemistry laboratory experiments demonstrated the ability to perform quantitative spectroscopy without the need for calibration standards and the ability to extract pure-component spectra of spectrally active chemical species in heterogeneously mixed samples. Now, we are adapting robust multivariate calibration to identify and quantify materials in remote spectral sensing subject to instrumental, environmental, and atmospheric variations. We will evaluate the utility of new augmented multivariate-curve resolution (MCR) for extracting pure components from mixed spectra. We will test prediction-augmented classical least-squares (PACLS) and PACLS with a partial least-squares (PLS) post processor for online calibration augmentation and model updating. We expect that incorporating these robust calibration techniques will significantly improve the performance of the identification and quantification algorithms. Developing the ability to identify spectra in the presence of atmospheric, environmental, and instrumental variations will enable us to use remote spectral imaging to recognize facilities, identify chemicals and biological agents, and detect man-made anomalies.

- Robust method accomplishments.

— Investigated alternative sensors for remote hyperspectral data collections, including Kestrel Corporation spectral imagers.

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- Redesigned experiments because of information-efficient spectral-imaging system (ISIS)—limited spectral range to focus on discrimination between vegetation and infrared (IR) camouflage.

- Constructed new camouflage fabric board.
 - Tested instrumental and environmental variability factors, including focal-plane cooling, heating of spatial light modulators (SLMs), lighting modifications, neutral-density color filters, polarization filters, SLM offset voltages.

- Selected significant variability factors to include various neutral-density filters and distance and direction of illumination.

- Acquired library spectra of vegetation and camouflage.

- Investigated source of intermittent ISIS artifacts and devised median filter solution to remove the artifacts.

- Collected training and test data from camouflage and vegetation samples, both with minimal variability and with controlled illumination variability.

- Applied dry lab mixing to emulate subpixel mixing of vegetation and camouflage spectra.

- Applied principal component regression (PCR) and PLS methods to estimate the quantity of the component spectra.

- Conducted a study to confirm correlation between radiometric intensity level and the vegetation spectral shape.

- Compared quantification results of regression training with and without environmental variabilities.

- Collected ISIS image data from 700 nm to 1000 nm of common plant and IR reflective camouflage sample using a sequence of neutral-density filters and composed training sets with and without variations in illuminations and a test set with illumination variations.

- Simulated subpixel mixing of camouflage and vegetation spectra for a random selection of mixing ratios.

- Applied PCR to predict the mixture quantities of the two components within the test set and demonstrated the improved quantification performance of training the regression with variabilities; training with variabilities reduced the standard deviation of the error by a factor of 3.7.

- *Pure component extraction accomplishments.*

- Using equality constraints ensures the conservation of known intensities, spectral signatures, or abundances; only mathematically rigorous equality-constraint methods produce the true least-squares solution.

- Implemented rigorous equality constraints in MCR algorithm and demonstrated that rigorous methods are more accurate than approximate methods.

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- Demonstrated better accuracy and improved execution speed of applying inequality constraints directly rather than converting inequality constraints to equality constraints with the addition of a “slack” variable, which increases the problem dimensionality.

- Non-negative least-squares (NNLS) and inequality constraints.

- Developed improved implementation of NNLS and other inequality-constrained algorithms: recognized limited number of unique combinations of passive set variables and applied single-factorization computation for each combination rather than performing factorization and solution steps column-by-column to increase computational efficiency; developed and implemented orthogonal factorization methods, which have the potential to significantly reduce the number of NNLS floating-point operations as compared to the normal equation solution.

- Developed a general method for combining linear equality and inequality constraints derived from Lawson’s and Hanson’s algorithms for the single right-hand-side case. We transform the constrained least-squares problem through a series of steps to a least-distance programming problem, which the NNLS algorithm can solve.

- Uncertainty estimation of MCR–derived pure components.

- Applied linear unmixing to an HSI containing two highly overlapping pure components; showed that repeated MCR analysis using different random starting points establishes uncertainty bounds for pure component spectral shapes; provides improved reliability assessment for identification and quantification using MCR–derived components.

- Weighting for soft constraints.

- Showed that use of weighted least-squares to impose soft constraints during data analysis can assist the MCR process in finding a lower error solution and reduce the number of iterations required to converge, which portends predictable MCR performance improvements.

We developed a comprehensive White Paper that describes Sandia’s capabilities and recent developments and associated operating assumptions that address the challenges of extracting meaningful information from hyperspectral sensor data and that pave the way for a demonstration of functional hyperspectral data exploitation.

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26578

Deployable Large-Aperture Optics System for Remote-Sensing Applications

J. W. Martin, J. C. Wehlburg, J. M. Redmond, B. T. Macke, H. Sumali, M. P. Teague

Large-aperture optics are critical for improving sensitivity and ground resolution of future space-based telescope systems, such as those needed to monitor global proliferation of weapons of mass destruction (WMD). While many researchers are considering on-orbit assembly of conventional rigid optical mirrors to circumvent geometric limitations imposed by launch vehicles, their approach does nothing to alleviate the tremendous cost penalty associated with the added weight of the overall system. In stark contrast to such incremental technologies, Sandia has been developing a revolutionary new enabling technology for large-aperture optics. The key element of this research is an electron-gun-controlled piezoelectric thin-film mirror that can be compactly stowed for launch, deployed on orbit, and shaped to optical tolerances.

An integrated program of computational modeling and experimentation yielded a solid foundation for the demonstration of closed-loop thin-film shape control. The enormous potential of this technology has captured the interest of the remote-sensing community, and further research is needed to develop a fully deployable optical system based on this concept. Under this research, we are collaborating with the University of Kentucky to develop the technology needed for a deployable electron-gun-controlled imaging system.

Thin-film mirror technology has proven to be a challenging task. The greatest difficulty to date with closed-loop electron-gun control of thin-film mirrors is receiving feedback from the system. Drawing from various research efforts, we made steady progress with our research. We were awarded a patent for our unique electron-gun control strategies that hurdle several obstacles. Efforts are still ongoing in the areas of full-figure closed-loop surface-control experiments and modeling.

To date polyvinylidene fluoride (PVDF) is the only currently available material for electron-gun control of thin-film mirrors. We completed research on the material and control validations of PVDF. We analyzed samples that represented one pixel in an overall control scenario. This breaks the problem down into its basic unit of control. This is based on the idea that every thin-film mirror in an optics system can be mapped to individual pixels on a corresponding charge-coupled device

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(CCD) imaging camera. This means that to reduce aberrations in the system, the mirror-control capabilities need to be, at a minimum, subpixel.

Research shows that each pixel behaves as a linear control system. As the control input amplitude increases, the output deflection increases, and conversely, as the control input frequency increases, the output deflection decreases. Further, we characterized the control-system lag response. As control frequency increases, the response lag increases exponentially. For the case of a thin-film mirror system where we control approximately 2000x2000 pixels, the control system would have to refresh the whole system on the order of 0.02 Hz to maintain steady state.

We examined several optical metrology systems. The most reliable/applicable system proved to be a Shack-Hartmann sensor. In this system, light bounces off the surface being analyzed and passes through a system of micro-lenslet arrays. The light then focuses on the focal plane. As the curvature changes on the mirror surface, the individual points of focused light move along the focal plane. These changes provide a direct measure of the change in curvature on the mirror system. The range of the system is from 50 mm to 10 nm with an accuracy of 10 nm. We created a test platform incorporating this system and are currently incorporating it into our research needs for real-time closed-loop control.

We developed a deployable mirror-demonstration system test-bed. We established this system to provide a real-time closed-loop thin-film mirror-demonstration system. Being able to create optical-quality tolerance thin-film mirrors and then having the ability to adjust the optical prescription are just what we need to create further interest in this research from outside sources.

We further analyzed the light-detection and ranging (LIDAR) design chosen previously. Like all earth-viewing and space-viewing space-based optical sensor systems, LIDAR would benefit from a larger optical-collecting aperture. The LIDAR system requires surface accuracy on the collecting mirror of a few microns and therefore provides a challenging goal for the deployment and shape-correction technologies. Here we designed a 5 m Cassegrain optical telescope with a 5% central obscuration to act as the front-end collection optics for the ultraviolet laser-induced fluorescence (LiF) LIDAR system. A space-based LIDAR system could detect both bioaerosols and biosolids from a low-earth orbit with laser energies as small as 30–40 mJ at 355 nm wavelength with at least a signal-to-

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noise ratio of 4. This system would be very achievable with today's technology.

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26579

MicroChemLab Technologies for Early Detection of Pathogen Exposure

V. A. Vandernoot, J. S. Schoeniger, R. Behrens, Jr., J. V. Volponi, S. A. Pizarro

Sandia seeks to develop a more rapid means of determining exposure to a pathogen. The central questions of this project are whether there are early biological hallmarks that coincide with the ramping up of the immune system and whether we are able to measure these hallmarks of immune activation in a field setting. The earliest indicators of immune-system activation include changes in the phosphorylation or levels of key signaling proteins. We proposed selectively collecting the phosphorylated proteins from cultured immune cells by affinity chromatographic techniques and to subject them to a variety of sensitive separation techniques that are amenable to miniaturization into field devices. We need to determine whether there are separation patterns or “fingerprints” of phosphorylated proteins that are indicative of the resting state of the cells and whether there are demonstrable changes in the fingerprints when the cells have been activated. This work will provide an essential basis that could lead to the creation of a field device to track pathogen exposure to be used by first responders and emergency medical personnel.

- *Activation protocols for T-cells.* T-cell receptor antibody (anti-CD3) was found effective for Jurkat cells when either immobilized to a solid surface or cross-linked to another protein (avidin using biotinylated antibody). We found *Staphylococcal enterotoxin B* (SEB) to be ineffective; we later determined that this particular cell line produces a variant of receptor that was reactive to other staphylococcal enterotoxins. We generated dose response curves for both phytohemagglutinin-(PHA) and anti-CD3 by monitoring cytokine production overnight.

- *Phosphoprotein enrichment.* Additional antibodies to phosphoserine and phosphothreonine recently became commercially available. This allowed for the collection of larger numbers of phosphoproteins and increased the complexity of the fingerprints.

- *Separations development.* Capillary zone electrophoresis did not demonstrate sufficient resolution due to compression of the isoelectric point (pI) range of the proteins; this results from the phosphorylation (acidic phosphate groups at one or more sites) as well as the labeling process (fluorescent

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tag reacts with basic residues and inserts an acidic dye molecule).

Although isoelectric focusing (IEF) separates proteins based on pI and is subject to the same pI compression mentioned above, it is an extremely high resolution technique and is amenable to very narrow pH ranges. We developed laser-induced fluorescence (LiF) detection (for high sensitivity) coupled to IEF. The first step was the development of peptides that would serve as fluorescent pI markers. We optimized conditions for LiF-IEF with respect to ampholyte used, pH dependence of dye, and focusing/mobilization conditions. The technique has proved useful for test proteins, although it is not fully optimized for cell lysates.

Capillary gel electrophoresis (CGE) proved very successful for the determination of phosphoprotein signatures, and we gathered the bulk of the data comparing signatures using this technique.

- *Capillary gel electrophoresis and phosphoprotein fingerprinting.*

- *Phosphoprotein signatures versus stimuli.* Distinct differences are seen in the electropherograms of resting cell and overnight-PHA-activated cell lysates. We also observed differences in resting and stimulated T-cells with anti-CD3, which stimulates T-cells via a different mechanism. Moreover, the data show patterns that appear to be different from those obtained with PHA stimulation. This is very important to a key premise of this project; it suggests the possibility of pathogen specificity inherent in the phosphoprotein patterns.

- *Time courses.* Phosphorylated protein signature differences begin very rapidly in cultured T-cells. To study this, we collected the phosphoprotein patterns after very brief exposures to optimized concentrations of PHA or anti-CD3 (0 to 40 minutes). There are clear differences that appear in the stimulated traces in as little as 10 minutes. This is extremely important to the ultimate “rapid diagnosis” application of this work.

- *Reproducibility.* We addressed reproducibility of the CGE traces to get an estimate of the degree of variability that is expected from such experimental parameters as sample handling and fluorescent labeling. We prepared replicate samples that show very good similarities.

- *Pathogen signatures from tissue samples.* The final stage of this work is the collection and analysis of phosphoproteins from more complex systems. We benefited from a collaboration with the University of New Mexico, which developed mouse infection models for a number of pathogens.

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We established a procedure to take spleens, a rich source of T-cells, from resting and challenged mice, harvest the cells, which are actually a mixture of T-cells and B-cells, homogenize them, and then lyse the cells to release the phosphoproteins. This type of approach is very exciting, as it represents a big step in addressing the complexity associated with the phosphoproteins of a whole animal and how they will respond to a pathogen.

The stimulation/pathogen being evaluated for this phase of work is SEB. Based on previous research by our collaborators, this stimulus is expected to produce large changes in phosphoproteins. Experiments are under way and are scheduled to be completed soon.

This type of approach is very exciting, as it represents a big step in addressing the complexity associated with the phosphoproteins of a whole animal and how they will respond to a pathogen.

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26580

Intelligent Tracking of the Telepresent Rapid-Aiming Platform

C. L. Nelson, J. J. Carlson, M. A. Martinez

The Telepresent Rapid-Aiming Platform (TRAP) is a remotely operated weapon system. TRAP offers significant force multiplication and enhancement by enabling near-instantaneous response to attackers, increasing targeting accuracy, removing personnel from direct weapon fire, providing immunity to suppressive fire, and reducing security-force size needed to effectively respond. Test results have been exceptional, and response from the Department of Energy (DOE) sites and the U.S. Air Force is enthusiastic. Testing shows that the TRAP performs comparably to a trained marksman except for target-acquisition speeds, which are up to three times longer. Currently, the platform is enslaved to a remote operator's joystick. Tracking moving targets with a joystick is difficult, depending on target range, movement patterns, and operator skill. Even well-trained operators encounter difficulty tracking moving targets. A remote-response platform modified from the TRAP system is installed at Sandia. This installation supports an operational test and evaluation with inert ammunition. With the enhancement of intelligent tracking, the installation may form the basis for significantly improving security-force response in terms of effectiveness and numbers of responders.

We will develop automated, intelligent targeting capabilities for the TRAP—capabilities that will integrate machine-vision-based tracking with sensor- and model-based control. These developments will offload low-level targeting details, allowing an operator to focus on the immediate threat before deciding whether to issue firing commands. Our approach will integrate three-dimensional video motion detection (3DVMD) under development at Sandia. This technology is already undergoing evaluations at several DOE and Department of Defense facilities where the TRAP could be deployed. We will use 3-D information in lieu of the joystick to automatically manipulate the TRAP's pointing angle and keep the target within weapon sites. Video from the 3DVMD system would provide immediate assessment capabilities for the operator to determine the appropriate response.

We added a second, off-board video camera to the system. We enhanced the sensor- and model-based control techniques with information integrated from both on-board and off-board

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cameras. We also added a second platform, similar to the first, to the system.

We added more intelligence to the system to provide for graduated response, accurate lead times to hit moving targets, and exclusion zones where shooting was not allowed. We investigated several approaches for selective tracking and targeting. These included, but were not limited to, the selection of valid targets and the filtering of nonvalid targets. We developed several demonstration applications. We developed a point-and-shoot mode of operation using either the on-board or off-board camera. This allows the operator to manually use the mouse button to select a target within the field of view (FOV) of the camera. The weapon moves to the selected location and shoots. We implemented an ambush mode that automatically detects targets when they move within the FOV. The weapon shoots when a target reaches the line of sight. We developed an automatic targeting demonstration that automatically selects, tracks, and shoots targets as they move throughout the FOV. Another demonstration involved the coordinated control of two platforms using a single off-board camera. We added safety mechanisms to all applications such that the weapon would fire only if input were provided by the operator.

The direction of the project changed slightly from the original goals. First, a TRAP did not become available for development work. Hence, we continued all development on the new laboratory platforms rather than pursue algorithm integration with a TRAP. The TRAP itself is relatively slow and does not provide the speed necessary to track and shoot multiple targets in an actual attack. The high-speed pan-and-tilt unit used for the laboratory platform is capable of automatically acquiring, tracking, and shooting multiple targets (one at a time) within a matter of seconds.

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38695

Passive-Legged, Multisegmented Robotic Vehicle

D. R. Hayward, M. C. Reineke, P. R. Klarer, J. H. Buttz

Mobility of sensor packages and access to traditionally denied areas for the purpose of intelligence gathering present challenges that we are beginning to address. The desired destinations can be impeded by both natural and man-made obstacles. Traditional efforts stress autonomous behavior development based on processing sensor information and path planning rather than using simple processing and extreme terrain agility. Sandia seeks to develop a robotic vehicle that is very terrain-agile and is small enough to gain access to normally denied areas by passing through small openings.

This concept for a terrain-agile robotic platform is a simple legged vehicle that is modular and scalable, but will initially be sized to fit through the fabric openings of a chainlink fence. The vehicle will be composed of multiple segments, each of which has fixed appendages (legs) that resemble oars extending from a boat. Motion is achieved by pushing with these legs, which can flex to fold next to the body when passing through a constricted area. Each segment is attached to another segment using a two-axes-of-motion actuated joint. The joint can be moved vertically or horizontally. In flat terrain, horizontal joint actuation will provide the forward force. The minimum number of segments is two, but greater mobility benefits will be realized by using three or more segments. Each joint will be controlled by a microprocessor with driver circuits. Power and data will be bused to all the segments to allow synchronization of joint motions. The major effort of the project will be the mechanical design of the joints and the development of the control architecture and algorithms to provide synchronized motion for forward motion and climbing. A further goal is to include obstacle detection in the lead segment to determine when vertical actuation is needed to "step" over an obstacle.

Our activities emphasized conceptual design followed by dynamic analysis to determine if the conceptual design would indeed yield meaningful motion. The conceptual design began with a basic idea for motion and evolved to include the necessary detail for input to the dynamic-analysis software. As we conceptualized the ideas, we designed them in SolidWorks (a three-dimensional computer-aided design [CAD] package). We mated the SolidWorks parts into assemblies that contained the proper mechanical constraints to be imported into Dynamic

Accomplishments and planned future work.

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Designer (the dynamic-analysis software package). We provided the assembly with various velocities, phases, and torques to cause joints to move within their mechanical constraints. This yielded motions that could be evaluated to determine if and how meaningful motion could be achieved.

The results indicate that one-axis motion (horizontal or vertical) where the joints between the modules are phased angularly 90 degrees apart with a total of four modules will produce the desired mobility.

The summary of the progress to date includes a completed conceptual design, a completed prototype mechanical design, a dynamic analysis yielded and a potential solution, a completed prototype electrical design, mechanical components built, electrical components assembled, and several leg designs tested.

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38696

Low-Cost Photonic Lattice Structures for Remote Sensing

W. C. Sweatt, S. Y. Lin, T. R. Christenson, M. B. Sinclair, M. B. Ritchey, D. W. Peters

A first photonic bandgap (PBG) material has been designed and fabricated of nickel (Ni). Ni's large complex emissivity will reflect essentially 100% over a very wide reflectance band and will transmit well outside the band. These materials could be useful in remote sensing for infrared (IR) "tags." They could also be used as attachable "skins" that could modify the IR signature of aircraft, satellites, clothing, etc. The IR signatures of the PBG could make the equipment either easy or very hard to find. The emphasis of this project is to demonstrate the manufacture of large, flexible photonic lattices at reasonable cost.

Using deep x-ray lithography (DXRL), Sandia fabricated $> 5 \text{ cm}^2$ of Yablonovite in Ni. Photomicrographs showed that the structures were well made. They are a three-dimensional (3-D) array of cylindrical holes in a matrix. Unfortunately, reflectance measurements did not show the desired band structure. Calculations indicate too little communication between the features in the structure. We concluded that we should make the negative of this structure—a 3-D lattice of rods in a diamond-shaped arrangement. A new mask is designed and in fabrication.

Photonic lattices made of metal are hard to model because of resonances in the metal. Thus, our Yablonovite design is suspect, and we looked for alternatives. A metal PBG designed by the University of Iowa was fabricated using surface micromachining (SMM). Measurements show it has quite a wide bandgap. We conceived a method of fabricating this structure using DXRL. Our scheme is simple and quite similar to that used for making Yablonovite, so making large sheets should be relatively inexpensive.

Using DXRL to make small, sloping features (e.g., photonic lattices) has been problematic. The masks are 5–10 μm thick, and the x-rays approach from significant angles. With a micron-sized hole, no flux can get through. We developed a method of sloping the holes in the mask so very crisp, slanting images can be created in the photoresist. This is critical to making PBGs for near-infrared (NIR) applications because the features must be smaller than a micron.

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Other Communications

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38698

Security Monitoring and Management with Information Technology (SUMMIT)

L. A. Cano, G. N. Conrad

When designing or updating secure facilities, an ad hoc collection of stand-alone, but related, subsystems emerges. These subsystems can include physical security, access control, cyber-security, safety systems, and infrastructure (air/water/power) monitoring. Each of these subsystems holds information about the security posture of the facility. However, separate reporting systems can prevent operators from determining this posture. If managed as a complete system with appropriate anomaly detection, an integrated system could increase operational security and possibly detect against some insider activities.

The Security Monitoring and Management with Information Technology (SUMMIT) system will collect data from these various systems. In addition, SUMMIT will have a native data-collection capability. The system will move collected data to a rule-engine and facility model. The rule-engine will filter data for security content and will detect anomalous behaviors. The overall security status of a site will be displayed along with any anomalies. Thus, human operators will have a better understanding of the security posture of their facility.

When fully implemented, SUMMIT will provide data for future modeling/simulation tools. The SUMMIT architecture may also allow a modified rule-engine to filter for other customers, such as safety or process operations. The effort would clearly establish Sandia as the leader in high-consequence security information-management systems. SUMMIT has the potential to protect facilities against insider activity, a capability that no commercial system currently has.

- *SUMMIT accomplishments.*
 - Gathered data from various sources, e.g., turnstile, phone logs, classified network access, delivery of hazardous materials.
 - Developed a methodology to organize these data for analysis.
 - Obtained a tool (Clementine) to correlate data collected to develop a library of patterns of behavior.
 - Developed a computer simulation using ARENA to model various types of activities. We used output from this model to develop an initial database of activities to investigate.
 - Presented our current results using the ARENA simulation.

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- On track to develop a methodology to detect insider activities based on current data available as well as to develop criteria for what data should be collected. Our goal is to develop methods for implementing near-real-time systems for identifying insider threat activities.

- *SUMMIT—current status.*

Currently working to develop a database requirement for ARENA modeling of a facility to focus on

- Insider threat.
- Malicious insider.
- Anomalous behavior patterns.

To do this work, we are currently gathering data from various sources, including classified computing access, phone records, turnstile data, and hazardous-materials delivery schedules.

We are currently developing a methodology that maps relationships between individuals, facilities, and the use of Sandia resources. Our next steps are to develop a simulation using ARENA, which will duplicate the various activities we wish to track, then use a data-correlation tool (Clementine) to develop pattern-recognition schemes and probabilities for different sequences of behaviors.

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Other Communications

Cano, L. A. 2002. Identifying the insider threat using computer simulation. Paper presented at the INMM Conference 2002, July, Orlando, Florida.

38699

Novel Methods for Ultracompact, Ultralow-Power Communications

R. C. Ormesher, A. L. Schauer, J. J. Mason, R. M. Axline

Sandia seeks to develop a new Turbo-decoding algorithm and hardware for use in ultralow-power, covert, mobile-communications systems. With a new algorithm, we believe we can operate at a bit-energy-to-noise ratio (E_b/N_0) of 1.5–2 dB, yielding transmitter power savings of 4–5 dB (with respect to existing methods). The algorithm design poses two major challenges: (1) eliminating the use of phase-lock loops (PLLs) and delay-lock loops (DLLs) that cannot operate at lower power levels, and (2) handling receiver-processing complexity for real-time applications.

Time, phase, and frequency estimation, normally performed by PLLs and DLLs, would be combined within the symbol-by-symbol Turbo decoder to reduce computational complexity and improve the estimation results. After developing the algorithm, we would implement it in a high-level software language. Finally, we would implement the algorithm on a programmable gate array (PGA) to demonstrate the capability to support high data rates at extremely low E_b/N_0 values on a single chip.

Successful demonstration of transmitter-power savings would represent a breakthrough for radio-frequency (RF) communications applications. The key points are to (1) reduce required user-segment transmit power by 4–5 dB, (2) decrease user-segment probability of intercept and increase ability to hide signal, and (3) decrease physical size of the user-segment transmitter, thereby decreasing the size of a man-carried radio.

We reviewed the requirements for several systems, including the GPRS. Several key requirements make implementing a Turbo encoder at low signal-to-noise ratios (SNRs) very difficult. These include the clock stability and velocity requirements of the mobile transmitter.

We searched the literature and believe that we are current on the latest technology for Turbo decoding and encoding. To date, we have not found an approach that meets our specific requirement for an LPI (low probability of interception) system with requirements similar to those specified by GPRS and similar systems.

We proposed a new algorithm that we believe will solve our problem. There are really two new algorithms for both Viterbi and Turbo decoding. Our interest is in the Turbo decoding, but the building block for this is the new enhanced Viterbi

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algorithm. The new decoding algorithm incorporates the phase- and time-delay estimators within the encoder.

We found several papers that describe how to implement Turbo decoders on PGAs. We can use these as a starting point for implementing the new algorithm on hardware. Also, we found a chip designer, IMEC, that claims to have implemented Turbo decoder that runs at 100 Mb/s. If we could use this design in a custom application-specific integrated circuit (ASIC), then at a data rate of 20 Kb/s, we would have significant overhead to implement a new algorithm.

We implemented part of the new algorithm in MATLAB and in C. The part that we implemented contains the delay estimator integrated into the Turbo decoder. The phase estimation should require a slight modification to this algorithm. We performed Monte Carlo simulations to verify the algorithm implementation, and so far, results look very promising. We demonstrated that the new algorithm, where the delay estimate is integrated into the decoder, performs significantly better than the existing techniques of a tracking loop followed by a Turbo decoder. We will require more simulations to completely quantify the new algorithm.

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38700

Collaborative Approach in System Design and Protection

T. Q. Thai, K. C. Nichols, Z. L. Lovelady, J. L. Ziegler, N. R. Copperman, S. T. Jones, J. M. Childs, D. P. Ghormley

This is a classified project.

38701

Novel Tagging Technologies for the Tracking and Authentication of Documents, Property, and Other Items

M. C. Wanke, M. M. Manginell, S. A. Kemme, S. M. Brozik, P. Esherick, M. E. Warren, F. T. Mendenhall

Recent global events have continued to foster interest in the development of more-sophisticated technologies for the control and monitoring of many items, including, but not limited to, classified documents and computer media, government property, personnel (e.g., friend or foe identification), and different types of contraband. Such tagging can serve to verify authenticity, maintain a record of chain of custody, or monitor changes in an environment over the course of time. Ideally, tagging technologies should be covert, passive (i.e., not giving away the location of an important item or person), unique, and extremely difficult to replicate. Sandia seeks to demonstrate and develop advanced tagging technologies that have some or all of the above characteristics. Optical tagging research will likely focus on experiments to demonstrate the potential uses of infrared (IR)-retroreflecting microspheres for a wide variety of applications, including dispersal over loose ground to determine whether or not objects have passed since the microspheres were put into place. Biological tagging research will be carried out in a number of areas, all with the overriding goal of demonstrating the use of specific deoxyribonucleic acid (DNA) sequences as covert, unique tags for important documents.

This project focused on optical tagging technologies. The original idea was to develop a tag that reflects IR light and could be identified upon illumination with an appropriate light source. This tag was to be based on either microcornercubes or “cat’s-eye” microspheres. We identified a commercial source of tape based on microspheres of this type and performed characterization studies on the tape and, more recently, the free microspheres. We recently demonstrated that the microspheres can be placed on loose ground, allowing the area where they have been placed to be identified, based on on-axis light reflectance. Furthermore, the reflectance goes away if the ground has been disturbed, e.g., by footprints created by a passing person, vehicle, or other object. This suggests a powerful application to monitor human activity at places such as border crossings.

In our biological tagging work, we demonstrated that a unique DNA sequence can be placed on a paper among 20 other

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DNA sequences that serve as “false” tags and then be detected using a polymerase chain reaction (PCR). We accomplished this using paper that we subjected to various chemical treatments prior to running the PCR. We also made some progress in the evaluation of a hybridization approach to detecting the bio tags. We optimized the spotting buffer used in printing the DNA to get the lowest background signal and developed a new hybridization protocol using a condensing agent (dextran sulfate) and mixing it to reduce hybridization times.

38702

A Revolutionary Long-Lived Power Supply: The Icosahedral Boride Semiconductor (IBS) Beta-Cell

T. L. Aselage, M. P. Siegal, D. P. Adams, G. Nagasubramanian, D. T. Berry, G. L. Zender, P. H. Helmick, M. A. Rodriguez

Beta cells are solid-state devices to convert the immense energy capacity contained in beta particles emitted by decaying radioisotopes directly into electricity. Realizing their full potential, beta cells would be reliable, self-contained, long-lived power sources of enormous capacity. Within Sandia missions, beta cells could replace currently used power sources and offer the possibility of applications that are not currently feasible.

Beta cells are analogous to solar cells. A beta ray passing through a semiconductor creates many (about 100,000) electron-hole pairs. The local electric field within a semiconductor junction separates these pairs into electrons and holes, thereby generating an electrical current.

However, beta-radiation damage quickly degrades the electrical output of beta cells made with conventional semiconductors. Thus, beta cells fabricated from conventional semiconductors have very limited utility. By contrast, beta-radiation damage spontaneously self-heals in an unusual class of semiconductors—icosahedral borides. With self-healing, the life of a beta cell would depend on the lifetime of the beta emitter rather than being limited by radiation damage.

This project will create prototype icosahedral-boride beta cells. We will use chemical vapor deposition (CVD) to grow device structures. We shall attempt to control the doping of the icosahedral-boride semiconductor to optimize the device's electrical response. We will then measure and assess the radiation-induced output of these devices. These findings will establish the applicability of particular beta cells for specific Sandia systems. We will engineer electrical storage and delivery systems associated with beta-cell usage.

Growth of crystalline films of icosahedral-boride semiconductors for beta cells requires unconventionally high temperatures. Our Kansas State University (KSU) collaborators completed modification of their CVD reactor, demonstrated reliable substrate temperatures of 1450°C, and are now beginning to grow films. We measured and analyzed x-ray rocking curves and pole figures of existing B₁₂As₂ films to provide a baseline for KSU improvements in film quality.

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We identified transition-metal diborides as suitable and advantageous electrical contact materials. We prepared and supplied bulk diboride samples to KSU for CVD of icosahedral-boride films. We are developing the technology of thin-film diboride deposition.

Electrical transport measurements of $B_{12}P_2$ films in which silicon (Si) atoms substitute for some phosphorus (P) atoms show Si's effectiveness as a *p*-type dopant. Theoretical analysis of similar S or selenium (Se) substitutions for pnictide atoms suggests that these substitutions would also produce holes, rather than serving as *n*-type dopants. These results direct our initial efforts, in keeping with our project plan, toward Schottky-barrier devices.

We are exploring two types of Schottky-barrier beta cells. The first utilizes different metal contacts to an icosahedral-boride semiconductor to produce a net electrical output under beta bombardment. We prepared a simple $B_{12}As_2$ -film device with four different metal contacts: aluminum (Al), gold (Au), TiB_2 , and TaB_2 . We tested this device by individually bombarding each of the metal contacts with 20–40 keV electrons in a scanning electron microscope (SEM). Each of the four metal contacts produced a different open-circuit electromotive force (emf) when bombarded with an electron beam. As a result of this asymmetry, uniform bombardment of two different metal contacts on an icosahedral-boride semiconductor will produce a net emf.

The second type of Schottky-barrier device uses asymmetrical doping of the semiconductor near the two metal contacts to produce a net electrical output. The feasibility of this device was demonstrated by the dramatic difference in electron-bombardment-induced emf of Au contacts on undoped and heavily doped icosahedral-boride films.

We identified a suitable, commercially available source of high-energy beta rays. We designed and will manufacture a fixture to employ this source in the beta irradiation of icosahedral-boride semiconductor devices. Upon completion of the final design and safety approval stages, we will purchase the beta source and commence beta-irradiation testing.

We obtained rechargeable lithium batteries with long shelf-cycle lifetimes. We are testing their electrochemical properties at room temperature and at higher and lower temperatures. We also obtained small ultracapacitors to undergo similar testing.

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Refereed

Emin, D. 2002. Icosahedral borides in direct and indirect solid-state nuclear energy to electric energy conversion. Paper presented at the Defense Sciences Research Council Meeting, 8 July, San Diego, California.

38703

Remote-Sensing Data Exploitation for Geologic Characterization of Difficult Targets

M. M. Moya, A. R. Lappin, G. L. Peace, C. L. Walker, J. L. Smith

Determining the geology and rock properties is a significant component of characterizing an underground facility site. Analysts use geologic and rock property data to assess facility characteristics and destruction potential under a variety of attack scenarios. Current assessments use a variety of imagery, but the full potential to exploit the wealth of data from remote-sensing platforms for geologic characterization is as yet unrealized.

This effort focused on developing the initial pieces of a methodology to investigate geologic features and near-surface rock characteristics critical to planning nuclear weapons–attack scenarios. Because of the accelerating rate of identifying new sites, we need to develop a capability to exploit data rapidly from remote-sensing sources and integrate it with traditional data sources to create a robust geologic characterization. We will collaborate with investigators at the Defense Threat Reduction Agency (DTRA)/Springfield Research Facility (SRF) to develop a new set of experiments using the multispectral thermal imaging (MTI) satellite and other remote-sensing platforms. We focused on three activities: (1) identifying key geologic features and rock characteristics that could be detected, identified, and measured using remotely sensed data, (2) developing data-processing techniques to extract information from image data that would allow detection and measurement of key geologic characteristics, and (3) planning a series of field ground-truth studies, in conjunction with the SRF, that will provide confirmation of data-interpretation methods. Subsequent efforts will concentrate on refining these data-processing techniques, developing additional methods to broaden the range of geologic features addressed, and applying these methods to specific sites where extensive ground-truth data are being collected.

We focused on three activities: (1) identifying key geologic features and rock characteristics that could be detected, identified, and measured using remotely sensed data, (2) developing data-processing techniques to extract information from image data that would allow detection and measurement of key geologic characteristics, and (3) planning a series of field ground-truth studies, in conjunction with the SRF, that will provide confirmation of data-interpretation methods.

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This effort focused on developing the initial pieces of a methodology to investigate geologic features and near-surface rock characteristics critical to planning nuclear weapons–attack scenarios.

- *Digital elevation modeling (DEM)*. To attain our objectives of characterizing the geology for sites of interest in denied areas, it is necessary to have slope information at as fine spacing as our multispectral information. In addition, it is essential that our multispectral data remain in its most native form so that the small perturbations that we will exploit are not removed from the data in a resampling process. To this end, we developed a novel idea for obtaining elevation information directly from the multispectral imagery (MSI). Rather than using the traditional stereo method, we plan to exploit the MTI's pointing capability to obtain a minimum of three images of a site to obtain more accurate elevation information than a stereo pair. We are entering into collaboration with a leader in this field that will result in a new and innovative DEM.

- *Spectral signatures of geomaterials*. We are conducting a material separability study to understand the potential and limits of using multispectral data to separate general classes of rock type. MTI's small ground-sample distance (GSD) affords the potential for a greater number of pure pixels of interest; however, the multispectral nature of the data limits our ability to identify fine absorption features that uniquely identify materials. We are collecting libraries of mineral spectra and creating mixture recipes for appropriate materials. We applied principal component reduction to library spectra of the minerals of interest and examined relevant clusters. We computed Pearson correlation coefficient for each pair of materials. We are investigating sensor-band combinations that provide optimal separation of these geological materials of interest.

- *Thermal/physical properties of rocks*. We are investigating a novel method to determine thermal rock properties using MTI thermal imagery by exploiting the differential heating histories of pixels in the vicinity of shadows. Simulations of a one-dimensional heat-transfer model with time-varying boundary conditions (heat flux at surface) predict surface rock temperatures with significant differences (5°–15°C) as functions of local sunrise/sunset times and thermal rock parameters. The pixel-by-pixel sunrise/sunset times within a thermal image depend on the date of collection and the site's location and topography. Estimating the thermal rock parameters (e.g., emissivity, reflectance, thermal conductivity and thermal capacity or equivalently thermal inertia and diffusivity) from the model requires optimization code that searches the space of rock parameters to minimize the sum-of-squares difference between model-predicted temperatures and temperatures estimated from the MTI thermal bands over a number of spatial pixels. We demonstrated, in a

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no-noise simulation, that the optimization code DAKOTA (Design Analysis Kit for Optimization and Terascale Applications) can invert the model estimation and accurately predict the rock parameters. We are currently investigating the sensitivity of rock parameter estimation due to errors in temperature, radiance, DEM, and sunrise/sunset times. Sensitivity analysis for both bias error (all pixels have same offset from true) and random errors (each pixel has an independent error offset) is considered.

38706

Detecting and Tracking the Active Insider Using 3-D Detection Technology

C. L. Nelson, C. Q. Little, J. P. Luck

Vulnerability-analysis studies show that one of the worst threats against a facility is that of an active insider during an emergency evacuation. When a criticality or other emergency alarm occurs, employees immediately go along evacuation routes to designated areas. Procedures are then implemented to account for all material, classified parts, etc. There is currently no method to detect or track an insider during this situation in which items could be removed and either hidden for later retrieval or thrown over the fence. A developing technology, 3-Dimensional Video Motion Detection (3DVMD), could be used to detect and track insider activities during alarm situations. 3DVMD technology uses multiple cameras to create 3-D detection volumes or zones. Multiple zones are defined to monitor a large volume of space such as a room or hallway. Movement throughout detection zones could be tracked, and various levels of information, such as the number of people moving about and their direction of motion, could be extracted. During an alarm, anomalies of evacuation procedures taken by an individual could be immediately detected and relayed to the central alarm station (CAS). The insider could be tracked, and any items removed from the area could be flagged. 3DVMD could also be used to monitor items such as machines that are used to build classified parts. During an alarm, detections could be made if items were removed from the machine. Overall, the use of 3DVMD technology during emergency evacuations would help to prevent the loss of classified items and would speed recovery from emergency situations. Further security would also be added by analyzing tracked behavior (motion) as it corresponds to predicted behavior. This information would be valuable for detecting a possible insider not only during emergency situations, but also during times of normal operation.

Our overall goal is to enhance 3-D sensing technologies to enable an automated system to track and record actions of multiple people in a monitored area and to alarm upon suspected insider activities. We set up a test-bed system to monitor an entire room with a 2 in. 3-D resolution. We found this resolution sufficient to extract needed information such as the presence of a person(s) and tracks of multiple people. We are able to determine the presence of two (or more) people to enforce a two-man rule. We can monitor the path taken by

Vulnerability-analysis studies show that one of the worst threats against a facility is that of an active insider during an emergency evacuation. ...the use of 3DVMD technology during emergency evacuations would help to prevent the loss of classified items and would speed recovery from emergency situations. Further security would also be added by analyzing tracked behavior (motion) as it corresponds to predicted behavior. This information would be valuable for detecting a possible insider not only during emergency situations, but also during times of normal operation.

individuals to detect deviations from normal operating procedures. We can detect loiter situations in which a person lingers too long at a location, and we developed initial asset protection capabilities.

We made significant advances in algorithm development, including adaptive models of motion in 3-D space and the representation of 3-D motion in 2-D space. We developed a clustering technique based on a projection of 3-D space into two dimensions to separate and track moving objects (or people). We developed algorithms for tracking clusters for purposes of detecting path deviations and loiter situations. We also developed clustering algorithms in 3-D space using different camera views to recognize and separate objects. We implemented initial tracking algorithms operating on raw 3-D data and added the capability for exclusion zones, which define boundaries that cannot be crossed.

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38707

Microfabricated Dielectrophoretic Sample Preparation System

E. B. Cummings, R. Shediak, A. K. Singh, G. J. Fiechtner, B. A. Simmons

Sample preparation is the most critical standing issue in the implementation of microanalytical systems. Sandia plans to exploit a recent discovery to prototype a front-end sample-preparation system for filtering, sorting, concentrating, and lysing biological macromolecules, including bacteria and viruses. The device, which discriminates by external and internal physical particle structure (hence, is insensitive to genetic modification), also has potential applications in rapid, first-response pathogen detection. Other applications include cell manipulation and identification for clinical diagnosis of cancer, human immunodeficiency virus (HIV), and other diseases.

The proposed device utilizes a recent discovery (U.S. patent application filed, SD-8318) in which an electric field applied across a two-dimensional (2-D) array of microfabricated insulating posts separates, isolates, and concentrates 0.1–10 μm particles dielectrophoretically, based on their polarizability, geometry, and structure. A water sample or aerosol-collector eluent can feed the device in a continuous or batch mode. During sample collection a moderate applied electric field traps or redirects bacteria and viruses into specific zones of the device containing carefully sized and shaped insulating posts. Bulk liquid and smaller molecules flow unimpeded to a waste stream. During sample recovery and analysis, a lowering of electric-field releases trapped particles in a concentrated stream to a subsequent detector, separation, or other analysis stage. Alternatively, a sharply pulsed applied field can lyse trapped cells, releasing their contents to an affinity-based analyzer, or protein-separation device such as $\mu\text{ChemLab}^{\text{TM}}$. These devices will be microfabricated in commercially available polymer substrates that display minimal nonspecific adsorption of biological material to minimize fouling.

We accomplished the following:

- Released designs of primitive devices for spatial separation using filamentary dielectrophoresis in uniform arrays and trapping dielectrophoresis in nonuniform arrays, and time-of-flight separations in uniform arrays.
- Fabricated in glass (> 6 copies) and silicone (2 copies) of post-arrays for initial tests.

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- Teamed and met with the director of medical diagnostics at the U. S. Army Medical Research Institute for Infectious Disease (USAMRIID), the viral pathologist at the Wildlife Conservation Society, and others to obtain meaningful specifications of raw samples and flowrates. This teaming led to a memorandum of understanding with USAMRIID.

- Modified the Laplace simulation software to handle filamentary and trapping dielectrophoresis. These modifications allowed us to simulate flow past arrays of circular posts, illuminating both enhancement and depletion-mode dielectrophoretic device operation. Importantly, simulations of dielectrophoresis in arrays of sharp-angled, e.g., square, posts fail to reproduce experimental data. Further study clearly suggests that the particle polarization is not in equilibrium near the corners, leading to the observed differences with the equilibrium-based simulations. Work is under way to add finite polarization-rate kinetics to the particle motion in Laplace. This work is complicated by hydrodynamic lift effects caused by rotation of the particles induced as a result of this nonequilibrium. This work is important to achieve a theoretical understanding of the operation of these devices and a simulation capability that is adequate for device optimization.

- Filed a continuation-in-part patent and patent cooperation treaty (PCT) patent detailing filamentary dielectrophoretic devices (SD-8347).

- Developed a new design methodology and several families of novel low-dispersion devices and filed a provisional patent for “method for providing conduction-like flow channels and applications therefore,” U.S. 60/387,684, 06/10/02.

Device optimization.

- Extended Laplace to handle uniform square arrays of completely general posts (including multiple-post unit cells) and modified the grid-generation algorithm to ignore unconnected channel segments to prepare for numerical optimization.

- Ported a command-line version of Laplace to UNIX for use with Sandia’s powerful optimization package OPT++ and formed a team to develop optimized post and array geometries.

- Created a general design procedure for filamentary dielectrophoretic microsystems that uses Laplace simulations to derive a complete optimized microdevice design given a post shape and array angle.

We began developing a novel mass-microfabrication technology because of our comparatively high flowrate and high-liquid-conductivity specifications and our experimental needs for test devices. We developed tooling for this technology

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and recently used it to produce device primitives in-house. Unfortunately, we encountered technical obstacles, simultaneously maintaining device fidelity and sealing the tops of the microdevices. To help solve these technical problems, we held a meeting to set up a collaboration with a major plastic-film manufacturer and fabricator.

Other Communications

Cummings, E. G. 2002. A comparison of theoretical and experimental electrokinetic and dielectrophoretic flow fields. *Proc. AIAA Conference on Fluid Dynamics, AIAA 2002-3193* (June, St. Louis, Missouri): 1–17.

38708

Automation of Microelectronic Physical Analysis

T. J. Drummond, R. P. Fleming, D. L. Barton, E. A. Walther, C. R. Jorgensen, V. R. Yarberry

This project is classified.

38712

Nonlinear Optical Limiters Using Photonic-Bandgap Structures for Sensor Protection

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Development of multifunction battlefield lasers increases the potential for accidental or intentional damage from laser radiation to optical systems. In addition, the recent evolution of military laser technology toward the use of parametric amplifiers and pulse sources capable of high-intensity propagation has created new performance requirements for sensor protection and threat warning systems that stress conventional passive optical limiters and multiline rugate filters. Future systems must exhibit rapid response, broadband spectral coverage, high radiant strength, wide dynamic range and field of view (FOV), and high optical transmission at low ambient-light levels without impacting operational capability of the sensor. These challenges can be met by integrating photon localization and nonlinear optics in a photonic lattice to produce a nonabsorptive structure whose refractive index profile and spectral reflectivity are regulated dynamically by light intensity. This project is fabricating a distributed multilayer system composed of alternating high and low nonlinear materials to respond actively to radiation intensity wherein the transmission of low-intensity light is determined by the linear refractive index, and the onset of high-intensity light induces a change in the index of refraction through the Kerr effect. The interaction changes the interface reflectance at the band edge and randomizes the phase shift of each layer, contributing to the spectral response. Sandia modeled the limiting spectrum of a device operating in the near infrared (NIR) and began modeling the internal propagation dynamics. We fabricated and partially characterized initial nonlinear materials using both linear optical metrology and Z-scan and femtosecond continuum spectrophotometry.

The key issues in developing a photonic lattice optical limiter are materials characterization and device fabrication, test, and modeling. We accomplished the fabrication of initial materials for characterization, designed a typical device, and developed a crude device model.

In device design, we pursued the fabrication and modeling of a one-dimensional (1-D) photonic crystal (PhC) composed of alternating layers of nonlinear and linear material. We identified porous silicon (poSi) as the nonlinear material with Si

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oxynitride as the likely mating material. A typical device design is twenty pairs of layers, each approximately 120 nm thick.

In the fabrication of materials, we electrochemically transformed 20 mm-thick crystalline Si (c-Si) into poSi using 20 mA/cm² of current at 48 V for 38 minutes in a 1:1 bath of 49 w/o HF : H₂O. The linear optical properties estimated based on the linear transmission spectra indicate a substantial layer of unanodized Si beneath the poSi. While nonlinear analysis by Z-scan and self-phase modulation are encouraging, indicating a large nonlinearity of femtosecond time scale, the underlying layer has made the interpretation of the nonlinearity difficult. Future samples should have no such underlying layer.

In device modeling, we considered the propagation of an optical pulse through an initially transparent quarter-wave nonlinear dielectric mirror in the limit that the intensity of the pulse is uniform throughout the structure. The modeled transmitted intensity was (1) the incident intensity for incident intensities less than the limiting intensity or for spectral components outside the induced reflection bandwidth or (2) the limiting intensity. This model made clear that it is important for the induced reflection bandwidth to be large compared to the incident pulse.

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38713

Secure MPLS Control Plane for Internet Connectivity

T. D. Tarman, J. T. Michalski, M. D. Torgerson, W. F. Young, L. G. Pierson, J. D. Tang, S. P. Black

As rapid Internet growth continues, global communications becomes more dependent on Internet availability for information transfer. Recently, the Internet Engineering Task Force (IETF) introduced a new protocol, Multiple Protocol Label Switching (MPLS), to provide high-performance data flows within the Internet. MPLS emulates two major aspects of the asynchronous transfer mode (ATM) technology. First, each initial Internet Protocol (IP) packet is "routed" to its destination based on previously known delay and congestion avoidance mechanisms. This allows for effective distribution of network resources and reduces the probability of congestion. Second, after route selection, each subsequent packet is assigned a label at each hop, which determines the output port for the packet to reach its final destination. These labels guide the forwarding of each packet at routing nodes more efficiently and with more control than traditional IP forwarding (based on complete address information in each packet) for high-performance data flows.

Label assignment becomes critical in the prompt and accurate delivery of user data. However, the label-distribution method is not secure. Thus, if an adversary compromises a node by intercepting and modifying, or, more simply, injecting, false labels into the packet-forwarding engine, the propagation of improperly labeled data flows could create instability in the entire network. In addition, some Virtual Private Network (VPN) solutions take advantage of this "virtual channel" configuration to eliminate the need for user-data encryption to provide privacy. VPNs relying on MPLS require accurate label assignment to maintain user data protection.

This research is developing a working distributive-trust model demonstrating how to deploy confidentiality, authentication, and nonrepudiation in the global network label-switching control plane. Similar to Sandia's early investment in ATM security, an opportunity exists today to impact MPLS control plane security and the security of optical network control plane protocols.

The project team studied the various protocols that are used by MPLS and all-optical networks to provision and route new label-switched paths (LSPs). Part of this analysis included an

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analysis of the following: (1) available security mechanisms, (2) implementation feasibility within the operating network (OPNET) modeling and simulation package, and (3) which of multiple contending label-distribution and -routing protocols will likely gain favor within the optical network vendor community. The result of this analysis shows that this project should focus its efforts on securing networks that use the Resource Reservation Protocol (RSVP) for signaling, and the Open Shortest-Path First (OSPF) protocol for routing.

During this analysis, we developed an architecture that addressed the principal threats to control plane protocol security in an MPLS or optical network. This architecture uses encrypted/authenticated IP Security (IPSec) tunnels to secure control channel links between label-switching routers (LSRs), and an auditing/monitoring mechanism to allow a policy monitor to determine whether new LSPs are being established in accordance with network policies. We selected this architecture because it shows the best properties for scaling to large networks.

In addition, this project was responsible for impacting work within the Optical Internetworking Forum (OIF) for securing control plane protocols for optical networking equipment (such as all-optical switches and dense wavelength division multiplexers [DWDM]). Sandia is working with its collaborators, carriers, and equipment vendors to ensure that the security techniques developed under this project are applied to the control plane protocols, which use the MPLS control plane protocols that have been adopted for optical networks.

Refereed

Tarman, T. D., and E. L. Witzke. 2002. *Implementing security for ATM networks*. Norwood, Massachusetts: Artech House Publishers.

Other Communications

Tarman, T. D., G. Woodard, R. Graveman, R. Esposito, and J. Naegle. 2002. Auditing and logging requirements for optical network elements. Paper presented at the Optical Internetworking Forum, July, Copenhagen, Denmark.

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38714

Integrated-Sensor Network Chip

B. A. Brunett, V. A. Hamilton, M. R. Daily, J. V. Wolf

In this project Sandia explored the technology necessary to produce a single-chip solution that would allow robust wireless peer-to-peer communication. The envisioned system would include a versatile sensor interface, advanced processing capability, and a secure, reliable, radio-frequency (RF) communication path. To accomplish these goals, we researched several independent components that would comprise the integrated-sensor network chip. To address the overall processing capability, we pursued several topologies, including digital signal processors (DSPs), field-programmable gate arrays (FPGAs), and microprocessors. Additionally, we addressed hardware and firmware solutions to the robust RF communication path. The reduction of the selected baseline hardware/firmware solution into a single chip was pursued in parallel to the hardware analysis.

We focused on exploring alternative wireless topologies, enhanced processing algorithms, and hardware volume-reduction approaches. As a baseline hardware design, we coupled a 2.4 GHz digitally controlled radio modem and an FPGA with a serial bus sensor module interface. The sensor interface is versatile in that any number of sensor modules can be monitored. This allowed us to explore various RF protocols and processing capabilities. We tested the performance of the specific radio chosen under varying RF circumstances and defined various algorithms to minimize the data error rate. At the same time, we defined a roadmap for reduction of the baseline design into a single chip. In addition, we provided algorithms for improved data and sensor authentication, which included elliptical-curve techniques. We built several copies of the baseline design and tested them for potential use in an integrated-sensor network chip. The strengths and shortfalls found in the baseline design will guide any subsequent work in this area.

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Refereed

Liu, H. (Oregon State University), V. Venkatesan (Oregon State University), C. Nilseny (Sandia), R. Kyker (Sandia), and M. E. Magana (Oregon State University). 2002. Performance of frequency-hopped noncoherent GFSK in correlated Rayleigh fading channels. *Proc. IEEE International Conference on Communications (ICC 2003)* (May, Anchorage, Alaska).

41194

Cognition-Driven Augmented Analyst

J. S. Wagner, P. G. Xavier, K. W. Boyack, E. M. Raybourn, S. E. Jordan, M. K. Snell, C. M. Pancerella, H. H. Hirano, J. C. Forsythe, J. H. Ganter, K. W. Larson, P. C. Reeves, N. G. Brannon

A common problem cuts across national security applications. The relentless proliferation of data, combined with the increasing demands on humans, has resulted in a nearly intractable problem involving human effectiveness and critical decision making. Scales of required understanding range from spatially—nano to stellar, and temporally—ultrashort to extremely long. Current approaches exacerbate the problems. Noise-filtering algorithms often suppress important aspects of, and especially changes in, patterns of interest. Complex processing algorithms mask the basis of conclusions and associated data uncertainties. Inflexible constraints hinder the innate human abilities to explore, recognize patterns, detect changes, resolve ambiguity, and connect disparate pieces of information.

Sandia proposes to implement a processing architecture for an “organic” systems approach to data exploitation—one in which human abilities/variabilities are embraced and exploited rather than negated. This architecture parses the problem space into object recognition (the “what”) and situation recognition (the “why”). In this approach, the human is the central element of the system rather than simply a user of the system. We will represent data in naturalistic, adaptable topologies allowing hypothesis testing and exploration. The human capability will be augmented beyond the traditional human-computer interface to one that more closely resembles a human-human interface. Representation of data will go beyond visualization of similar types of data to include the ability to visualize and otherwise experience the character of disparate types of data. Humans will not be replaced, but rather “supercharged,” as a result of utilizing naturalistic patterns of memory, reflectivity, and learning. Tiny cues will lead to large visions as a means of setting context for interpreting data.

This architecture could be applied to a number of important problems: characterizing/exploring nuclear weapons data archives, enhancing intelligence/homeland security analysis tools, modeling of human-in-the-loop systems, and battlefield automatic target recognition (ATR) and damage assessment.

We developed a computational architecture for augmenting human cognition and enhancing human performance in complex, data-rich environments. The architecture integrates

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perceptual (the “what”) and cognitive (the “why”) subsystems with tailored generative displays and other adaptive interfaces within an infrastructure “backbone” that enables interactions between the computational components and the human system elements. This architecture can be instantiated in three use modes: (1) a development environment where data sources, perceptive-cognitive components, and human interfaces can be engineered and integrated, (2) a test and validation environment in which the augmentation technologies are validated through experimentation, and (3) an operational environment where the technology is actually used in an application unencumbered by the details of the architecture or its implementation.

We researched, conducted preliminary design analyses for, and developed high-level requirements for the following:

- Perceptual systems (object recognition and characterization) toolkits based on fourth-generation artificial neural structures. These systems close the phenomena-to-phrase gap (from environmental sensors and other data sources to the computational environment) and feed the semantic knowledge base that is necessary to initiate cognitive augmentation.
- Cognitive models that will enable cognitive systems (situation recognition and interaction) toolkits to answer the “why” questions: importance, causality, intent, sequence, etc., and provide the basis for human cognitive augmentation.
- Interaction systems and protocols (tailored generative displays, other adaptive interfaces) that integrate the human into the system.
- Infrastructure backbone elements (based on Sandia’s UMBRA framework) to integrate the system elements from development to operational levels.

Other Communications

Forsythe, J. C., and P. G. Xavier. 2002. Human emulation: Progress toward realistic synthetic human agents. *Proc. 11th Conference on Computer-Generated Forces and Behavior Representation 1* (Orlando, Florida): 257–66.

Forsythe, J. C., N. G. Brannon, K. W. Boyack, and P. G. Xavier. 2002. *Concept development for cognitive components in next-generation intelligent systems*. Sandia Technical Report SAND2002-2128. Sandia National Laboratories, Albuquerque, New Mexico.

We developed a computational architecture for augmenting human cognition and enhancing human performance in complex, data-rich environments. The architecture integrates perceptual (the “what”) and cognitive (the “why”) subsystems with tailored generative displays and other adaptive interfaces within an infrastructure “backbone” that enables interactions between the computational components and the human system elements.

Schoenwald, D., P. G. Xavier, E. Thomas, J. C. Forsythe, and E. Parker. 2002. Simulation of a cognitive algorithm for a distributed robotic sensor network. *Proc. International Society of Robotics and Automation*, accepted.

48341

Chemically Stressed Glass Structural Elements

S. J. Glass, R. G. Stone, C. S. Newton, E. Hoover, J. E. Kooi, S. T. Reed, R. Tandon, K. J. Schwing

Sandia possesses a technology for producing stressed glass by a two-stage salt-bath immersion that produces product of uncommonly high strength and reliability. The stressed glass, when forced to failure, destructs in a fashion that leaves very small fragments of glass rather than large shards. The salt-bath immersion process is not restricted to flat sheets, as is the usual process for producing thermally tempered glass such as that used in windows. In fact, the process seems to be amenable to tubing or even objects of complex cross section. We believe we can produce simple structural elements such as beams, rods, and tubes on a scale of meters that we can incorporate into complex structures. We envision producing a representative number of samples of several different structural shapes for rudimentary strength and fragmentation tests as a means of proving the applicability of this technology.

We determined optimized ion-exchange strengthening treatments for soda lime silicate (SLS) and sodium aluminosilicate (SAS) glass compositions. Small diffusion depths limited the amount of strengthening and internal tension that could be developed in the SLS glass. We made calculations to determine how compositional changes in the SLS could enhance the diffusion depths. We could obtain high levels of internal tension (> 100 MPa) for the SAS glass at elevated treatment temperatures, long ion-exchange times, and for small glass thicknesses. The level of internal tension was so high in some samples that we could not measure it using the optical birefringence technique. The minimum level of internal tension to obtain dicing behavior (complete fragmentation into cubelike particles) appears to be in the range of 30–40 MPa. For short exchange times the surface compressive stress appears to exceed 1000 MPa. The prism-coupling technique could not determine the compressive surface stress for samples exchanged for the long times and high temperatures likely, due to surface stress relaxation. The fragmentation tests showed that we could obtain submillimeter-size fragments for a range of treatments for the SAS glass. The largest fragments were located close to the fracture initiation site. Strength measurements showed that the strength of the ion-exchanged glass was four to five times higher than the as-received glass.

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We made large complex-shape glass parts from flat SAS plate and then ion-exchanged them. Cutting and machining damage sometimes caused spontaneous failure of the parts during the ion-exchange process.

Refereed

Abrams, M. B., D. J. Green, and S. J. Glass. 2002. Fracture behavior of engineered stress profile soda lime silicate glass. *J. Noncrystalline Solids*, accepted.

Kamat, S., E. K. Beauchamp, S. J. Glass, and C. S. Watson. 2002. Crack shielding effects on the dynamic strength of engineered stress profile (ESP) glass. *J. American Ceramic Society*, in preparation.

Other Communications

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Watson, C. S., S. J. Glass, and S. Kamat. 2002. Crack morphology in engineered stress profile glasses. Paper presented at the 104th Annual Meeting of the American Ceramic Society (SAND3904A), 28 April–1 May, St. Louis, Missouri.

48746

Digital Signal Processing for Acoustic-Seismic Target Identification

K. T. Malone, M. W. Koch, G. B. Haschke, A. A. Yee, M. D. Ladd

Sandia has developed a number of new signal-processing techniques in the area of automatic target identification for synthetic-aperture radar (SAR) activities; it is from these types of Sandia programs that we plan to draw for innovation. The goal of this research is to provide a solid technical signal-processing foundation for acoustic-seismic target identification in harsh environments and to demonstrate the feasibility of an integrated acoustic-seismic measurement and signature intelligence (MASINT) untended sensor system into the widest possible applications. This project focuses on the algorithms and software foundation essential to all future hardware development. Expected results are that Sandia can successfully develop new algorithms to meet the needs of acoustic-seismic target identification applications.

The major accomplishment of this project was the development of a hybrid target-classification algorithm to aid in the “unknown” target problem and also to provide a meaningful confidence level associated with the target-identification result. We implemented the hybrid algorithm in MATLAB (a technical computing environment) and tested it using real acoustic data. The results to date show a slight decrease in performance for those targets in the target library. However, the algorithm was able to greatly improve the ability to declare a target as “unknown” if the target’s signature was not in the target library. The hybrid algorithm was, in most cases, also able to provide a meaningful confidence level for the identification result.

The performance of the tracked/wheeled classifier developed under this project is promising. More work is required to increase performance and determine the robustness of the algorithm.

We simulated several other modifications to the target-identification algorithm in MATLAB. The significant modification is a technique to implement the identification metric only when the fundamental frequency estimate is reasonably assured to be correct.

We identified MATLAB as the appropriate platform to develop a wavelet-based target-identification algorithm. MATLAB has existing wavelet tools, and all team members have prior experience with MATLAB. We are evaluating previous work on wavelet-based target-identification techniques. Preliminary work suggests that discrete Meyer wavelets may be a suitable wavelet family.

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48751

Terahertz Propagation in Telecommunication Optical Fibers

M. E. Warren, M. C. Wanke

Terahertz radiation ($\sim 10^{12}$ Hz) falls between the far-infrared (FIR) optical wavelength part of the electromagnetic (EM) spectrum and the millimeter-wave high-frequency radio-wave part of the EM spectrum. Because of the difficulty of performing experiments in this frequency band and the lack of convenient sources and detectors, this part of the spectrum is relatively unexplored. There is growing interest in this frequency range for chemical sensing as terahertz frequencies correspond to many molecular bending and vibrational energies. A capability to propagate terahertz radiation in waveguides would be useful for developing chemical sensors and instrumentation. However, optical fibers have polymer coatings outside the glass cladding and are usually inserted into polymer jackets for mechanical protection. Some polymers are relatively transparent to terahertz radiation and were used as waveguide materials in some previous terahertz experiments. Sandia performed several experiments with a variety of optical fibers as well as the cable jacketing materials to determine if they would serve as a waveguide structure for terahertz propagation.

The original report of terahertz propagation in optical fibers was based on measurements with an ultrawideband system that emits free-space pulses of terahertz radiation. This was a surprising report, as the glass used in optical fibers is known not to transmit well in the terahertz. However, all optical fibers have additional polymer layers that might allow for propagation along the fiber. Especially considering that the wavelengths in the terahertz are significant fractions of a millimeter, it seemed likely that jacketed fiber cables might be able to guide radiation. We did not have a similar broadband-pulsed terahertz generating system available, so we used a FIRL100 molecular laser from Edinburgh Instruments that we had purchased for another project. This laser was pumped by a CO₂ molecular laser and emitted a continuous-wave beam. We determined the wavelength by the gas mixture in the laser and tuned it slightly by varying the cavity length. We used a chopper and lock-in amplifier with a pyroelectric detector to detect the terahertz beam. While setting up this laser, we procured a variety of optical fiber samples. Some were connectorized cables and some were unterminated lengths of cable. We also purchased segments of “bare” fiber that is actually covered with a thin

There is growing interest in this frequency range for chemical sensing as terahertz frequencies correspond to many molecular bending and vibrational energies. A capability to propagate terahertz radiation in waveguides would be useful for developing chemical sensors and instrumentation.

polymer buffer coating. We inserted short samples of a variety of single-mode and multimode commercial optical fibers, as well as some samples of polymer cable-jacketing material, into the beam and measured the presence of any radiation transmitted around a shallow 90-degree bend. Since changing the wavelength of the laser was an involved process, including changing the gas used in the laser after an overnight purge, we used only a few wavelengths for the measurement. The wavelengths tried were 513 μm , 394 μm , 163 μm , and 118 μm . The first two used HCOOH and the second two used CH₃OH as the laser gas. We observed no propagation in any of the fiber samples at any of the wavelengths. To verify proper function of the system, short pieces of straight, hollow-cable jacket material did transmit radiation as expected. Early in the experiments we observed strong attenuation of the beam in air, presumably due to water vapor absorption. We enclosed the experimental setup in plastic sheeting and used dry nitrogen to purge the enclosure to reduce these losses, then repeated the experiments. We still did not observe any evidence of guiding of the terahertz laser radiation. The measurement system noise floor was about 10^{-5} of the unattenuated beam, so if there is any guiding, the losses are very high. The coupling procedure used for the beam was primitive, but the long wavelength of the terahertz radiation should be insensitive to the quality of the fiber end. Since this was a low-power, narrowband measurement, as opposed to the original pulsed experiments, we were unable to sample a wide range of wavelengths simultaneously. The spread of the four wavelengths that we tried does span most of the terahertz band. Additionally, we contacted the professor leading the university group that reported the original claim, and he claims to be unaware of any such observation. At this point we have concluded that the original report was likely due to experimental error on the part of a student, probably detection of stray radiation propagating a short distance through the atmosphere to his detector, and the result was reported prematurely.

There are alternative approaches to guiding terahertz radiation. Good results have been reported with small metallic waveguides fabricated from copper foil. We intend to try that structure in our measurement system soon, but were unable to fabricate the guides in time for the result to be reported here. Although those structures are not as convenient to use as dielectric fibers, they would still be usable for sensor applications.

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48764

Rapid Screening for Biological Infection

D. L. Osborn, J. P. O. Bood, A. McIlroy

This project addressed rapid screening for biological infection by detection of nitric oxide (NO) gas, which would be present in the exhaled breath of infected individuals. The technique developed to detect NO is cavity-enhanced frequency-modulation (CEFM) spectroscopy. Sandia's goals were twofold: first, to detect NO at a wavelength of 790 nm (using an existing apparatus) and calculate the sensitivity of detection at 1780 nm, the wavelength where breath testing measurement would be done; and second, to quantify whether the sensitivity, selectivity, and precision of this technique is sufficient to make this technology promising for rapid infection screening.

We succeeded in detecting NO at 790 nm, quantified its absorption strength, and calculated the sensitivity of detection at 1780 nm. We also compared the achieved sensitivity, selectivity, and precision with the requirements for successful use as a rapid screening technology for biological infection.

In the event of a large-scale bioterrorism attack, there is a need for rapid biological infection screening to separate the “worried well,” who think they have been exposed, from those people who are, in fact, developing an infection. We proposed that a rapid, noninvasive method for such screening is breath-testing for exhaled NO. NO is produced by the body as a response to inflammatory conditions typical of bacterial infection. Therefore, the rapid detection of NO could provide a first screening to largely eliminate the “worried well.”

A review of the medical literature shows that healthy humans have NO concentrations in their breath of 6–22 parts per billion by volume (ppbv), while those with a respiratory-tract infection show levels of 40–80 ppbv. Therefore, we chose our performance goal for NO detection to be an absolute sensitivity (minimum detectable amount of NO) of 1 ppbv, with a precision of 1 ppbv in a 1 s integration time. In other words, the goal is a detection limit of 1 ± 1 ppbv in 1 s. Selectivity is the ability to detect NO in the presence of other compounds (notably water and carbon dioxide [CO₂]), with the goal that the detection limit is unchanged by the presence of these other molecules in amounts that we expect in human breath.

We used CEFM spectroscopy to detect NO on the sixth overtone vibrational transition (i.e., the 0 to 7 band). We chose this band because the required wavelength of 790 nm is easily reached with an existing laboratory laser. Higher sensitivity

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could be attained using the CEFM technique on the second overtone ($3 \leftarrow 0$ transition) at 1780 nm. Since we do not possess a laser in this region, the goal of the project was to evaluate detection at 790 nm, extrapolate these data to predict values at 1780 nm, and compare with the sensitivity, precision, and selectivity goals described above.

The sixth overtone of NO has never been measured; therefore, to perform the extrapolation, we need to first establish the line intensity of several rotational lines in this band and compare these with known line intensities for the second overtone band. The achieved detection sensitivity for a 1 s time constant is $2 \times 10^{-11} \text{ cm}^{-1}$. This corresponds to detecting a density of $1.3 \times 10^{15} \text{ molecules/cm}^3$ (i.e., 40 mtorr), or 50 ppm at 1 atmosphere. We measured a line intensity of $3.7 \times 10^{-28} \text{ cm/molecule}$ for the strongest line in the sixth overtone. This line is a factor of 108,000 weaker than the corresponding line at 1780 nm. Based on these values, we predict a detection limit at 1780 nm of 0.5 ppb. This is our sensitivity estimate at a signal-to-noise ratio of 1, which in turn yields an estimated precision of 0.5 ppb.

We obtained the selectivity goal by passing the mixture of gases through a cold trap at -95°C . This trap removes essentially all water and CO_2 , leaving a signal due purely to NO. We believe that a thermoelectric cooler could perform this job adequately on a field instrument.

We predict that the CEFM technique, employed at 1780 nm, would have sufficient sensitivity, selectivity, and precision to be useful as a rapid screening technique for biological infection by detecting NO gas in exhaled breath.

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48765

Investigation of Bluetooth Capabilities and Vulnerabilities

R. P. Weishuhn, W. A. Amai, J. L. Etzkin, K. C. Nichols

Bluetooth (BT) is a wireless technology for data and voice transfer between personal computers (PCs) and devices such as personal data assistants (PDAs), cell phones, and printers. One can synchronize data manually or automatically between PCs and PDAs by placing the PDA into a cradle connected to the PC. With BT, one would need only to carry the PDA within range of the PC (< 10 meters) to initiate this synchronization. Similarly, one may be able to print from a BT-enabled laptop to a similarly enabled printer in range, without having to be in direct line of sight, as with the infrared digital assistant (IrDA) protocol. The built-in voice-transmission capability makes this technology compelling for use in wireless headsets, cell phones, and other voice communications devices.

BT devices operate in the 2.4 GHz frequency band, one of the bands where transmissions can be made without a license. In some respects, Bluetooth is similar to the Institute of Electrical and Electronics Engineers (IEEE) 802.11 (RF [radio frequency] Ethernet) standard, in that they both use the 2.4 GHz frequency band and can be used for connectivity between computing devices. A key difference is that BT has a much lower cost per unit than IEEE 802.11 devices, which will lead to greater proliferation. It also has a somewhat simpler set-up process that includes the ability to automatically determine what other BT devices are in range and what services each provides, and then to begin communications with them. A local BT network, called a piconet, can consist of up to eight devices. Piconets can then be chained together into scatter-nets to support greater numbers of devices over larger areas. Because of the likely widespread use of BT-enabled mobile communications devices and the dynamic self-discovery capability, security is of paramount importance in BT networks. The BT specification does provide for some security during device discovery and data transmission.

BT devices operate in the industrial, scientific, and medical (ISM) band (2400–2483.5 MHz). It is a globally available, license-free band and has many non-BT users. The BT system, or any other system that would use the ISM band, must therefore be very robust. BT devices use 79 specific frequencies. To keep interference on any one channel from stopping the flow of data, each BT radio in the piconet hops

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between 79 channels. The sequence of this hopping is known by each member of that piconet. A piconet is defined as a network of BT radios—a master with up to seven slaves. Outsiders to this piconet must “join” the piconet before being able to communicate within that piconet. The sequence length is 2^{27-1} . This sequence repeats, at most, once per day, making it impractical to listen for a repeat of the sequence. However, given enough receivers at different locations in the sequence, it may be possible to determine the sequence, “listen in,” and capture data.

The BT specification outlines the algorithm that is used in generating the hop sequence; however, unless the master’s BT device address is known, along with the other parameters used to determine the hop sequence, the specific hop sequence being used is difficult to determine. The slave device does obtain these parameters from the master, but the method that each slave device uses to obtain these parameters requires that their presence be revealed to the master device, and the master device must allow them to participate in the piconet.

If the device can be present prior to the formation of the piconet, it may be possible for an adversary device to obtain the BT device address of one of the slave devices by acting as a master, connecting with the slave, then dropping the connection. The adversary’s device will then configure itself to act as a “ghost” slave using the real slave’s BT device address. This is essentially having two slaves with the same address. If the master reaches this “ghost” slave before the real slave, it will begin a conversation with it and send all the required data for the device to track the hopping sequence. The “ghost” device can then terminate the conversation while still tracking the hopping sequence. The master will then reach the real slave device and reestablish a conversation with it. Subsequently, the “ghost” device should be able to monitor the conversation. However, it should be noted that this assumes that the master will discover the “ghost” slave before the real slave.

Since knowing “the sequence” is required to perform any communications within the piconet, it is difficult to listen in or to disrupt. Transmitting on any given channel will cause only a few bit errors, which will be corrected. The more frequencies that are jammed, the lower the data throughput will be. If all of the 79 frequencies are jammed, communications can be stopped.

A possible weakness exists when the host user is not notified when a new slave joins the piconet. In other words, the user of the equipment may not be notified. This may be mitigated by having all notifications enabled.

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In the BT protocol, authentication and privacy are handled in the software protocol layer as well as the physical layer. In addition to 79-channel frequency-hopping, the BT standard uses the publicly available encryption and authentication algorithm SAFER+, which provides authentication through a challenge/response system with key lengths of 8–128 bits. Key management is left to the software layers. It is worth noting that SAFER+ is rumored to have been broken. For highly sensitive applications, the BT group recommends utilizing more advanced algorithms in the network transport or application layer.

In addition to these software layer protections, BT devices can be specified to require authentication and can be set up to communicate only with specific devices.

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49168

Spectral Tagging

H. A. Smartt

Sandia's purpose in this project is to examine the feasibility and application of spectral tagging, particularly in the near-infrared (NIR) region. Uniquely tagging an item is an area of interest and need in the prevention of nuclear smuggling, safeguards and security, nonproliferation, and materials management.

The activities associated with this project were to examine the spectral signatures of various powdered minerals and to determine which minerals could be used for unique identification. We added the minerals to paint and studied the modified signature. The results of this project include a list of minerals that are unique in the NIR, spectral signatures of the minerals combined with paint, and conclusions concerning the feasibility of unique identification based on spectral tagging.

Spectral tagging involves placing unique signatures on a container or item to identify and track them. The project capitalized on the emerging field of remote sensing, but had the distinct advantage of locating a signature known only to the investigators at a specific location. The advantage is that the spectral tag is mechanically integrated with the container or item without alerting adversaries (for example, by modifying the spectral signature of the paint), and the tag is queried with a spectrometer.

This project investigated a layer of security that was not obvious and was therefore easy to conceal. The result is a tagging mechanism that is difficult to counterfeit.

We examined the U.S. Geological Survey (USGS) spectral database for minerals that had unique signatures in the 0.5–0.9 μm region. From this list, we chose several minerals, mostly based on availability, and purchased them at a mineral store. We analyzed the rock segments with the spectrometer to verify uniqueness in the desired band (0.5–0.9 μm) or visibility to NIR. The purchased minerals appeared differently from those in the USGS spectral database. This is due to the variety of exact compositions of minerals. We narrowed the list to the couple of minerals, olivine and lapis lazuli, that remained unique in the region of interest. The minerals were powdered by the Geology Department at the University of New Mexico. Grain size of minerals is important. Reflection tends to go up as a result of decreasing grain size. We saw this with both minerals—both had increased reflection with decreased grain size.

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In parallel to the above effort, we analyzed various paints using the spectrometer. We originally assumed that the paint should have low reflectivity so the minerals would stand out more and chose flat Army-green paint.

We next mixed the minerals with the paint and studied it with the spectrometer. The mineral/paint mix did not appear much different from the paint mix alone. Further research explained that absorption is dominant, not reflection. Therefore, the darker-colored nonreflecting paint absorbed the light before the light could reach the minerals.

As a result of the above discovery, we tested different paints with high reflectivity (at least in some region of our spectrum) with the lapis lazuli and olivine so the mineral absorption could stand out. We added lapis lazuli to red paint, light blue paint, dark blue paint, and orange paint. We added a large concentration to the red paint, which caused the color to shift to purple. The light blue paint mixture became lighter. The orange paint mixture remained visibly nearly the same, and the dark blue paint mixture remained identical to the eye. We added the olivine to the orange paint, which caused it to become lighter. Different concentrations and mineral colors (olivine was almost white, and lapis lazuli was blue) had different effects on the visible colors of the paints. By lowering the concentration and/or matching the mineral color to the paint color, the tagged paint sample can remain the same visible color as the paint sample alone. The mineral additives were apparent using the spectrometer in all the mixtures. Therefore, the project succeeded in demonstrating the feasibility of tagging an item with a mineral and not necessarily affecting the visible (to the human eye) colors.

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49864

Aviation Security

M. K. Snell, J. E. Parmeter, D. W. Murray, F. A. Bouchier, S. E. Jordan, C. L. Rhykerd, Jr., K. L. Linker, D. W. Hannum

The events of 9/11 demonstrated the importance of airport security to the nation. As the nation's recognized leader in airport security, Sandia has the opportunity to advance the state of the art for airport security and to assist the nation in immediately implementing technologies developed over the last decade. Most airport technologies have remained the same for many years. Advances in computing capabilities, including much faster processors, image-processing techniques, and signal processing, hold the potential to significantly increase the effectiveness of current and planned technologies. In addition, most detection technologies today are used in isolation, and thus are easily defeated. For example, success in increasing the probability of contraband detection lies in using complementary technologies in parallel. Given the defeat mechanisms for most x-ray technologies, particle/vapor technologies offer excellent compensation.

This project focuses on three critical technology areas: (1) security modeling and simulation of the commercial aviation system with a primary focus on airports, (2) using the Sandia explosives preconcentrator and detection technologies for checked-baggage screening, and (3) software and hardware enhancements for commercial x-ray systems to provide automatic indications of dangerous contraband in baggage.

We identified the benefits of the integrated computed tomography (CT) system, which combines multiple technologies, i.e., CT, dual-energy x-ray, chemical trace, radiation monitoring, and quadrupole resonance as the following:

- (1) Reduces the nuisance alarm rate
- (2) Increases the probability of detection of explosives
- (3) Reduces the time to perform a baggage scan
- (4) Reduces the overall size of the system
- (5) Reduces the cost of the system
- (6) Adds the capability to scan for terrorist nuclear weapons.

The benefits of a prototype system to screen baggage for both explosives and radioactive materials are the following:

- (1) It detects several common high explosives (HE), including TNT (2,4,6-trinitrotoluene), RDX (cyclomite), PETN (pentaerythritol tetranitrate), NG (nitroglycerin), and AN

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(ammonium nitrate). Sensitivity to particle contamination should be at the subfingerprint level (a “typical” fingerprint contains on the order of 10–100 μg of HE). Sensitivity to vapor should be at or near the parts per billion (ppb) level. This would mean that vapor detection of TNT, NG, and AN is realistic, while detection of RDX and PETN will rely on particle detection.

(2) Screening speed will be 450 bags per hour, or 7.5 per minute. This would make the system speed compatible with current x-ray screening systems.

(3) Bags will move through the system on a conveyor belt, as is the case with current x-ray systems. The system could be inexpensive enough to be developed as a stand-alone system to be deployed at airport check-in counters, or fitted with a conveyor belt and integrated with the baggage-handling system.

The benefits of modeling and simulation to aviation security fall in the area of distributed simulations, allowing simulations of various subsystems and security personnel to participate in simulations of security-related events (e.g., closing concourses for various reasons).

The risks of the three systems were similar: technical feasibility, cost, and length of time to achieve the objectives.

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50000

Protection of Sensitive Computers

S. T. Jones, T. Q. Thai, V. E. Echeverria, IV

This is a classified project.

50395

Assessment and Identification of Appropriate μ Power Technologies for μ Sensors and Other Applications

A. C. Marshall, W. K. Schubert, C. P. Tigges, D. Ingersoll, J. J. Hudgens

Micropower sources are critically needed in several project areas of strategic importance to Sandia: microsensors, micro-mechanisms, and meso-/microrobotics. Multiple research efforts are under way in the laboratory to develop micropower devices. These incorporate a large range of approaches from radioactive sources to fuel combustion to electrochemical energy storage, and beyond. How these devices will be married to the applications that require them is problematical, however. The specifications, requirements, and permissible tradeoffs for micropower sources have not been clearly defined. Past and present work has not necessarily covered the performance space that will be required by future microapplications. This project will do the following: (1) carry out a comprehensive assessment of what microsystems of the future will require from power/energy sources, (2) assess what ongoing research and development micropower devices are capable of, and identify how they can or cannot meet the requirements of Sandia and other National Nuclear Security Administration (NNSA) microapplications needs, and (3) make recommendations on the direction of future funding for micropower studies and generate performance specifications and requirements, including environmental specifications.

Our approach will be to perform a literature search, review ongoing research programs within NNSA laboratories, and interview scientists and system developers both internal and external to Sandia programs, with a focus on systems important for national security missions.

We completed a very broad survey of potential micro- and mesopower sources and components. We completed concept summaries and Ragone plots for most power sources and power-conversion technologies. Summaries include advantages and issues, maximum power and energy densities, specific power and specific energies, concept options, technical risk, and development level (within 5 years, within 10 years, and ideal.) We are developing system-level Ragone plots for comparison with projected needs. The system-level comparison is developed by combining specific power and energy data for various components and energy sources. Comparison of

Micropower sources are critically needed in several project areas of strategic importance to Sandia: microsensors, micromechanisms, and meso-/microrobotics. Multiple research efforts are under way in the laboratory to develop micropower devices.

projected needs with possible sources includes comparisons of development time and required date for micropower sources and includes other factors and considerations.

50973

Multispectral Data-Exploitation Advancements

B. R. Stallard, R. L. Bilisoly, J. C. Davidson, N. D. Fabian, B. N. Post, J. G. Taylor

As more multispectral and hyperspectral sensor systems become available, there is great potential for gain in integrating the data from the same or different sensors to extract additional information. Each sensor brings some unique capability such as spatial resolution, spectral region, spectral resolution, temporal information, etc. Typically, each multispectral or hyperspectral sensor utilizes one or many registration techniques to perform interband registration for that sensor's data. The accuracy required and achieved for this interband registration varies, depending on the sensor and the application of the data. This project is an effort to provide the initial piece for a future toolkit suite that can be used to automate and integrate multisensor multitemporal data for further analysis. This effort will concentrate on multitemporal data from the multispectral thermal imager (MTI).

In the first quarter of 2002, the progression of the MTI satellite across the Earth gradually slowed, coming to an apparent halt sometime in March before reversing its procession (retrograding) from west to east across the Earth. During this unique event, the MTI satellite had the historic and unprecedented ability to image a ground target on consecutive days for up to a month. This provided an excellent opportunity to collect multitemporal datasets.

The goal was to get 0.25-pixel overlay accuracy between two A-band images without human intervention. Performance evaluation would be by cross-correlation, explained below. The first task was to choose four pairs of MTI images and prepare them to fit the following ground rules: (1) coarse alignment is assumed to be about 2 pixels or better, (2) magnification error is assumed to be no greater than 0.5%, and (3) the image is no greater than 500 pixels on a side. All work was done by hand in environment for visualizing images (ENVI). We are assuming that registration is already in the ballpark and are focusing on fine alignment. We expect that the coarse alignment could be automated with the same procedure if the image were deresolved. This combined algorithm could give us a complete automated registration within two or more steps.

These are the steps for coarse hand registration:

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(1) Z value transform, if needed (example: atmospheric correction, edge detection).

(2) Orthorectification, if needed (could be as simple as perspective correction, assuming flat Earth).

(3) Coregistration of band images—use PRISM (Polymer Reference Interaction Site Model) for now.

(4) Chip to about 100 to 400 pixels on a side from a single sensor chip assembly (SCA). Warp should be 20% larger on a side than the reference.

(5) Coarse warp—use ENVI rotation/scaling/translation (RST), cubic interpolation with 5–10 manually chosen points. Save table of tie-points to pass to fine overlay.

These are the steps performed by the program produced in this project:

(1) Intensity standardization between the two scenes. This was done by histogram parameter fitting between the two scenes. The degrees of freedom were gain and offset for the warp image. This should account for atmospheric transmission, atmospheric scattering, sensor calibration, and small differences in sun illumination.

(2) Explode the pixels by five on a side (choice available) with various options for interpolation.

(3) Pick features and find their position in the warp image relative to the reference image. This step assumes that only translation is required to match local areas in the reference and warp images.

(4) Combine all steps requiring resampling into a single tie-point table.

(5) Model and fit.

(6) Output the warped image that is trimmed to the same size as the reference image.

We stress that resampling is done only a single time, starting with the original warp image. The procedure lends itself to tiling so that an entire large image may be processed in pieces and then stitched together. One should give some thought to smooth transitions in Z values at the tile edges, but the main work is done by this project.

A team member suggested breaking the image into regular segments, e.g., 25 (5 on a side), and then finding which segments correlate between the reference and warp image. If the correlation is high, it should be retained, and if poor, it should be ignored. Hence, we do not use all of the possible 25 tie-points, but only those that have a correlation above a selectable threshold. We also explored other schemes for selecting the tie-points. This approach suggests that our program could be used for interband coregistration of a single

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image. While many features do not appear the same in all wavelength bands, there are usually a significant number of highly correlated regions between certain bands. Our project uses only the good regions to overlay the various band images. The computer could produce a new scheme for each image, where certain bands were aligned to certain others until the whole stack was aligned.

Extremely limited performance testing indicates about 0.25-pixel registration error. The performance number has to be confirmed, and it is very possible that performance will improve with small tweaks to the program.

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51538

Response Analysis Tactical Simulation

J. W. Purvis, N. M. Winowich, J. F. Jones

The events of 9/11 increased the need for easily usable vulnerability-assessment tools to be used in the fight against terrorism. Present vulnerability-modeling technology ranges in two extremes: a very simple model, ASSESS (Analytical System and Software for Evaluating Safeguards and Security–Neutralization Module), to a very complex model, JTS (Joint Tactical Simulation.) Neither of these two models can be used in the field to rapidly and accurately determine the probability of a resident guard force's or response force's ability to defeat a dedicated terrorist attack with the goals of sabotage or theft of nuclear assets. ASSESS is too simplistic to adequately cover the complexity of a terrorist attack, and JTS requires multiple operators, digitization of complex terrain, and extremely rigid quality controls to obtain accurate results. To fill this void, Sandia developed a new simulation tool—RATS (Response Analysis Tactical Simulation). RATS is an EXCEL-based tool that can be used easily in the field to obtain valuable insight into a facility's ability to defend against terrorist attacks. RATS uses a digitized representation of a facility and can model response forces, terrorists, vehicles, helicopters, many common military firearms, and explosives. The tool can be run in the batch mode to obtain valuable statistics and perform sensitivity analysis. We will debug the code, document the analytical engine calculations, and expand the weapons databases that are used by the code. Completion of this code will enable Sandia to respond rapidly to the multitude of vulnerability-assessment requirements and significantly expand our ability to assist in the fight against terrorism.

The tool is operational and has already been used in a limited version with a revised format to investigate options. We enlisted specialists in certain disciplines vital to the accuracy of the tool, such as small-arms effectiveness experts, to review and correct the databases used in the tool. These specialists determined a more efficient method of storing and accessing arms data and also contributed a comprehensive but unclassified and unrestricted database for use in assessments. Preparation of a user's manual and a technical description manual are under way. Refinement of the set-up and engagement models used in the tool led to the preparation of another software model that may also be either patentable or copyrightable. International Training Course personnel have

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also expressed interest in using some of the concepts in the RATS methodology in their training programs. We expect to file two or more technical advances.

51541

Optical Tagging Technologies

M. R. Ackermann, M. E. Warren, J. P. Wilcoxon, T. J. Drummond

In this project, Sandia seeks to make a preliminary assessment of materials and technologies suitable for use in a liquid-based optical tag. The basic idea is to mark an object with some liquid that can either dry or remain moist (or oily). Later, through optical means, the object can be queried and simple imaging optical detectors used to determine if the object in question was the one tagged.

We explored material combinations suitable for use in either the ultraviolet (UV), short-wave infrared (SWIR), or near IR (NIR) portions of the spectrum. We found a number of materials with properties suitable for eventual use in an optical tag.

We investigated several material systems for use as a nonvisible optical tag. The primary materials of interest were nanoparticles of metals and semiconductors; these materials could be engineered to fluoresce in the NIR and SWIR. As an alternative, we also examined materials systems that could give either a high contrast or unique signal in the UV.

In our UV work, we identified a number of materials systems already in use for optical marking (not necessarily tagging) in private industry. However, not confining our investigation to commercial products, we identified a small number of readily available commercial materials that could be adapted to making a UV optical tag. One available polymer binder identified has a rather unique signature in the UV, varying from highly reflective to highly absorbing over about a 50 nm range of wavelengths. This material could give a very unique signal and easily be queried by a two-color UV system.

We also looked at possibilities for including rare-earth (RE) oxides in some form of paint or binder to form a unique tag operating primarily in the NIR. Here there are a myriad of possibilities, and the RE oxides give a sufficiently narrow absorption line that various combinations of several dozen materials could give roughly the equivalent of a hyperspectral bar code, easily observed by simple spectrographic equipment.

For operation in the SWIR, our goal was to identify materials that would fluoresce when illuminated by one of the common SWIR laser wavelengths. The fluorescence had to be at a longer wavelength than the illumination, but sufficiently close that common detector technology could be used. The material technology selected consisted of nanoparticles of metals and various semiconductors.

Sandia seeks to make a preliminary assessment of materials and technologies suitable for use in a liquid-based optical tag. ...We found a number of materials with properties suitable for eventual use in an optical tag.

We chemically fabricated and tested a few material samples. While additional work and more measurements are required, results of laboratory measurements indicate that solutions containing nanoparticles of metals and semiconductors suspended in an oil-like binder are environmentally stable and do fluoresce in the SWIR. They could eventually be engineered into some form of optical tagging technology.

...results of laboratory measurements indicate that solutions containing nanoparticles of metals and semiconductors suspended in an oil-like binder are environmentally stable and do fluoresce in the SWIR.

52216

Thermobaric Weapons Signatures

L. A. Boye, J. D. Corey, M. J. Kaneshige, R. D. Wickstrom

Thermobarics is an important new class of highly energetic explosive materials that were first developed by the Russians for urban warfare. Somewhat different from classic high explosives (HE), these systems are considered volumetric explosives and are similar to fuel air explosives (FAEs), a single-detonation event that is distributed over a large volume. These materials burn brighter and longer than conventional explosives. Thermobarics are designed to enhance blast overpressure conditions, which results in localized atmospheric-oxygen depletion. As a result, explosive chemistry of the event differs from that of conventional explosives, and observable signatures may be altered. As an organization nationally recognized for its expertise in detection of transient electrooptical events, Sandia provided in this project a means to gain knowledge of the optical signatures of these highly energetic materials (EMs) for development of subsequent discrimination techniques of thermobarics from other explosive events. This project seeks to understand thermobaric material content, and to identify the current use and testing of such materials and/or systems. Through these efforts we analyzed some signatures collected during thermobarics testing, to collect radiometric signatures of explosive calibration events for the identification of distinguishing characteristics of thermobaric materials from C4 and Comp-B, and to identify a series of tests that can provide an opportunity for future radiometric signature collection.

The research conducted on thermobaric weapons systems through this effort encompassed many areas: literature searches, communication with military and government personnel, explosive-test signature assessment, radiometric equipment deployment and signature collections at interior chamber explosive testing, and test planning for future radiometric deployment at interior and exterior testing.

Sandia's thermobaric project personnel reviewed signatures collected by systems of recent thermobaric event tests to assist in analysis. Sandia developed guidance for the incorporation of relevant parameters in the analysis efforts and in the assessment and successful interpretation of these signatures.

We conducted several explosive calibration tests ranging from 50 to 500 grams of explosive. These events provided a unique opportunity for "piggy-back" radiometric equipment deployment and optical signature collection, which have never

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before been conducted under these conditions. The optical data collected thus far show potential for materials identification and explosive parameter scaling. The optical collections are a unique complement to the suite of typical temperature and pressure measurements currently conducted at Sandia.

Other Communications

Boye, L. A., J. D. Corey, and M. M. Hoffman. 2002. Thermobaric weapons LDRD: Review of Sandia explosive signatures collections. Briefing to Lt. Col. Tom Ward, USAF, and Mr. Eric Rheinhardt, DTRA, 26 July, Albuquerque, New Mexico.

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52974

Class B Fire-Suppression Capabilities of a Modified Sandia CBW Decon Foam

R. G. Betty, M. D. Tucker, C. V. Williams

Sandia developed a nontoxic, noncorrosive aqueous foam with enhanced physical stability for the rapid mitigation and decontamination of chemical/biological weapon (CBW) agents. This technology is attractive for the protection of the nuclear weapons facilities, as well as for civilian and military applications for several reasons, including (1) it requires minimal logistics support, (2) a single decon solution is effective on both CW and BW agents, (3) mitigation of agents can be accomplished in bulk, aerosol, and vapor phases, (4) it is deployed rapidly, (5) it exhibits minimal health and collateral damage, (6) it is relatively inexpensive, and (7) it has minimal run-off of fluids and no lasting environmental impact. The foam can be delivered by a range of methods, including systems that yield desirable properties for fire-suppression foams.

The Sandia decon foam was effective in extinguishing Class A fires, but not Class B fires. Extinguishing of Class B fires is important because terrorists use petroleum products as accelerants. We identified surfactants that show promise in being effective against Class B fires and are compatible with the Sandia decontamination formula. This work includes addition of these surfactants to DF-200 and testing for CBW and fire-suppression capability.

This research will have three primary benefits to Sandia, including the following:

(1) Expand the understanding of the basic phenomenology underlying Sandia decon foam technology through a preliminary assessment of its properties in these novel environments.

(2) Initiate a new line of research in the interaction between fire and low-water-content foam, thus extending Sandia's basic understanding of fire phenomenology that underlies many nuclear weapon certification efforts.

(3) Establish a new technological approach within the overall technology base available for the protection of critical nuclear weapon facilities.

We used three modified formulations for CBW surrogate testing for destruction of chemical-agent simulants for HD, a mustard gas, and VX, a nerve agent. The results of the modified formulation that demonstrated the most favorable destruction of phenyl mustard, a surrogate for HD mustard, were 14%, 51%, and 83% destruction at 1, 15, and 60 minutes, respectively. The

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most favorable results for the destruction of the VX surrogate, O,S-diethylphenylphosphonothioate were 32%, 60%, and 84% destruction at 1, 15, and 60 minutes, respectively.

The modified formulations did not meet the efficacy for CBW simulant neutralization at the level of DF-200, the current decontamination technology of choice. DF-200 performs as follows: for destruction of the mustard simulant, 55%, 91%, and 100% destruction at 1, 15, and 60 minutes, respectively; and for destruction of the VX simulant, 79%, 99%, and 100% destruction at 1, 15, and 60 minutes, respectively. Because the modified formulations did not meet the efficiency of DF-200, we decided not to pursue the testing of the fire-suppression capability at that time.

Pulsed Power Sciences

The Pulsed Power Sciences investment area researches concepts and technologies for advanced pulsed-power systems and applications critical to important DOE and national priorities. Our mission is to support experimental and computational capabilities for application to stockpile stewardship, emerging threats, basic science, industrial competitiveness, and future energy production. Pulsed-power research includes all aspects of pulsed-power technology, electromagnetics (EM), and devices to convert EM energy into directed particle beams and into Z-pinch implosions and magnetically driven shock physics.

Advanced computer codes developed under the Accelerated Strategic Computing Initiative (ASCI) are being used to understand the mechanical behavior of new nanomaterials. These materials must be studied at the mesoscale where the material behaves as a system of distinct grains with individual properties. Currently, there are no high-fidelity dynamic data for the mechanical properties of individual grains for comparison with these simulations. The purpose of the "Determination of Microstructural Properties with Isentropic Compression" project is to

demonstrate the ability to detect microstructural and defect properties of well-characterized single crystals using the recently developed Isentropic Compression Experiment (ICE) method on the Z and Saturn accelerators. This technique might also be applied to LIGA (the acronym for the German words for lithography, electroforming, and molding) materials, welded and brazed joints, and aged materials.

28763

Use of Intense Ion Beams for Surface Modification and Creation of New Materials

T. J. Renk, G. A. Torres, G. A. Mann, P. P. Provencio

Pulsed intense ion beams can be used to modify material surfaces through fast heating, followed by equally fast quenching, or to create thin films by ablating target material and depositing it onto other surfaces. A detailed understanding of the modification process requires materials science-based analysis. Unlike pulsed laser deposition (PLD), which also provides a high kinetic energy process for modifying materials, ion beams can lead to much higher production volumes. Applications chosen for this evaluation have potentially high payoff for the neutron tube (NT), materials programs, and pulsed-power programs. Improvements to source and target films in NTs can significantly improve NT performance and life span. Successful formation of high-dielectric constant thin films of barium titanate oxide (BaTiO_3) can lead to more compact energy-storage devices.

The surface alloying and hardening of platinum (Pt) into titanium (Ti) shows strong improvement in wear characteristics; we initiated further work to understand the microstructural changes that lead to this performance enhancement. In addition, we are alloying hafnium (Hf) into Ti to compare the performance and microstructure with the Pt/Ti system. The use of the ion beam to ablate and redeposit coatings produced interesting results. The deposition and post-annealing of yttrium-barium-copper oxide (YBCO) superconducting film look promising in the initial experiments. We found a highly oriented layer after the post-processing, a necessary requirement for superconducting performance. A BaTiO_3 layer suffered premature breakdown upon voltage testing, apparently due to a porous structure to the thin film. We will again attempt to produce a higher-density BaTiO_3 layer. We produced metallic thin films of Pt and erbium (Er); cross-sectional transmission electron microscopy (XTEM) studies confirm that the grain structure of both films is nanocrystalline. This is presumably because the high deposition rate (> 100 A/pulse) produces contiguous layers, unlike conventional techniques like sputtering, or even PLD, which produces columnar grains. The fine grain structure of Er is promising because the layer may be better able to retain helium (He), which is proving to be a problem with current NT target films. We produced an Er layer doped with aluminum (Al) and are now studying it. Prior

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Russian work funded by Sandia indicated that addition of Al to Er reduces He migration. The ion-beam ablation method provides a potentially easy way to dope Er with Al.

Refereed

Renk, T. J., and R. Peterson. 2001. Chamber dynamic research with pulsed power. *NIM A* 464:172–79.

28764

Low-Intensity Laser Triggering of Spark Gaps

G. M. Loubriel, F. J. Zutavern, M. W. O'Malley

Extremely low energy (< 1 mJ) laser-triggered spark gaps have been demonstrated by injecting magnesium (Mg) aerosol particles into the gap. This result could revolutionize optically triggered gas-switching technology by enabling direct control of plasma breakdown-based systems such as high-power spark-gap arrays with remote, optically isolated semiconductor or fiber-optic lasers. This project seeks to demonstrate this effect and study the viability of using such a system to reduce laser-energy requirements for future pulsed-power inertial confinement fusion (ICF) drivers and other optically triggered spark-gap systems. Sandia seeks a low-level effort since we have suitable lasers and diagnostics (harmonic generation of $1.06\text{ }\mu\text{m}$ Nd:YAG or tunable titanium-sapphire [Ti:sapphire] with 200 fs to 15 ns pulsewidths, and fiber-amplified or gain-switched semiconductor lasers with pulsewidths as short as 30 ps under development), a variety of spark-gap housings, and a generator for the Mg aerosol particles. The idea is to suspend a very low density ($10^5/\text{cc}$) cloud of 100 nm size Mg particles in an argon (Ar)/SF₆ gas mixture and then illuminate the gap with unfocused laser radiation. The effect of the laser is to generate seed electrons by photoemission from the Mg particles, which then allow for a multichannel discharge. Our unique contributions to this research would be advanced spark-gap technology, short-pulse laser technology (solid-state, semiconductor, and fiber lasers), and a wide range of electrical and optical diagnostics for modeling and optimizing optical triggering. Since this is a nonlinear process, shorter, higher-power optical pulses may decrease the optical energy requirement and/or improve triggering stability. This is a proof-of-principle experiment that we believe can be achieved at low cost.

We designed, assembled, and tested a pulsed-power system (thyatron-switched capacitive discharge through a pulse transformer). We purchased and modified a new optically triggered spark gap to provide variable gap lengths and an optical viewport for optical diagnostics.

We acquired the aerosol-generating components, and they are ready for testing. We aligned a 100 mJ, tunable, Q-switched, Ti:sapphire laser and calibrated it in energy, wavelength, and pulsewidth. We installed frequency-doubling and -tripling crystals optimized for 1 mm and procured crystals for 800 nm.

While testing harmonic generation and aligning the ultraviolet beam to the spark gap, the laser flashlamps stopped simmering.

This result could revolutionize optically triggered gas-switching technology by enabling direct control of plasma breakdown-based systems such as high-power spark-gap arrays with remote, optically isolated semiconductor or fiber-optic lasers. This project seeks to demonstrate this effect and study the viability of using such a system to reduce laser-energy requirements for future pulsed-power inertial confinement fusion (ICF) drivers and other optically triggered spark-gap systems. ...Our unique contributions to this research would be advanced spark-gap technology, short-pulse laser technology (solid-state, semiconductor, and fiber lasers), and a wide range of electrical and optical diagnostics for modeling and optimizing optical triggering. ...This is a proof-of-principle experiment that we believe can be achieved at low cost.

28769

Z-Pinch Power-Plant System Development

G. E. Rochau, S. A. Slutz, P. C. Mickey, C. L. Olson, M. S. Derzon, R. E. Olson, W. A. Stygar, A. R. Parker, K. W. Struve, C. W. Morrow

The Z-Pinch Power Plant (ZP-3) is the first concept to use the spectacular results at Z in a power-plant application. While the initial concepts and calculations applying high-yield fusion look very promising, there are significant technical issues to be addressed. The highest-priority issues are system studies for creating a definition of the system, integrated blanket design for absorbing the fusion energy, cartridge manufacture of all the recycled materials, and cartridge installation/replacement to maintain a reasonable duty cycle. An effective system design for ZP-3 requires (1) an integrated blanket, which can shield the permanent structures from the high-energy neutron flux and the strong shock wave, then breed tritium, and (3) in the process absorb the released fusion energy. Through this technique, Sandia intends to minimize the shock propagation by dispersing the energy absorption over the volume of the blanket structure. The generation of this energy requires a fusion fuel cartridge to couple the repetitive pulsed power to a replaceable load using a recyclable transmission line (RTL). Innovative engineering will be required to economically manufacture the required cartridge. The ZP-3 represents a fifth-generation nuclear-power source without the burden of long-lived radioactive waste or nuclear proliferation. As such, this system description will provide a cornerstone for launching a concept exploration initiative in fusion energy and potentially lead to large experimental and pilot facilities.

Sandia's specific objective for current work was to identify high-current pulsed-power driver designs and repetition rates (rep rates). We delayed work on this project until the next fiscal year because of programmatic conflicts. In the interim, review of Russian research indicates the availability of low-cost linear transformer drivers (LTDs) that will reduce the capital cost and improve the availability of driver systems. Sandia has experience with LTDs from other work being done by the pulsed-power group. Thus far, we have accomplished the following:

- We developed a detailed road map of studies that will lead to an IFE (inertial fusion energy) for RTL manufacture and steel system recycle and for a tritium cartridge and associated assembly.

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- We refined the design of the RTL insertion mechanism, including equipment movement, electrical connection, and vacuum maintenance, while protecting permanent equipment from blast damage.
- We refined the design of a high-energy-yield driver technology for six shots/minute (in process).
- We began a detailed analysis of the RTL structure, including mass and strength.

Refereed

Rochau, G. E., C. W. Morrow, C. L. Olson, P. J. Pankuch, P. F. Peterson, E. I. Mogahed, I. E. Golovkin, G. L. Kulcinski, R. R. Peterson, I. N. Sviatoslavsky, and M. E. Sawan. 2002. Containing IFE pulses in a Z-pinch-driven power plant. Paper presented at the 2nd IAEA Technical Meeting on Physics and Technology of Inertial Fusion Energy Target and Chambers (17–19 June, San Diego, California).

Rochau, G. E., G. L. Benavides, M. S. Derzon, C. L. Olson, R. E. Olson, A. R. Parker, G. A. Rochau, S. A. Slutz, K. W. Struve, P. J. Pankuch, C. R. Gibson, C. W. Morrow, P. F. Peterson, J. S. DeGroot, H. D. Tran, E. A. Mogahed, I. E. Golovkin, G. L. Kulcinski, R. R. Peterson, I. N. Sviatoslavsky, and M. E. Sawan. 2002. ZP-3, a power plant utilizing Z-pinch fusion technology. *Proc. Inertial Fusion Science and Applications: State of the Art 2001* (September, Kyoto, Japan): 706–11.

28770

Recyclable Transmission Line Concept for Z-Pinch IFE

S. A. Slutz, W. A. Stygar, G. E. Rochau, C. L. Olson, R. B. Spielman

Sandia accomplished a rapid development of Z-pinch loads on the Z-machine, which led to outstanding progress in the last few years, resulting in radiated powers of 280 TW in 4 ns and a total radiated x-ray energy of 1.8 MJ. The goal of this project is to demonstrate single-shot, high-yield fusion capsules. Inertial fusion energy (IFE) requires a repetition-rated (rep-rated) capability. Recent developments led to a viable conceptual approach for a rep-rated Z-pinch power plant (ZP-3) for IFE using a recyclable transmission line (RTL) to provide the necessary standoff between the fusion target and the power-plant chamber. In this approach, a portion of the transmission line (the RTL) near the capsule is replaced after each shot. The RTL should be constructed of materials that can be separated easily from the liquid-coolant stream and be refabricated for subsequent shots. One possibility is that most of the RTL is formed by casting fluoride lithium beryllium (FLiBe), a salt compound, which is an attractive choice for the reactor coolant, with chemically compatible lead (Pb) or tin (Sn) on the surface to provide conductivity. Another possibility is ferritic steel, which is immiscible in molten FLiBe. We need to determine if transmission lines constructed from these materials using rapid, inexpensive fabrication processes will efficiently transport electrical power at the large currents required of a fusion driver. This project will investigate the power-flow characteristics of several candidate RTL materials, the structural integrity of the RTL, design of appropriate high-yield targets to connect to the RTL, and an initial plan to develop Z-pinch IFE. We will conduct power-flow experiments first on the SATURN accelerator at 10 MA to study electrical turn-on and electrical conductivity characteristics of various candidate RTL materials. We plan future studies of RTL structural integrity, design of high-yield targets to connect to the RTL, and an initial plan to develop Z-pinch IFE. This project is leading into a large-scale energy program on Z-pinch IFE.

We completed the SATURN experiment to test the low-mass limit for the RTL concept. Based on RTL electrode motion due to the B field, calculations show that the RTL mass could be as low as 1 kg (compared to 5 tons for the Z magnetically insulated transmission line [MITL]). Such low-mass electrodes would have a thickness an order of magnitude less than one

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resistive skin depth. SATURN experiments at the 10 MA level measured the electrical-conductivity properties of 25 μm Mylar, and 50, 100, and 250 μm carbon steel. The results scale to show that for a power plant, an RTL mass as low as 2 kg could be used, and that with an RTL mass of 80 kg, the resistive losses would be very small (10%). This is good news for the RTL power-plant concept.

We worked on the development of a suitable high-yield target concept for Z-pinch IFE. We envision a target with a yield of 3–4 GJ and performed a series of one-dimensional (1-D) Lasnex calculations on the dynamic hohlraum concept. In this concept, a Z-pinch wire array collapses onto a cylindrical foam that contains the spherical fusion capsule at its center. As an example of present calculations, we use an initial wire-array radius of 5 cm with a wire mass of 45 mg/cm. The initial capsule radius is 0.49 cm, and it contains 26 mg of solid deuterium-tritium (DT). For a driver current of 95 MA, approximately 45 MJ of x-rays are produced, 9.1 MJ of x-rays are absorbed in the capsule, and a yield of 3.8 GJ is obtained. These are very acceptable values for a ZP-3. We are now directing work toward the key issue of radiation symmetry. We started to investigate the structural integrity of thin ferritic-steel RTLs to the vacuum differential pressure expected in a power plant. For a cylindrical coaxial RTL, we found that for the case of a vacuum in the RTL, and atmospheric pressure inside the inner cylinder, the inner cylinder remains intact due to the acceptability of the hoop stress. The outer cylinder will buckle unless the outside pressure is on the order of a few Torr. This means that for thin ferritic-steel RTLs, the power-plant chamber operating pressure should be in the few Torr range. We are determining what research elements are needed for a long-range plan to develop Z-pinch IFE.

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Refereed

Slutz, S. A., C. L. Olson, and P. Peterson. 2002. Low-mass transmission lines for Z-pinch inertial fusion energy. *Physics of Plasmas*, submitted.

Other Communications

Olson, C. L. 2002. Z-pinch IFE. (Invited) Paper presented at 19th Symposium on Fusion Engineering, 22–25 January, Atlantic City, New Jersey.

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Olson, C. L., *et al.* 2002. Z-pinch IFE. (Invited) Paper presented at BEAMS DZP 2002, 24–26 June, Albuquerque, New Mexico.

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28771

Suppression of Electron Emission from Conductors

D. J. Johnson, W. A. Stygar, K. W. Struve, W. E. Fowler, D. H. McDaniel, J. L. McKenney

This research effort consists of testing surface-treatment processes on 304L and 316L stainless steel (SS) and anodized aluminum (Al) for the purpose of suppressing electron emission over large planar surface areas to improve the high-voltage (HV) hold-off capabilities of the materials. The work with SS is relevant to the vacuum transmission line near the final power-flow section on the Z accelerator. Improvements to voltage holdoff with SS will allow smaller transmission line spacing and lower inductance in the final convolute region. This reduction results in higher currents to the Z-pinch load and more efficient x-ray production. The work with Al is relevant to the Al grading rings at the vacuum insulator stack on the Z accelerator. Improved holdoff here will allow an upgrade to the power transmitted across the vacuum interface.

To allow testing at higher voltage, we designed, fabricated, and installed a 20 μH ring-up coil to increase the voltage by 50%. This gave a 1 cos pulse shape with 160 ns full-width half-medium (FWHM) and voltage peak of 260 kV. We also installed a voltage monitor to directly measure the voltage on the gap and faster current monitors. We determined the gap voltage and current to be accurate to 1% and 5%, respectively, after extensive calibrations and comparisons to Sandia SCREAMER code circuit model calculations.

We acquired HV test data for 304L SS machined to $R_a < 0.4 \mu\text{m}$ with five surface preparations. These were solvent-cleaned, electropolished, H-fired, Au-coated, and the Z-protocol combination of these. We tested the preparations for both a flat (without ring-up coil) and the 1 cos pulse. We acquired the flat-pulse data, starting at 200 kV/cm with E-field increased in 10 kV/cm steps until breakdown. We acquired the 1 cos pulse data starting at 400 kV/cm, which was near the breakdown threshold for nonelectrically conditioned electrodes, with the E-field raised in 40 kV/cm steps. The results for the hydrogen (H)-fired and Z-protocol, using the flat pulse, show improved reproducibility and a 20% increase in holdoff compared to the solvent-cleaned surface. With the 1 cos pulse, the holdoff for the Z-protocol was 20% lower than the solvent-cleaned 304L. The solvent-cleaned 316L electrodes tested gave about 10% lower results than the 304L. We determined cathode plasma

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expansion and area growth rates by assuming a Child-Langmuir space-charge limited emission from a single cathode plasma spot with area expanding and moving toward the anode linearly in time. The data indicate typical closure and area growth rates of 3 cm/ μ s and 2 cm²/ μ s. The closure rates were $\sim$ 10% higher when the breakdown occurred at a factor-of-2-higher E-field. We have to acquire more data to say conclusively if the surface treatments reduce or increase electrical-breakdown thresholds. The requirement to condition the surface by slower-rising voltage suggests that residual dust particulates are limiting performance.

Four types of SS electrodes were treated and HV tested, totaling 120 electrodes. These were 304L and 316L rod stock and 304L plate stock with and without H firing in 12 cm- and 8 cm-diameter sizes. The Institute of High-Current Electronics (IHCE) completed the HV testing of 8 cm electrodes to ensure an optimum electron (E)-beam treatment protocol. The data showed that the E-beam treatment only allows E-fields to $\sim$ 900 kV/cm without breakdown for a 50 ns FWHM duration pulse. Prior to E-beam treatment, the maximum threshold E-fields for the 304L and 316L (rod stock) electrodes were about 700 kV/cm. The electron-beam surface treatment (EBEST) + H-fired electrode holdoff increased from 900 to 1050 kV/cm, whereas the ion implantation + EBEST hold-off increased from 770 to 1170 kV/cm.

Four types of SS electrodes were treated and HV tested, totaling 120 electrodes.

Other Communications

Johnson, D. J., W. E. Fowler, M. E. Savage, and W. A. Stygar. 2002. Suppression of electron emission from large surface area stainless-steel electrodes. *Proc. 20th International Symposium on Discharges and Electrical Insulation in Vacuum* 1 (1–5 July, Tours, France): 131.

28772

Solid-State Switch for Advanced Pulsed Power

F. J. Zutavern, M. W. O'Malley

The next-generation driver for advanced pulsed-power accelerators, Z-pinch, weapons effects, or radiography could be greatly improved and simplified by the use of low-jitter, low-inductance, solid-state switches coupled to a very fast prime power stage. If successful, such a system would not require the use of gas-breakdown switches and intermediate storage capacitors or other pulse-forming lines. Sandia seeks to build and demonstrate such a high-current switch based on laser-triggered photoconductive semiconductor switches (PCSS). In this project, we are demonstrating the capability to discharge an 8 nF, 200 kV direct current (DC)-charged capacitor bank through PCSS producing 100 ns-wide 20 kA current pulses (optically triggered with 1–10 mJ). This bank will be composed of eight 4 nF capacitors, each charged to 100 kV. Optically isolated, low-inductance, high-current PCSS will connect the capacitors in series and parallel. PCSS previously were demonstrated to switch 220 kV at 8 kA[1] and 1 kV at 1 kA[2]. For 220 kV and 8 kA, we used six switches (each 3.4 cm long, 4 cm wide) in parallel to carry 8 kA for ~ 30 ns, at 10 Hz for >10,000 pulses. The 1 kV result was higher current density, longer pulses (~ 100 ns), and DC holdoff. It also demonstrated excellent switch longevity (> 1,000 pulses) and can be scaled to the voltages, currents, and size required for this application. The high-current-density scaling would result in a switch length of 6.6 cm and a width of 5 cm for the parameters of this project. The high-gain PCSS are based on a high-field (> 5 kV/cm), avalanche-like effect in gallium arsenide (GaAs) that is triggered with low-energy optical pulses. We placed particular emphasis on semiconductor trigger lasers for the PCSS, as efficient triggering improves PCSS synchronization and lifetime and reduces the overall switching-system size and cost.

We completed the following tasks to achieve our final PCSS switching goals.

We designed, fabricated, and tested a 100 kV, 200 J, thyatron-switched transformer-based test-bed and the appropriately sized PCSS required to charge, discharge, and diagnose eight 100 kV, 4 nF capacitor modules.

We planned and initiated epitaxial growth procedures for *n*- and *p*-type contacts on GaAs for large, high-voltage, long-lifetime switches. These procedures, which we derived from

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previous research on smaller low-voltage PCSS, include several new methods to improve the switches and simplify the growth process for large switches. We neutron-irradiated high-resistivity GaAs substrates to fabricate DC-chargeable switches.

After we carefully measured and analyzed the requirements for reliable multifilament triggering, we down-selected PCSS-triggering options to semiconductor laser-diode arrays (LDAs) located at each switch. We tested two sizes of PCSS at 67 kV/cm and 50 A/filament, and 15 mm-long switches at 100 kV and 7.5 mm-long switches at 50 kV.

To improve PCSS triggering and develop efficient optical triggers, we are exploring many triggering options. Sandia has developed and demonstrated the technique of using stacked, wide-stripe, edge-emitting lasers to trigger multiple parallel current filaments in PCSS. We purchased several types of stacked, wide-stripe, edge-emitting semiconductor lasers from different vendors and tested them for uniformity, output energy per laser, and PCSS triggerability. We modified and improved the electronic circuit required to drive the semiconductor lasers for higher-current and faster-risetime operation. We are determining the optimum trigger wavelength in PCSS experiments with a tunable, Q-switched, titanium-sapphire (Ti:sapphire) laser. We are pursuing potential triggering improvements with shorter laser trigger pulses using a mode-locked, 140 fs pulsewidth fiber oscillator and Ti:sapphire regenerative amplifier.

Sandia designed, fabricated, and tested a new vertical-cavity surface-emitting laser (VCSEL) for PCSS triggering that will provide the capability to fabricate trigger lasers that match the size, wavelength, and energy requirements of the PCSS. Hundreds of 1 cm-long, parallel, line-emitting lasers can be fabricated on a single wafer with VCSEL technology, eliminating the tedious task of stacking edge-emitting lasers. Presently, twelve 8-stack edge-emitting lasers and twelve $7.5 \times 7.5 \text{ mm}^2$ switches are required to switch one module with a $> 10,000$ -shot lifetime. If the VCSELs can demonstrate reliable multifilament triggering, this requirement may be reduced to two 50-element VCSELs and two $30 \times 7.5 \text{ mm}^2$ switches, reducing component count, cost, size, and assembly time.

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39669

Determination of Microstructural Properties with Isentropic Compression

M. D. Furnish, C. C. Henderson, H. E. Fang, R. J. Hickman, J. J. Mason, T. R. Christenson, W. M. Trott

The goal of this project is to demonstrate the ability to detect microstructural and defect properties of well-characterized single crystals and structured materials such as LIGA (the German term Lithographie, Galvanoformung, und Abformung, for lithography, electroforming, and molding) parts, micro-welds, and forced-porosity lead zirconate titanate (PZT) ceramics using the recently developed Isentropic Compression Experiment (ICE) method on the Z and SATURN accelerators. We built a line-imaging velocity interferometry system for any reflector (VISAR) that provides spatially and temporally resolved motion with several-micron resolution over about 1 mm linewidth to resolve local intergrain motion. We also developed a remote micropositioning capability for this piece of instrumentation, although demonstration is at an early stage. Methods to interface these parts with tens of microns thickness and approximately 1 mm width to the standard ICE drive plates, while maintaining their fidelity, are under development and include diffusive bonding and gluing. We will conduct ICE experiments in the coming year on both Z and SATURN as add-on experiments as much as possible to minimize expense.

(1) Complete line VISAR development with 10 μm spatial resolution. This includes the optics of the VISAR *per se*, as well as the relay system. The optical relay system for Z converts a 1 mm line on the target to a 17 mm line in the VISAR; this is suitable for the present resolution needs.

(2) Remote positioning of the imaged line on the target. We are meeting this requirement with a piezoelectric mirror mount at the entry to the Z/SATURN center section. Although parts are in hand, this has not yet been checked on Z. It has proved important to have a reference mark on the sample to use as the line end to allow re-indexing of the instrument as shot time approaches (vacuum strain compensation).

(3) Technique to interface LIGA scale parts to ICE panels. We started three paths of investigation: a gluing optimization matrix, diffusion bonding (bringing two polished surfaces together and pressing under some heat), and direct plating of LIGA materials onto the ICE panels. These efforts are not yet complete.

Effect of grain size on calcium carbonate phase transitions under isentropic compression.

The goal of this project is to demonstrate the ability to detect microstructural and defect properties of well-characterized single crystals and structured materials such as LIGA...parts, micro-welds, and forced-porosity lead zirconate titanate (PZT) ceramics using the recently developed Isentropic Compression Experiment (ICE) method on the Z and SATURN accelerators.

(4) Demonstrate the ability to detect material property variations over regions of interest to LIGA manufacturers and microjoining researchers. This is part of objective (1) above.

In addition, we conducted an experiment on Z (one panel on an ICE experiment) with carefully characterized calcite samples of dramatically different grain sizes to assess grain-size effects on phase-transition behavior (e.g., calcite I/II/III transitions at 14, 17 kbar). The effect of grain sizes was substantial; for the single-crystal material, we observed clean steps for the separate transitions, while for the fine-grained ($< 1 \mu\text{m}$) material, we smeared the transitions into a single-transition region. This shows that the ICE technique may resolve structural information under certain conditions, with signatures that should be observable over a wide range of scales.

Preparation of carefully characterized samples of nickel/titanium (analogous to LIGA materials) was unsuccessful due to diamond-machining difficulties.

Finally, we realized a significant portion of an upcoming objective in the successful development of an explicit Lagrangian code for extracting stress-strain paths for ICE experiments. This will be required in the quantitative interpretation of the ICE data from planned experiments.

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39670

Simulations of Intense Petawatt Laser Pulses with Dense Z-Pinch Plasmas

R. B. Campbell

Sandia used LSP (Large-Scale Plasma, a simulation code) for studying fast ignitor physics. We made good progress in the areas of laser-plasma interaction, transport of relativistic electron beams in solid-density plasma, and the generation of energetic ion beams from the backside of exploded foils.

The Z machine experiment has become renowned for attaining ultra-intense x-ray pulses, which can be used to obtain high densities. There is now considerable interest in using short laser pulses to study laser-plasma interactions in an as-yet unexplored parameter regime. Sandia is pursuing a modification of the Z-Beamlet laser facility to enable a near-term high-energy petawatt (HEPW) capability for high-energy radiography and fast-ignition physics. The combination of an HEPW laser and an inertial confinement fusion (ICF) fuel-compression facility (Z) will be unique within the National Nuclear Security Administration (NNSA) community. In keeping with Sandia's paradigm of science-based stockpile stewardship, simulation must be an integral part of utilizing such a facility to its full potential, and designing and understanding experiments carried out in this new physics regime.

We discovered that the implicit algorithms and hybrid physics in LSP do indeed allow us to begin unique research into the interaction and transport physics of the fast particles generated by the laser-beam-plasma interactions. They might also allow us to study the interaction of intense lasers with solid- or near-solid-density targets. We made good progress in extending the simulations to conditions beyond those already simulated by standard particle-in-cell (PIC) codes.

The specific knowledge areas that will benefit from these simulations include ICF, weapons physics, weapons effects, high-pressure dynamic material properties, and basic light-matter interaction physics.

We added energetic materials (EMs) boundary conditions (BCs) to LSP to treat an incident uniform plane EM wave.

We formulated and implemented an algorithm to create a Gaussian laser beam from a uniform plane wave using a dielectric lens.

We confirmed that LSP algorithms can treat the laser/plasma interaction (LPI) problem in the high-power, over-dense regime relevant to ICF, both direct drive and fast igniters.

Sandia is pursuing a modification of the Z-Beamlet laser facility to enable a near-term high-energy petawatt (HEPW) capability for high-energy radiography and fast-ignition physics. The combination of an HEPW laser and an inertial confinement fusion (ICF) fuel-compression facility (Z) will be unique within the National Nuclear Security Administration (NNSA) community. ...The specific knowledge areas that will benefit from these simulations include ICF, weapons physics, weapons effects, high-pressure dynamic material properties, and basic light-matter interaction physics.

We performed an LPI problem at high intensity and high target density that compared favorably with published simulations (ZOHAR code from Lawrence Livermore National Laboratory).

We performed a series of simulations of a (laser-generated) relativistic electron beam propagating through a solid-density plasma. We are studying plastic and metal plasmas.

We performed a calculation of daughter-wave generation in an under-dense plasma through the stimulated Raman-scattering (SRS) process.

We selected LSP as the sole code tool for the project.

We presented the initial results of the electron-beam generation and transport and ion-energy extraction from exploded foils at the Advanced Accelerator Concepts Workshop in June.

We performed a calculation of daughter-wave generation in an under-dense plasma through the stimulated Raman-scattering (SRS) process.

Refereed

Welch, D. R. 2002. Simulations of laser-produced electron propagation in a thin foil. *Proc. Beams/Dense Plasma/Z-Pinch Conference* (June, Albuquerque, New Mexico).

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Corporate Objectives

Sandia collaborates with universities to create new science and engineering for the Laboratories' science and technology base, to train the next generation of scientists and engineers, and to employ complementary resources and skills for achieving common goals. These collaborations improve Sandia's ability to recruit top students for Sandia's work force and to ensure Sandia's future as a leader in science and technology.

“Pseudostationary Separation Materials for Highly Parallel Microseparations” is developing new materials for performing separations in highly parallel microseparation systems. The materials synthesis and initial testing are being performed in collaboration with the New Mexico Institute of Mining and Technology. The materials being developed are specialized chromatographic materials known as *pseudostationary phases* that are easily introduced into micro-fabricated channels, enable high-performance chemical separations, and can be tailored to provide a high

degree of chemical diversity. These developments support a number of Sandia efforts in microanalytical devices based on highly parallel separations. One example is the “Accelerated Molecular Discovery Arrays” project. This project will develop and apply microscale techniques to the analysis of biomolecules that carry the “signals” that control life processes such as growth, aging, memory, and emotion. The development and implementation of new separation methodologies and materials are central to this project.

10729

Ultraminiaturization of RF Circuitry

G. R. Sloan, C. E. Sandoval, K. W. Plummer, G. A. Wouters

Many synthetic-aperture radar (SAR) and radar-responsive tag applications now require microwave electronic miniaturization that is well beyond Sandia's current state of the art. However, recent advances in Lockheed-Martin's (LM) high-density interconnect (HDI) technology, in conjunction with Sandia's new research in microwave microelectromechanical systems (MEMS) and solid-state devices, position us for a major breakthrough. This project seeks to develop a revolutionary radio-frequency (RF) capability by adapting HDI to advanced Sandia technology and applying the result to a multitude of advanced radar applications. Potential new applications for the national interest that these advances would make possible are legion. Next-generation SARs for guided munitions and small unmanned aircraft must be reduced in size by 5x to 10x. Similarly, this technology has been deemed critical to next-generation RF tag programs at Sandia.

Our previous evaluation and testing led us to conclude that this technology is best suited for those applications that require extreme miniaturization and that benefit from the package/substrate integration that HDI offers. An ideal application is a radar-responsive tag. Thus, we decided to focus our effort on the design and fabrication of the RF subsystem for a SAR tag. The circuitry is basically a design that detects and downconverts the incoming signal, runs it through a switched delay line, and then upconverts and retransmits. The module includes 11 Ku-band monolithic microwave integrated circuits (MMICs) and several distributed structures. The resulting size was less than 1.25 x 1.25 in. This represented a 10x miniaturization over a comparable surface-mount design.

We completed the basic design and layout and procured, prepared, tested, and delivered the MMICs used to fabricate the design.

One frustration we encountered in the design process is that LM did not have good data on the actual thickness of the glue and kapton layers. The glue thickness can vary with the number of die, and the kapton thickness is affected by the fabrication processes, such as heating cycles. At ku-band and higher frequencies, the thickness parameters have a significant impact on RF performance. To obtain good design parameters, we cross-sectioned a previous module using ion milling and then used scanning electron microscopy (SEM) imaging to make

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actual measurements. The result facilitated more accurate modeling and provided better agreement for the test data from the first module.

We observed two mechanical concerns in the previous design: (1) the modules are so thin they have a tendency to “potato chip,” and (2) the corners of the module tend to delaminate over time. Working jointly with LM we implemented a potential solution to these problems: We embedded an aluminum wall structure in the module. This structure makes the module more rigid, and it prevents delamination by effectively riveting the laminate to the wall by means of vias. Two versions of the wall structure were used in this fabrication run: one version has wall metal only under the module’s ground strips; the second type has metal everywhere except for die cutouts. The risk of the second type is that it may short out the bottom-most traces (MT0 metallization) if the glue layer becomes too thin. Cross sections of previous modules indicate that this should not be a problem. Ultimately, this effort should verify the validity of this assumption.

Finally, it was a goal of this project to prove out and adapt HDI to the packaging of RF MEMS. Specifically, we were to obtain and package custom devices designed at Sandia, but we currently have no functioning devices available for trial insertion.

The effort this year focused on continued evaluation of the technology, process, and model improvements, and the design and miniaturization of a functional tag RF subsystem. Due to fabrication delays, the test results were not available as of this writing.

The result facilitated more accurate modeling and provided better agreement for the test data from the first module.

10795

Surface-Micromachined Mechanical Timer

K. A. Klody, F. J. Peter, J. L. Dohner, G. E. Vernon, M. W. Jenkins, M. A. Polosky, L. L. Lukens, J. A. Nevers, R. D. Habbit, Jr., R. A. Renn, J. A. C. Zamora, S. S. Mani

This project sought to develop a surface-micromachined (SMM) micromechanical timer. Weapon systems utilize mechanical timers for various functions. Typically, mechanical timers are used in lieu of solid-state oscillators because mechanical timers can physically interrupt electrical or optical paths. In addition, solid-state timing devices possess two distinct weaknesses: They are inherently sensitive to radiation, and they require uninterrupted external power. Solid-state oscillators have been widely used and are well suited for many applications. Their principle advantages are related to their size and cost. New SUMMiT™ SMM technologies allow the manufacturer of micromechanical devices to use silicon (Si) batch-processing techniques. An SMM mechanical timer offers a small, elegant, cost-effective solution for applications where a solid-state oscillator is not suitable. In addition, micromechanical timers offer a suite of attributes that are quite attractive, e.g., small, lightweight systems that are insensitive to mechanical shock and vibration environments due to their nearly massless part sizes.

This project developed mechanical timing mechanisms using Sandia's SUMMiT™ SMM process. The vision for each device is based on a wound spiral spring that stores energy and is connected to a gear train. Terminated at the end of the gear train is an escapement mechanism that we use to provide mechanical damping. The escapement mechanism retards the unwind speed of the spiral spring and regulates the device so that timing information can be measured as a function of gear position. Sandia fabricated and tested complete microelectromechanical systems (MEMS) timing devices. In addition to complete timer devices, we performed component analysis to improve not only the timer, but also MEMS in general. This project also proved the feasibility of combining solid-state devices with MEMS. The recent proof-of-concept MEMS devices developed through this project demonstrate the feasibility of developing MEMS weapon components.

Since SMM is in its infancy, all of the supporting technologies and tools are also in their infancy. The project team had to develop the supporting technologies and tools along the way. We successfully fabricated and operated a

This project sought to develop a surface-micromachined (SMM) micromechanical timer. Weapon systems utilize mechanical timers for various functions. ...This project developed mechanical timing mechanisms using Sandia's SUMMiT™ SMM process. ...

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complete timer and completed and submitted several new designs for fabrication. We developed and demonstrated the use of Sandia's advanced force-measurement capabilities. Finally, the team expanded the automated testing capability. But most important, all of these accomplishments demonstrated the feasibility of producing a micromechanical timer.

- *Fabricated FP28901A and B.* This reticle set features a comparison between various microengines driving a transmission. Due to a design flaw in the transmission, we were unable to test most of the devices. However, we tested a modified torsional ratcheting actuator (TRA) and compared it to TRAs in the standard components library. This TRA actuated at the lower end of the typical operating range (16–18 V with no load).

- *Fabricated FP29601A.* This reticle set featured a comparison between transmissions with pressure angles of 10, 20, and 25 degrees. Unfortunately, the tested dies from the initial release were “sticky,” and a thorough analysis was not completed prior to this project summary.

- *Designed and fabricated FP32901 A and B.* This reticle set featured one and two TRAs winding spiral springs, hairspring escapement test mechanisms, and a full timer design actuated by a TRA. We tested the TRAs winding the springs at various voltages to observe angular displacement. We recorded the hairspring escapement test mechanisms with a high-speed camera; this footage helped to fully analyze the devices. We also determined the amount of damping in the system. We were unable to test the full timer design due to a design flaw.

Additionally, we took high-speed camera footage of the timer devices unwinding on FP22701A Module 3. This footage allowed us to determine the amount of time that was stored on these devices after they were wound to 150 degrees.

We successfully fabricated and operated a complete timer and completed and submitted several new designs for fabrication. We developed and demonstrated the use of Sandia's advanced force-measurement capabilities. Finally, the team expanded the automated testing capability. But most important, all of these accomplishments demonstrated the feasibility of producing a micro-mechanical timer.

16167

Pseudostationary Separation Materials for Highly Parallel Microseparations (PECASE)

D. L. Lindner

This project is developing new materials for performing separations in highly parallel microseparation systems. Sandia will perform the materials synthesis and initial testing in collaboration with New Mexico Tech. The materials being developed are specialized chromatographic materials known as “pseudostationary phases” that are easily introduced into microfabricated channels, enable high-performance chemical separations, and can be tailored to provide a high degree of chemical diversity. The emphases of the project are the development of novel phases, the characterization of the phases to determine the factors that most affect chemical selectivity, and the application of the phases for the separation of model or representative compounds of interest to Sandia. These developments support a number of Sandia efforts in microanalytical devices based on highly parallel separations.

- *Synthesis of acrylamide methyl propane sulfonic acid (AMPS) analogues with ionic acrylate monomers.* Repeated attempts to synthesize analogues of AMPS copolymers using sulfopropyl methacrylate (SPM) and sulfoethyl methacrylate generated disappointing results. We identified several solvent systems that provide sufficient solubility of both the ionic monomer and the nonpolar dodecyl methacrylate comonomer. Multiple synthetic attempts using these solvent systems led us to conclude that the reactivity ratio of the monomers is not conducive to the formation of random copolymers. We obtained near homopolymers of the ionic monomer, with little evidence for copolymerization. We obtained a single copolymer of approximately 85% SPM, and preliminary studies with this polymer indicate that polymers of this chemistry can be used for electrokinetic (EK) separations, although higher fractions of SPM would yield better performance.

- *Application of AMPS and siloxane polymers with alternate detection strategies.* We made significant progress in the development of an electrochemical detector. However, since compatibility with instruments under development at Sandia was the primary goal, studies concentrated on the use of laser-induced fluorescence (LiF) detection. Poly(sodium undecenyl sulfate), AMPS copolymers, and siloxane copolymers have all been demonstrated to be compatible with LiF detection. We did

A novel siloxane polymer (left) with 20% of the silicon centers modified with dodecyl chains and the other 80% modified with a linker arm and sulfonic acid groups that can be used as pseudostationary chromatographic phase for separation of molecules such as TNT. The chromatograms (right) show separation of aromatic hydrocarbons using the polymer in micellar electrokinetic chromatography.

This project is developing new materials for performing separations in highly parallel microseparation systems.

not observe significant background signal for polymers that had been washed with spectrophotometric grade solvents.

- *Characterization of polymer-solute interactions by fluorescence studies.* AGENT siloxane polymers and taurine-modified maleic anhydride-dodecyl vinyl ether (MADVE) copolymers were characterized by fluorescence studies using pyrene to determine the polarity of the solvation environment, and 1,3-bis-(1-pyrenyl)propane to determine the microviscosity of the solvation region. Most significantly, the results indicate significant differences in the solvation environment afforded by MADVE polymers as a function of pH. We submitted these results for publication.

- *Synthesis and characterization of modified ionic siloxanes without tertiary amine spacer arm.* We developed synthetic protocols for the synthesis of siloxane polymers having no amino functionality in the spacer arm between the polymer backbone and the ionic sulfonate group. Various pendant group structures and densities do not significantly affect selectivity. There are significant selectivity differences, however, between these polymers and the siloxanes studied previously. The new polymers are more polar and have about the same acid-base chemistry as the previous materials. This latter result is surprising, given the absence of the tertiary amine functionality. We presented these results at an international conference and submitted them for publication.

- *Application of selected polymeric phases in chip-based instruments.* We used AMPS-Lauryl methacrylamide as a pseudostationary phase in a chip-based instrument with LiF detection. The polymer solution was easily introduced into the microchannel and did not interfere with detection. We separated and detected several derivatized amino acids in just over 3 minutes.

Most significantly, the results indicate significant differences in the solvation environment afforded by MADVE polymers as a function of pH. We submitted these results for publication.

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17230

Novel Coatings for Microelectromechanical (MEM) Devices (PECASE)

M. P. DeBoer

Sandia seeks to integrate new materials (in particular as thin films) into polysilicon (poly-Si)-based microfabrication technology. Specifically, we are pursuing two classes of new materials: superhard materials and metals. We are making a special effort to develop processes that integrate materials at the microstructure release step because such processes would afford a wider class of materials and a greater degree of flexibility to device engineers. Consequently, processes will have to allow conformal deposition.

We chose superhard materials with the following properties: wear resistance, hydrophobicity, lubricity, and chemical and thermal inertness. Our initial efforts focused on developing a process to coat poly-Si micromachines with a conformal layer of Si carbide (SiC)—a tough, radiation-hard, corrosion-resistant material, second only to diamond in wear resistance. Furthermore, in contrast to self-assembled monolayers (SAMs), which do not withstand temperatures employed in packaging technologies, we expect SiC to be much more thermally stable. We are exploring the use of C60 and its interaction with Si to realize a thin conformal SiC layer. Carbon nitride is predicted theoretically to be even harder. We are exploring ways of integrating it into micromechanical structures.

Integration of metals offers special opportunities for realizing devices such as microrelays. Standard metal-deposition techniques suffer from being line-of-sight (LOS). One way of circumventing this problem is to use electroless plating techniques, based on coating the structures with a self-assembled organic monolayer with a special end-group functionality that catalyzes the growth of a continuous metallic layer from solution.

In the aforementioned coating processes, little is known about the tribological properties of the resulting materials in thin-film forms. Therefore, we also are characterizing these films using surface analytical techniques in our laboratory and specially designed test microstructures. Metal surfaces may be hydrophilic, and hence, additional surface modification may be necessary to alleviate stiction.

- *Perform tribological studies of SiC overlayers using specially designed microstructures. SiC is well known as an attractive material for demanding mechanical and high-*

Sandia seeks to integrate new materials (in particular as thin films) into polysilicon (poly-Si)-based microfabrication technology. Specifically, we are pursuing two classes of new materials: superhard materials and metals. ... Our initial efforts focused on developing a process to coat poly-Si micromachines with a conformal layer of Si carbide (SiC)—a tough, radiation-hard, corrosion-resistant material, second only to diamond in wear resistance.

temperature applications and in abrasive, erosive, and corrosive media. We used the disilabutane (DSB) chemical vapor deposition (CVD) process successfully to coat released poly-Si microstructures. Using a tungsten (W) probe tip, the thin SiC coatings proved to be scratch-resistant, while an uncoated poly-Si surface was readily scratched. A SiC-coated micromachine remained intact following immersion in hot potassium hydroxide (KOH), indicating that the SiC overlayer is conformal, dense, and pinhole free. We are currently depositing thin conformal SiC films on various tribology microinstruments, such as cantilever-beam array and various friction microinstruments. We learned that the films must be thick enough to be void-free, but thin enough that they do not electrically short out the device since the coating also is deposited on Si₃N₄ isolation layer.

- *Investigate selectivity of DSB-based deposition process toward silicon dioxide (SiO₂) and silicon nitride (SiN).* We deposited SiC on Si(100), polycrystalline Si, SiO₂-coated Si(100), and Si₃N₄-coated Si(100). The deposition temperature explored was 700°–850°C. In this range, SiC film deposition is determined to be independent of the substrate. In other words, we obtained similar quality films based on x-ray diffraction (XRD) and scanning electron microscopy (SEM). It is possible that higher temperatures are needed to prohibit SiC growth on SiO₂, as reported for the methylsilane-based SiC-deposition method. Unfortunately, our system does not allow us to reach temperatures above 900°C. As a consequence, we have been working on developing fabrication technology for DSB-based SiC surface micromachining (SMM). We found that the beams suffer from the significant stress gradient when the SiO₂ sacrificial layer is used, and we observed much improvement with a Si sacrificial layer. We also fabricated high-aspect-ratio SiC flexures using our low-temperature, single-source CVD process. To date, high-aspect-ratio elastic flexures or Hexsil structures have primarily been fabricated from CVD poly-Si, as it is highly conformal and exhibits slow attack by the release-etch chemistry. The superior mechanical, thermal, and chemical properties of SiC make it an exceptionally attractive material for high-aspect-ratio microelectromechanical systems (MEMS) flexures. These preliminary results indicate that our SiC CVD method is adaptable to the processing steps required in the fabrication of high-aspect-ratio flexures. Currently, we are working on doping our SiC films and fabricating fully released structures from conductive, *n*-doped SiC.

- *Perform tribological studies of electroless-plated test microstructures.* Electrochemical processes at the core of

We used the disilabutane (DSB) chemical vapor deposition (CVD) process successfully to coat released poly-Si microstructures. Using a tungsten (W) probe tip, the thin SiC coatings proved to be scratch-resistant, while an uncoated poly-Si surface was readily scratched. A SiC-coated micromachine remained intact following immersion in hot potassium hydroxide (KOH), indicating that the SiC overlayer is conformal, dense, and pinhole free.

integrated circuit (IC) technologies have been the subject of extensive investigations. In contrast, metallization of MEMS remains a relatively unexplored subject. Potential applications of metals in MEMS technology range from reflective/conductive coatings for optical MEMS, microswitches, and microrelays, to catalytically active coatings in microchemical reactors. We recently reported on a new process for Si metallization, which offers several attractive features for MEMS applications. We based the method on galvanic deposition from fluoride-containing solutions. In contrast to electroless deposition, galvanic displacement deposition requires no prior activation of the surface and is truly selective to Si surfaces. We examined in detail several issues of concern in immersion-plating MEMS, namely the conformality of the coating process and the surface energy of deposited copper (Cu) films. In particular, we were able to Cu-plate cantilever-beam arrays. The Cu film obtained by immersion plating is hydrophilic, as are the surfaces of bulk metallic Cu. Fortunately, functionalization schemes for Cu surfaces can be used to render the surfaces hydrophobic. We use alkanethiol self-assembled monolayer passivation. We were able, for the first time, to successfully integrate this functionalization scheme with Cu plating and microstructure release process. Measurements on several different arrays yielded an average detachment length of about 1100 μm , or a work of adhesion of about 3 mJ/m^2 .

We use alkanethiol self-assembled monolayer passivation. We were able, for the first time, to successfully integrate this functionalization scheme with Cu plating and microstructure release process.

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22854

Theoretical Study of Sb as a Surfactant in Epitaxy of III–V Materials

E. S. Hertel, Jr.

A key direction for Sandia is the development of integrated microsystems. This project will advance the state of the art in new metal-organic chemical vapor deposition (MOCVD) reactor designs and in the development of new diagnostic tools. A key integration element of the silicon (Si) microchip module level will be an infrared (IR) laser produced via MOCVD techniques. In collaboration with the University of Utah, we will evaluate the current designs and optimize the next-generation reactors and diagnostic tools currently in development.

A principle mechanism by which surfactants affect epitaxial growth is modification of surface structure. We developed theoretical techniques to determine surfactant-induced reconstructions and applied them to investigate antimony (Sb)-covered GaP(001) (gallium phosphate) and InP(001) (indium phosphate) surfaces, with the goal of explaining interesting experimental observations for Sb/GaP. Here, we provide a detailed derivation of the technique and then discuss a specific application of the theory.

Free energy is a function of partial pressures and temperature. Temperature affects surface energy directly through configurational and vibrational entropy and indirectly through modification of chemical potential. For most epitaxial systems, the indirect temperature effects are dominant. Therefore, it is useful to neglect the direct dependence on temperature and express the free energy as a function of the chemical potential, where dependence on temperature and partial pressures is implied.

As long as the slab contains enough atomic layers to relax all surface-induced strain, the free energy of a slab can also be expressed as a sum of surface and bulk free energies.

We created a super-cell containing a reconstructed slab for each considered surface structure. We used the Vienna Ab Initio Simulation Package (VASP) electronic structure code to calculate total energies and forces within the local density approximation (LDA). We investigated convergence of computational parameters, including k -points, vacuum space, slab thickness, plane-wave cutoff, lattice parameter, and atomic forces.

We applied these methods to Sb-covered InP(001) and GaP(001) surfaces. We found the most stable of the considered

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reconstructions for allowable values and used this information to construct surface-phase diagrams.

For III-P(001) (phosphorus) surfaces, at a minimum value in the surface-phase diagrams, our calculations predict that the P-terminated surface can be reconstructed. As Sb is added to the surface, the structure is retained, and Sb substitutes for P atoms in the reconstruction. For high values, the structure changes significantly, and double-layer P and Sb reconstructions become stable. It is interesting that the structures are predicted to be stable despite violating Pashley's electron-counting rule.

The presence of surface structures in the limit may explain the recent observance of triple-period ordering in GaP grown by organometallic vapor-phase epitaxy (OMVPE) and corroborates the change in surface structure detected by surface photoabsorption. Previous calculations indicate that surface structures provide thermodynamic driving force for triple-period ordering.

We derived a general method for calculating surface energy and applied it to a relevant materials science problem. Following the prescribed method, we used density-functional theory (DFT) and the LDA to calculate total energies for Sb-covered InP(001) and GaP(001) surfaces. We determined surface energies and used them to construct phase diagrams, which will assist in developing theories to explain experimentally observed phenomena. In addition, identification or surface reconstruction is a critical first step toward investigation of growth processes such as add-atom diffusion, step-edge attachment, island nucleation, and morphological and compositional evolution.

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Refereed

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32817

Molecular Simulations of MEMS and Membrane Coatings (PECASE)

A. P. Thompson, A. C. Sun

Self-assembled monolayers (SAMs), which are ultrathin organic layers that are chemically and/or physically attached to solid inorganic supports, are important in many areas of technology. Two prime examples are microelectromechanical systems (MEMS) and gas-separation membranes.

SAMs are used in MEMS components as adhesion and friction reducers. Although their performance can be measured in situ on MEMS devices, the structure and dynamics of the SAM coatings is only partially understood. A better understanding of the molecular-scale phenomena will provide fundamental knowledge of performance and degradation mechanisms. Such knowledge is an essential requirement to predict the performance of MEMS devices with usage and aging.

SAMs have also been used as key elements in gas-separation membranes. In several laboratories, membranes were created by the deposition of SAM films on nanoporous supports, such as silica and alumina. These "hybrid" membranes show significantly increased selectivity for heavier organics and vapors, meaning that they will be useful for environmentally relevant separations such as the removal of volatile organic contaminants from air. However, the mechanisms that led to this increased selectivity have not been isolated; this is essential if better hybrid membranes are to be developed.

Sandia seeks to use molecular simulation as a means to study the structure-property relationships of SAMs in both MEMS devices and gas-separation membranes. The MEMS studies will use molecular dynamics (MD) simulations to study the effects of chain length and degree of fluoro-substitution on the ability of SAMs to reduce adhesion forces between silica surfaces. The membrane studies will use a combination of MD and Monte Carlo simulations to predict the transport rate of various gas species across a SAM-treated nanoporous membrane and examine the molecular-level transport mechanisms that occur. We will also carry out some experiments to validate the simulations.

We made significant progress on the hybrid organic-inorganic membrane project. We studied two mixed-gas systems, propane/nitrogen and methane/butane, and found the membrane performance to be generally better than that predicted by the corresponding single-gas experiments. Based

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on these encouraging results, we submitted a manuscript to the *Journal of Membrane Science*. We also demonstrated our ability to modify the membrane permselectivity via synthesis variables, such as the hydration state of the surface and the functionality of the organic reagent; we are preparing a manuscript on this topic for submission to *Langmuir*. We also set up a vapor permeation experiment for volatile organic compound (VOC) recovery applications and obtained data for toluene/nitrogen systems. We explored the use of dendrimers as the organic surface phase. With an aromatic dendrimer, we obtained excellent performance for the toluene/nitrogen separation; the selectivity was nearly equal to that of the best polymer currently used in industry, and the permeance was much higher.

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34692

Self-Assembly of Polymers in Confined Geometries

J. G. Curro

Self-assembly of molecules is nature's way of creating ordered structures on the nanometer scale. Depending on their architecture, certain molecules such as block copolymers will spontaneously order themselves on a scale that would be impossible to achieve by ordinary polymer processing techniques. This property makes self-assembly a powerful tool for producing nanostructure materials. Some applications include low dielectric constant materials, microfluidic devices, sensors, membranes, microelectronics, and microelectromechanical systems (MEMS) devices.

As polymers are used for these applications, it is necessary to understand how the confined geometry influences the properties of the polymer. It is well known that miscibility, viscoelastic properties, density, and the glass transition in thin films are quite different from the corresponding bulk properties. The purpose of this project is to develop computational tools to model the properties of polymers near surfaces and in confined geometries.

We wrote a density-functional theory (DFT) code that allows the modeling of tethered polymer chains in continuum and explicit solvents. We found the DFT code to be very accurate in describing polymer brushes in continuum solvents when it was compared to molecular dynamics simulations under athermal conditions. We used the code to predict experimental density profiles on poly n-isopropylacrylamide (PNIPAM) polymers grafted to substrates in the presence of water and acetone solvents. We compared these with the neutron reflectivity experiments at Sandia. We found good agreement for the acetone solutions, but the DFT did not agree with the density profiles measured in water. Further experiments are planned on higher-molecular-weight and better-characterized samples, and these results, when available, will be compared with the theory.

We also developed a theory to account for changes in the glass-transition temperature (T_g) of polymers in confined geometries. The theory is based on the fact that in confined geometries the density of the polymer is not uniform relative to the pure bulk polymer. We employed DFT theory to compute the density profile and made predictions for the T_g that are in good agreement with experiments.

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34693

Building Conscious Machines Based on the Architecture of Visual Cortex in the Primate Brain

J. B. Whitley, G. Yonas

Designing intelligent systems that can monitor and interact with complex, variable, and poorly modeled environments remains a challenge. This is particularly true for systems that need to be controlled in real time, such as autonomous robots, automated buildings, or traffic control in metropolitan areas. Sandia took an approach that sacrifices the time-consuming (and, for many physical systems, ill-defined) goal of searching for the global optimum in favor of a locally optimal solution in a small, restricted subset of the system. That is, an attentional mechanism selects a subset of all relevant data, in real time, as the best representation of the system status given limited computational resources. This central representation, akin to the content of consciousness, changes as the system and the environment evolve. The organization of this architecture model is reminiscent of the cognitive architecture of the primate brain and makes use of a notion similar to the hypothesized function of consciousness.

(1) We acquired an infrared (IR) video eyetracking system that we are using to record observers' eye positions with high temporal (120 Hz) and spatial (± 0.25 deg visual angle) accuracy. This allows us to focus in on the locally optimal subset of the global dataset.

(2) We collected eye-movement scan paths from observers as they viewed computer-generated fractals, rural and urban outdoor scenes, and overhead satellite imagery. We found that, with very high statistical significance (10 to 12 z-scores), the saliency model accurately predicts locations that human observers will find interesting.

(3) We adopted our model of short-range interactions among overlapping spatial orientation channels to better predict bottom-up stimulus-driven attention in humans. This enhanced model is even more accurate in its predictions of human observers' eye movements. This moves us toward predicting the optimal data subset in the evolving environment.

(4) We are currently incorporating biologically plausible long-range interactions among orientation channels, which will aid in the detection of elongated contours such as rivers, roads, airstrips, and other man-made structures.

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35376

Development of Experimental Verification Techniques for Nonlinear Deformation and Fracture

N. R. Moody

This project is a collaboration between Sandia and Washington State University (WSU). Currently few experimental testing methods exist that can assess nonlinear deformation and fracture phenomena on the micrometer- and submicrometer-length scales. Those that exist are often not verified using a second experimental approach. Nanoindentation techniques have been developed to probe failure modes, including film fracture and delamination, but these tests are difficult to verify without resorting to other indentation or scratching techniques. Therefore, a study that will allow for the development of testing using an independent technique (bulge testing and blister testing) will be applied to materials systems of interest to film-substrate systems that can be used as models for components in the stockpile. We will perform additional testing in materials that exhibit nonlinear deformation and shear band formation under high stresses. As both systems, nanoindentation and bulge testing, can be carried out in aqueous environments that are environmentally aggressive, we will perform testing correlation under various thermochemical environments to ensure the robust nature of the experimental procedure. We will then compare the results of all of these tests to simulations in projects supported in the Accelerated Strategic Computing Initiative (ASCI) program to show applicability of the testing methods to future verification of simulations for life-cycle engineering.

The project constructed a rapid film-fracture bulge testing system, which has brought the time for running a single-membrane fracture experiment from approximately 30 min to approximately 3 min. This enables much larger datasets to be collected on film fracture. With improvements in film fabrication methods, this project has been able to generate films that show no evidence of interfacial failure, only through thickness fractures are now observed.

WSU established finite-element (FE) simulations to correlate experimental nanoindentation data to simulations using the ABAQUS package. While the observed trends hold for out-of-plane deformation between the experiment and the simulations, more work is needed in mesh refinement to accurately capture the magnitude of the deformation in the hard film-soft substrate systems of titanium dioxide (TiO₂) on Ti

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and aluminum oxide (Al_2O_3) on Al. Effects such as tip geometry and film thickness appear to currently match experimental results, with sharper tips generating more significant out-of-plane deformation; blunter tips appear to be more likely to generate through thickness fracture events.

Cyclic loading during nanoindentation of the TiO_2 -Ti and Al_2O_3 -Al systems shows that the continuous stiffness method of testing can lead to film fracture, an effect that has not been documented in the literature. In both oxide-metal systems, monotonic loading was unable to generate film-fracture events, while an imposed sinusoidal displacement of between 3 nm and 9 nm generated film fracture in these systems at total penetration depths of 15–50 nm for oxides of 60 nm thickness. The expected cause of this is the motion of dislocations in the metal, removing the load-carrying support of the substrate from the film, leading to increased tensile stresses at lower displacements from the superposition of the load between the film and substrate.

The effects of the underlying crystal structure and oxide films on deformation around indentations may be influencing the film-fracture behavior, and this has led to a new area of study utilizing atomic-force microscopy (AFM), orientation imaging microscopy (OIM), and nanoindentation to track individual slip steps around a given indentation. These results demonstrated that it is possible to resolve slip systems that are active around submicrometer indentations, identifying slip steps spaced as closely as 250 atomic planes around indentations into body-centered cubic (BCC) Ti and a 304 stainless steel.

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36901

Microcontact Printing of Nanoparticle Arrays*P. G. Clem, S. Y. Lin*

Focused ion-beam (FIB) lithography is a powerful technique for low-cost, high-resolution topographical patterning of substrates. Unlike conventional photolithography, no mask is required, and the patterning is accomplished in one step. Additionally, “gray-scale” images, that is, features of varying depth on the substrate, can be patterned in the same lithography step. This pattern can then be used to nucleate large-area colloidal crystals with predefined orientation and defined-defect densities.

The ability to fabricate photonic crystals (PhCs) with predefined orientation and defects should enable the formation of surfaces with low observability and tailored reflectance, and photonic structures for waveguiding. Teams of researchers at both the University of Illinois (UI) and Sandia are performing the assembly and characterization of these materials. The UI group is assembling and characterizing the optical properties of the patterned surfaces and PhCs; the Sandia group will participate in optical characterization and in synthesis of the nano- and microparticles used in this study.

An important aspect of the colloidal assembly process is the inclusion of nanoparticles in the precursor suspension of nanoparticles. The nanoparticles modulate the interparticle forces between colloidal particles and thus enable formation of lower-defect colloidal crystals. This interaction is strongly driven by the charge on the nanoparticles, and thus the synthesis of nanoparticles with defined surface charge is highly important.

We successfully patterned substrates with periodic arrays of dimples and crystallized a colloidal crystal on this substrate. The colloidal crystal was settled out of a suspension of micron-sized silica colloids and 1–3 nm zirconia nanoparticles at a pH of ~ 2 . Normally, drying of colloidal crystals is problematic because capillary forces disturb the colloidal crystal when the drying front passes through the crystal. One significant advantage of the zirconia nanoparticle-containing system over other systems is that the zirconia-containing suspension can be gelled by raising the pH. After we pass ammonia gas over the colloidal crystal and gel the zirconia, the colloidal crystal can be dried without disruption.

By modulating the periodic spacing of the substrate, we found it possible to vary the lattice constant of the colloidal crystal and thus form noncubic colloidal crystals. In the

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experiments to date, colloids with a diameter of $1.18\text{ }\mu\text{m}$ were settled on substrates patterned with a periodic array of dimples with a pitch of $1.21\text{ }\mu\text{m}$ and $1.27\text{ }\mu\text{m}$. The resulting colloidal crystals had 100-plane spacings of 800 nm and 610 nm, respectively. This can be compared to a face-centered cubic (FCC) crystal of $1.18\text{ }\mu\text{m}$ spheres, which would have a 100-plane spacing of 830 nm. The ability to independently modulate the a , b , and c lattice constants (while maintaining a hard-sphere colloidal crystal) in the PhC should open up possibilities for new photonic materials with anisotropic optical properties.

A significant part of this project was the synthesis of nanoparticles with defined surface chemistries. To date, we have synthesized both gold and silica nanoparticles with a range of chemistries including aliphatic, ethylene glycol, amine, quaternary amine, and carboxylic acid groups. Currently, the majority of our nanoparticle effort is going into the formation of nanoparticles with mixed surfaces, and we have now successfully formed silicon dioxide (SiO_2) nanoparticles coated with 1% and 3% amine groups in a background of aliphatic groups. We believe this scheme should enable the fabrication of particles that attach to substrates in a defined fashion, as well as create nanoparticles that interact in controlled ways with colloidal particles, which should enable the assembly of colloidal crystals with lattice constants and defect densities outside of that commonly available.

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36902

Mathematical Analysis of Deception*F. B. Cohen*

This project involves theoretical research, development of technologies, experiments to confirm or refute theories, and publications and presentations related to the use of deception for information protection. Sandia is performing the work in collaboration with the University of California at Davis.

The work involves the creation of experimental test-beds based on theoretical results where those test-beds are designed to differentiate effects due to the presence or absence of deception and measure their efficacy against the theoretical models. We are adapting theories where appropriate to reflect the experimental evidence and will publish results. Developments of technology are required to perform some of these experiments, and those developments will yield additional value that can be re-applied to other needs to form increasingly effective technologies for protection through deception.

We developed several preliminary papers that go into mathematical details of deceptions. Perhaps the most important result was the development of generic attack graphs for computer system attack with and without deceptions and the generation of systematic methods for inducing human attackers to proceed through the attack graph in predictable ways.

Other results include the characterization of the space of deceptions relative to computer systems, the development of limited mathematics for analysis of that space, and the creation of a set of techniques for measuring attackers as they progress through that space.

This work also resulted in the creation of a set of patents that includes techniques associated with substitution of system calls, the use of process lineage for deception and detection of attacks, the creation of dual systems for deception, and a range of other techniques, all derived from the mathematical understandings developed in this project.

This work also resulted in the creation of a set of patents that includes techniques associated with substitution of system calls, the use of process lineage for deception and detection of attacks, the creation of dual systems for deception, and a range of other techniques, all derived from the mathematical understandings developed in this project.

36904

A System-Dynamics Approach to Modeling Water Demand

V. C. Tidwell, S. H. Conrad, H. D. Passell

Fresh water is central to the vitality of our society; however, national and international demands are increasingly being met through unsustainable practices. Unfortunately, management of this precious resource is complicated by the different values placed on water by various sectors of our society (e.g., industry, agriculture, environmental protection, recreation). Modeling tools are needed to quantify these differing value systems and their relation to supply.

Sandia seeks a system-dynamics approach to modeling freshwater demand. This approach provides a comprehensive framework for quantitatively modeling the values ascribed to water. Here, our concern is for market-driven values (economic) and nonmarket values (e.g., environmental, ecological, and cultural) alike. Efforts will be made to conceptualize, mathematically model, calibrate, and test key value systems. As these values tend to interact, we will explore the coupling or feedback between different values and their relation to water supply. Additionally, we will explore the legal and political constraints used to protect and promote particular values. Ultimately, our goal is to develop a freshwater-demand model accessible to water managers, policy makers, regulators, and stakeholders to help them understand the consequences of their decisions.

This work will be performed cooperatively with the University of Arizona and the National Science Foundation Science and Technology Center for Sustainability of Semi-Arid Hydrology and Riparian Areas (SAHRA). By leveraging our efforts with SAHRA, we will gain access to field data acquired from a variety of semi-arid river basins, including the Rio Grande. More importantly, this relation will provide new understanding and predictive models for implementation in our system-dynamics water-demand model.

We modeled the impact of groundwater pumping on Rio Grande flows, modeled a shallow aquifer intermediate between the basin aquifer and the Rio Grande, and reworked the model interfaces to facilitate public interaction. We also modeled two water conservation alternatives. One calculates the expected water saved and economic costs associated with Bosque restoration, where non-native plants are removed and thinning of the overgrown vegetation is performed. The second alternative considers the effects of different pricing strategies

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and structures on municipal and industrial water consumption in the basin.

Refereed

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38716

Self-Organization of Software

G. C. Osbourn

Sandia is currently exploring and developing a new statistical mechanics approach to designing self-organizing and self-assembling systems that is unique to Sandia. The primary application target for this ongoing research is the development of new kinds of nanoscale components and hardware systems. However, a surprising out-of-the-box connection to software development is emerging from this effort. With some amount of modification, the collective behavior physics ideas for enabling simple hardware components to self-organize may also provide design methods for a new class of software modules. Large numbers of these relatively small software components, if designed correctly, would be able to self-assemble into a variety of much larger, more-complex software systems. This self-organization process would be steered to yield desired sets of system properties. If successful, this would provide a radical (disruptive technology) path to developing complex, high-reliability software unlike any known today. This effort is aimed at appropriately generalizing these collective behavior physics concepts and testing their feasibility for achieving the self-organization of large software systems.

Dynamic self-assembly mechanisms in nonequilibrium physical systems provide models for how physical building blocks participate in the self-assembly of larger, hierarchical structures of which they are a part. The idea behind our feasibility study was to determine a way to adapt these physics mechanisms to a pure software environment and to carry out simple tests of the feasibility of the resulting self-assembly approach. We needed much of the project time to translate the physics ideas appropriately. We also completed a set of simulations to evaluate this self-assembly approach using the FORTH language. Our simulation results directly supported the feasibility of our idea. The results also help establish that special classes of nonequilibrium physical systems intimately combine physics and information-processing characteristics in a way that may not be well known to either the statistical physics or information science communities. Based on these results, we are developing an expanded “thrust” activity in our organization to develop the physics of highly nonequilibrium, self-assembling systems. Our early focus will be on developing the novel idea behind this small project, i.e., implementing a full-scale self-organizing software-development system.

This self-organization process would be steered to yield desired sets of system properties. If successful, this would provide a radical (disruptive technology) path to developing complex, high-reliability software unlike any known today. This effort is aimed at appropriately generalizing these collective behavior physics concepts and testing their feasibility for achieving the self-organization of large software systems.

38717

Nanoscale Energetic Materials by Inverse Micellar Synthesis

A. S. Tappan, J. P. Wilcoxon, W. M. Trott, R. Behrens, Jr.

Sandia is investigating inverse micellar synthesis (IMS) as a technique for preparing nanoscale energetic materials (EMs). Particle sizes of materials such as metals, oxidizers, and composite mixtures can be precisely controlled by this technique and result in particles as small as a few nanometers. The lower limit of useful particle size of conventional aluminum (Al) for EM formulations is being realized as the surface-area-to-volume ratio is increased, thus increasing mass percentage of the ubiquitous surface coating of nonenergetic aluminum oxide (Al_2O_3). This limit appears to be on the order of 30 nm. IMS allows for pure Al particles to be synthesized and should allow them to be passivated against oxidation by a coating of a compound that would contribute to the energy release. By careful selection of the passivation layer, composite EM energy densities twice that of high-melting explosives (HMX) are possible. Of particular importance are the precise control and enhancement of chemical energy release in overcoming dissipative processes at the small-length scales characteristic of microelectromechanical systems (MEMS) devices for future components. IMS is one application of nanotechnology that will result in higher energy-release rates and higher energy-densities in EM compositions.

Characterization of these materials is key to understanding the enhancement of EM performance and the mechanisms of this enhancement. We will use standard analysis techniques, such as standard safety tests, electron microscopy, calorimetry, light scattering, and chromatography, to characterize the chemical and physical properties of these materials. We will evaluate Fourier-transform ion-cyclotron resonance mass spectrometry (FTICR-MS) as an analysis technique for these nanoparticles. We will examine characterization of performance of EMs formulated with nano-EMs by shock studies, utilizing a line-imaging optically recording velocity interferometry system (ORVIS) to observe reactive-wave growth and evaluate the contribution of the nanoscale material to this reactive-wave growth.

Nanotechnology has been accepted throughout the EMs community as a means to access the higher-energy-density of composite materials such as pyrotechnics and thermites through strict particle-size control. IMS is an established technique for controlling particle size of chemically synthesized materials.

Sandia is investigating inverse micellar synthesis (IMS) as a technique for preparing nanoscale energetic materials (EMs). ...IMS is one application of nanotechnology that will result in higher energy-release rates and higher energy-densities in EM compositions.

This project is the first known application of IMS to the synthesis of EMs.

The approach of this project is to apply IMS to chemical reactions with literature precedent to create materials with desirable energetic properties. We chose Al as the first material to investigate due to its high heat of combustion and large existing body of information on its properties. We identified other materials, including boron, magnesium, titanium, and zirconium. Most nanoscale metals are pyrophoric in a nonpassivated state, and Al is no exception. Al is typically stable due to a several-nanometer-thick passivating oxide layer. This layer becomes more of the mass fraction of the particle as the particle size decreases and thus becomes a significant detriment to performance at particle sizes below 100 nm. The key to the success of this project is passivation of the Al particles to prevent oxidation before the material is ignited. It is desirable for this passivating material to contribute to the energy release of the material, rather than detracting from it, as is the case with Al_2O_3 . We chose materials as potential passivation layers, including oxides of transition metals such as molybdenum and tungsten.

The initial synthetic effort involved screening precursor materials and solvent/surfactant systems. We examined dissolution of the chloride and nitrate salts of Al in various solvent/surfactant systems, which led to certain acceptable systems. We successfully performed reduction with various reducing agents. We used dynamic light scattering and x-ray fluorescence to analyze the resulting samples. We will further analyze on passivated particles. We selected the thermal decomposition of alane (Al hydride) adducts as a route to nanoclusters of Al and also as a means to increase particle size of seed particles. We synthesized 1.8 nm Al nanoclusters by thermal decomposition of dimethylethylamine alane and analyzed them by transmission electron microscopy. We selected thermal decomposition of transition-metal carbonyls and subsequent controlled oxidation as a route to passivation layers. Future work will include optimization of the synthetic routes to passivated particles, characterization of these materials, and comparative studies with conventional materials.

This project is the first known application of IMS to the synthesis of EMs.

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Modeling of Rock Penetration

L. S. Costin, R. D. Hardy, W. A. Olsson, D. J. Frew, J. D. Rogers, A. F. Fossum, D. J. Holcomb

A basic approach to defeating a hard and deeply buried target (HDBT) requires the weapon to penetrate the target rock sufficiently so that adequate energy coupling is achieved. The mechanics of penetrating rock are poorly understood. The influence of such basic factors as porosity, hardness, stratification, and fracture density on penetrability are virtually unknown. The objective of this project is to develop a basic understanding of the mechanics of rock penetration that will lead to enhanced modeling capabilities to support the design of new penetrator systems. The project has four principal components. First, Sandia will develop an understanding of the physical mechanisms of rock deformation during penetration to provide a foundation for predictive modeling. We are undertaking this effort in the laboratory and focusing specifically on understanding rate sensitivity, coupled shear-volume response, the effects of three dimensional (3-D) stress states, and methods to upscale the results from laboratory to field scale. Second, we will develop a preliminary constitutive model for rock behavior during penetration that takes into account the principal deformational mechanisms controlling penetration as well as rock mass and structural features that could influence a penetration event. Third, we will run a series of intermediate-scale dynamic penetration tests to validate or calibrate the model under a variety of geologic and rock-mass conditions. Finally, we will integrate the experimental and constitutive modeling results with other ongoing efforts to develop dynamic penetration simulation capability so that 3-D probabilistic simulations of penetration can be run.

We made significant progress in developing a preliminary constitutive model that incorporates some, but not all, of the important behaviors. Laboratory work resulted in preliminary data on rate sensitivity and other effects that will be incorporated into the model in the near future.

- *Constitutive model.* The constitutive model includes two basic mechanisms: (1) compaction, dominated by pore collapse, and (2) dilation, caused by brittle microcracking, grain rotation, and overriding of asperities. As the mean stress increases, there is an increase in the value of shear stress at which microcracking initiates. Pore collapse is related directly to hydrostatic pressure and enhanced by shear stress. With

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increasing mean stress, the resistance to pore collapse increases as pore space is depleted. The model allows a smooth transition from one mechanism to the other. Because elevated strain rates are likely to exist during a penetration event, and because it is known that the strength of many geomaterials increases with increasing strain rate, the model was endowed with a strain-rate-sensitive capability. Using this capability it was possible to capture adequately the strength increase of Alaskan frozen soil in going from a strain rate of $1 \times 10^{-5} \text{ s}^{-1}$ to 500 s^{-1} . In addition, many sedimentary rocks and soils, such as frozen soil, exhibit anisotropic deformation. Because of the manner in which these rocks and soils were formed, the degree of anisotropy is often transversely isotropic. The constitutive model has therefore been formulated to handle transverse isotropy in the elastic and inelastic regimes.

Many brittle rocks contain joint sets, vugs, and other similar structural features that are not accounted for in standard laboratory-scale rock tests used to determine material constants. As a result, the strength of these rocks is overestimated. For rock structure that is comparable in scale to several times the penetrator diameter or less, the rock-mass properties could be extremely important. To accommodate the presence of rock joints, the model takes into account joint frequency and joint normal and shear stiffnesses in the elastic regime and includes a systematic reduction of strength determined by rock grade that incorporates joint frequency, weathering, hardness, and condition of core. We partially validated this model by comparing predictions against measured free-field velocity profiles for the "Hard Hat" underground nuclear test. When we do not use the rock-mass properties, the arrival times are too short, the wave amplitude is overestimated, and the pulsewidth is underestimated. When we use the rock-mass formulation, the predictions fully match the measurements.

- *Laboratory investigations.* We developed the testing techniques necessary for valid, confined split Hopkinson pressure bar (SHPB) experiments. We conducted an initial suite of confined SHPB experiments on the same limestone rock used in an extensive series of penetration tests. Results from the SHPB experiments show that this limestone is highly rate-sensitive over a wide range of confining pressures. Over approximately seven decades of strain rate, the strength of this rock almost doubles. We also conducted several tests using the new SHPB technique with confining pressure. Similar to the unconfined compression test results, we are seeing a substantial increase in rock strength with strain rate at all of the confining pressure levels tested to date. We used results from these initial

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tests to develop material parameters required for implementation into the rate-sensitive geomaterial model currently under development. We are implementing the model in finite-element codes such as SCE/PRONTO and ALEGRA to conduct validation calculations and predict the penetration performance of steel projectiles into limestone targets. We will compare model results to extensive test data acquired by other projects over the past several years.

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Nanoconverter*J. P. Brainard, T. R. Christenson*

Mechanical charging and voltage generation has been accomplished for over a hundred years. Usually these devices are large (meters in dimensions) and are capable of producing very high voltages (MeV). These machines use motors (some are hand-cranked) to transport small charges ($\sim$ mC) from a low-voltage electrode to a high-voltage electrode. The faster the charge is moved, the greater the current and voltage rise. Sandia's idea was to miniaturize such devices so that a few tens of volts could be generated from a few volts. This is done with a 6 mm wheel that transfers charge from a low-voltage source to a high-voltage shielded electrode. Because of the high-speed capability of nanomotors, we charged reasonable capacitance (a few nF) in reasonable times (a few tens of minutes) up to 200 V from a 20 V source.

We designed approximately 25 parts and made 25 replications of each part using microelectromechanical systems (MEMS) technology. The basic design is a small poly methacrylic acid (PMA) wheel (this rotor is 6 mm in diameter) on the shaft of a tiny high-speed motor (1.5 V DC). The rotor has 12 slots to insert electrodes, spring contacts, or brushes. A fixed outer ring (stator) also has 12 slots to accept electrodes, spring contacts, or brushes. In addition, the stator has 12 holes to support shields for Faraday cages over the high-voltage electrodes.

We fabricated and tested several designs. Unshielded high-voltage electrodes produced efficient charge transfer, but low step-up voltages. Shielded contacts produced high step-up voltages, but the charge-transfer efficiency was significantly reduced. For a 20 V input, we were able to charge a 2 nF capacitor to 200 V in a few tens of minutes.

We learned several lessons in this study. More work will be required to produce a viable device, but our work demonstrates that it is possible. By increasing input capacity (our design was not ideal), motor speed (our motor was relatively slow), number of contacts around the rotor (we used only one), and number of rotor/stator pairs (we used only one pair), we can charge large capacitors to high voltages in reasonable times. The packaging of such a device would be form-factor independent.

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Novel Proton-Exchange Membrane Materials for the Advancement of Direct Methanol Fuel-Cell Technology

C. J. Cornelius, J. M. Gee, C. J. Brinker

The advancement of direct methanol fuel-cell (DMFC) technology demands novel proton-exchange membranes (PEMs) that enable higher DMFC power outputs by minimizing methanol diffusion across the PEM. Currently, Nafion® is almost exclusively used as the PEM in a DMFC because of its excellent electrically insulating and high-proton conductivity properties. However, Nafion® is very expensive and suffers from a high rate of methanol diffusion across the anode to the cathode, which decreases DMFC efficiency by electrically shorting the cell. In addition, DMFC cells utilizing Nafion® must operate below or near 80°C to maintain proper hydration of the PEM for proton conductivity. Lower operating temperatures preclude the DMFC from attaining higher operating efficiencies, which occur at higher temperatures due to enhanced diffusion rates of water, methanol, carbon dioxide (CO₂), and minimization of carbon monoxide (CO) catalyst poisoning. These problems decrease catalyst efficiency and increase the cost of DMFC technology. The technical challenge for current DMFC technology is the discovery of PEM materials that increase the DMFC power output and the catalyst's efficiency. This can be realized immediately by preventing methanol diffusion across the PEM material to the cathode and increasing the operating temperature of the DMFC. This research addresses these technical challenges by utilizing hybrid inorganic-organic materials and self-assembled inorganic silica materials to inhibit methanol diffusion and increase the operating temperature, thereby increasing DMFC power output and catalyst efficiency and reducing the cost of a DMFC. These inexpensive materials will be assembled to create a barrier to methanol while maintaining good proton conductivity. We will controllably reduce mesoporous inorganic pore size with cross-linkable and functionalized polymers and coupling agents, and hybrid materials with significantly reduced chain mobility due to cross-links and covalent bonds with functionalized inorganic domains, to decrease methanol diffusion while maintaining good proton conductivity.

We synthesized the first generation of polyimide and polyimide hybrid inorganic-organic composite materials. We evaluated their physical properties, which included measuring the thermal stability in air, proton conductivity, swelling

DMFC LDRD data results.

This research addresses these technical challenges by utilizing hybrid inorganic-organic materials and self-assembled inorganic silica materials to inhibit methanol diffusion and increase the operating temperature, thereby increasing DMFC power output and catalyst efficiency and reducing the cost of a DMFC. ...We synthesized the first generation of polyimide and polyimide hybrid inorganic-organic composite materials.

characteristics, density, and gas-transport properties. Initial conductivities of these materials showed that they have increasing proton conductivities with increasing sulfonic acid content. At 20mol% diaminosulfonic acid (DASA), we observed a conductivity of 2×10^{-5} S/cm, which increased to 1.2×10^{-3} S/cm at 40mol% DASA. Results from this study demonstrated that a concentration of 60mol% DASA was necessary for conductivities to be equivalent to Nafion's® conductivity of 5×10^{-2} S/cm. Incorporation of inorganic particles by *in situ* sol-gel processing led to materials with significantly reduced swelling and increased thermal stability at higher DASA contents. Fully hydrated hybrid composite materials based on 20mol% DASA decreased in swelling from 10% to 2%, and 40mol% DASA hybrids decreased from 18% to 13%. Oxygen and H₂ gas transport decreased in these hybrid materials, which indicates that parasitic losses due to these fuels' diffusing from the anode to cathode would be reduced relative to Nafion®. These results are significant for H₂ fuel cells. Furthermore, the thermal stability characterized by the decomposition temperature of these hybrid materials improved by as much as 100°C, which may open areas of research for these materials in the air of thin-film protective coatings. The successes in this project led to several technical presentations, a technical advance, and a larger project focusing on novel materials based on hybrid composites that are aimed at conducting protons without the presence of water.

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Refereed

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Communicating with the *In Vivo* Sensor

T. A. Friedmann, J. P. Sullivan

The human body employs myriad sensors that efficiently communicate important environmental or internal status information to the brain. This is achieved by sending electrochemical signals along the nervous system (e.g., the sense of heat or temperature) or by sending chemical signals in the blood stream (e.g., the sense of hunger or exhaustion). Inorganic sensors can surpass some of the body's internal sensors in terms of sensitivity, but they have the distinct disadvantage that the information from the sensor must be consciously and deliberately acquired (e.g., reading a meter, listening to an audible signal, etc.). One ultimate goal is to implant the inorganic sensor within the body to provide precise analytical information about the in vivo environment (e.g., the presence of toxins, etc.). The dilemma is how to convey this information from the implanted sensor to the brain. One obvious approach is to interface the inorganic device with the nervous system of the individual, but there are formidable obstacles to achieving this. Such an approach would require directing specific cells to adhere to specific biocompatible sites on the inorganic device. In this project Sandia will do some fundamental preliminary studies on directed cell adhesion on amorphous diamond (a-D) microelectromechanical systems (MEMS) structures. Like silicon (Si), a-D can be used for the creation of MEMS and sensor structures, but unlike Si, a-D is inherently biocompatible. Sandia will perform the inorganic structure synthesis, while the studies of directed cell adhesion, using soft lithography-patterned fibronectin or other cell-specific extracellular proteins, will be performed at Harvard and Massachusetts Institute of Technology's (MIT's) bioengineering research labs. The short-term goal is to obtain directed cell adhesion and growth at specific sites on the inorganic device in a biological serum simulating the in vivo environment.

To be able to sense in the body requires that the implanted sensor have access to the analyte of interest. The natural reaction of the body to implanted foreign materials is essentially an immune response that causes cells to surround and encapsulate the implanted object. The degree of response can vary from no response to extreme dependence on the surface of the material implanted—its chemical composition, reactivity, size, and shape.

In this project Sandia will do some fundamental preliminary studies on directed cell adhesion on amorphous diamond (a-D) microelectromechanical systems (MEMS) structures. ... The short-term goal is to obtain directed cell adhesion and growth at specific sites on the inorganic device in a biological serum simulating the in vivo environment.

We used two strategies to assess the immune response of the body to a-D. First, to simulate the many small structures of thin, essentially two-dimensional (2-D) parts that could be made by surface micromachining (SMM), we synthesized a series of 1 μm -thick a-D particles with linear dimension varying from 1 μm to 30 μm in size on a sacrificial layer on Si; this process closely approximates the processing required to make MEMS structures. We released the particles in an acid etch from the substrate, cleaned them of acid, and injected them into live rat muscle tissue. We sacrificed the rats after varying times up to 6 months and assessed the immune response in the tissue. In all cases we found that there was no immune response to the injected particles.

We performed a second set of experiments using a series of a-D-coated Si die. These die were rectangular in shape with dimensions of $0.5 \times 0.5 \times 0.05 \text{ cm}^3$ —roughly simulating a standard die size for a MEMS device. We completely coated the die with a-D by repeated deposition steps where one face was coated in an off-axis technique that ensured that the sidewalls were also coated. We flipped and coated the die again. Finally, we annealed all die near 600°C to relieve stress. We then implanted these die in live rats for varying times up to 6 months to assess the immune response. In all cases we found the immune response to be minimal.

Finally, strategies for sensing in the body must be developed. One possibility for accomplishing this is to coat the sensor with a protein that will not cause an immune response and perhaps also facilitate in signal detection by concentrating the analyte material. We could also tailor the protein to cause directed cell adhesion of the cells of interest (e.g., blood cells) and no response from other cells. We progressed toward this goal by demonstrating directed cell adhesion. First, we exposed a-D-coated surfaces to a culture of bovine capillary endothelial cells. We found that these cells did not readily attach to the a-D surface. Next, we coated an a-D surface with fibronectin, a common extracellular cell-specific protein, and exposed it to the same bovine capillary endothelial cells. We found that the cells attached readily to the surface without a negative response.

We showed that the immune response to a-D surfaces implanted in rats is minimal or nonexistent. In addition, we showed that we can get directed cell adhesion to a-D surfaces using intermediary proteins. This establishes that a-D is a good candidate for *in vivo* sensor applications.

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Other Communications

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Agile, Microsystems-Enabled Receiver

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The goal of this project is to develop and integrate radio-frequency (RF) microelectromechanical systems (MEMS) and gallium nitride (GaN) device technologies to create an agile receiver front-end for applications such as synthetic-aperture radar (SAR), fuzes, tags, and active phased arrays. The intended module consists of a MEMS transmit/receive (T/R) switch, a MEMS tunable filter, and a GaN low-noise amplifier (LNA), providing significant advantages over existing radar front-ends. The low loss of the RF MEMS elements will allow tunable filters and T/R switches to precede the LNA without significantly degrading the noise figure, facilitating both jammer protection and real-time adaptivity. The GaN LNA offers high dynamic range and natural immunity to overload damage, eliminating the need for a separate limiter. The module, interconnected via monolithic and multichip-module (MCM) techniques, will be several times smaller than current radar front-ends.

Realizing these advances presents formidable technical challenges in electronic materials, processing, and devices. To achieve optimum performance, the RF MEMS components require careful design, well-controlled processing, and detailed characterization. The GaN transistors present challenges in materials growth, device processing and testing, and thermal management. Finally, the integration of these novel technologies into a single module will require accurate component characterization and electrical design. Once these challenges are met, the module will provide lower loss and higher power than existing packages much larger in size.

Sandia continued work on GaN high field-effect transistors (HFETs) to improve the power handling and frequency performance of the devices. Additionally, we fabricated several different RF MEMS switches to evaluate their suitability for high-power T/R modules and other applications. Also, we fabricated and characterized on-wafer passive devices and made significant progress toward demonstrating RF MEMS tunable capacitors. Finally, we designed and fabricated tunable filters using RF MEMS devices. With these accomplishments, we made good progress toward the final goal of this project.

In the area of RF MEMS T/R switches, we demonstrated one-million switching cycles with a metal-contacting

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micromachined relay on gallium arsenide (GaAs) and demonstrated metal-contacting RF MEMS switches with less than 0.15 dB of loss and 15 dB of isolation through Ku-band. In addition, we fabricated capacitive switches demonstrating switching lifetimes over one-billion cycles. To fabricate a suitable high-power switch for T/R applications, we identified self-actuation and heating at the contact surface as the primary issues facing high-power MEMS switches. To address these issues and provide state-of-the art RF power handling, we are in the process of designing a high-power, robust switch that we will fabricate in upcoming work.

To enable the GaN LNA microwave monolithic integrated circuit (MMIC), we fabricated and tested GaN field-effect transistors (FETs) on sapphire substrates with gate lengths as small as 0.1 μm . The focus of our GaN transistor effort was transferring the growth process from sapphire substrates to silicon carbide (SiC) substrates, which will provide superior thermal performance. This process has proven to be difficult, but we fabricated promising preliminary devices. After we grow and fabricate optimized devices on SiC substrates, we will measure the noise properties of the devices, allowing for their use in the LNA design.

To complete the technology required for the MMIC fabrication on the final aluminum nitride (AlN) integration substrate, we fabricated and characterized passive inductors and capacitors on GaAs and AlN substrates. We improved component yields to over 95%, with low loss and high self-resonant frequencies. In addition to fixed passive devices, we designed several different tunable RF MEMS capacitors. The simplest capacitors were fabricated and demonstrated loss below 0.2 dB, high self-resonant frequencies above 30 GHz, and 25% tuning with a maximum value of 200 fF with a 10 V actuation voltage. We designed other capacitors with improved tuning range, linearity, and other properties, but have not completed fabrication.

We designed and fabricated several filter topologies, using RF MEMS switches or tunable capacitors, on GaAs. We designed topologies containing fixed elements that are switched into and out of the circuit using RF MEMS switches and fabricated simple prototype circuits with metal shorts in the place of the switches. The best designs demonstrate tuning from 7.7 GHz to 12.2 GHz, bandwidths of approximately 2.0 GHz, and losses of approximately 3.5 dB prior to the addition of switches. We refined the filter design and will shortly begin fabricating the new filters using actual RF MEMS switches. In addition to the switched filter, we realized a continuously

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tunable distributed filter design using coupled lines and tunable capacitors. This filter demonstrated 1 GHz of fine-tuning around 6 GHz, with approximately 2 GHz of bandwidth and 4 dB of loss. We are refining all of these designs to improve the loss properties and frequency range and give Sandia a differentiating capability in the area of tunable RF MEMS filters.

We made significant progress in several critical technological areas, especially RF MEMS devices and circuits. Despite setbacks in the growth of GaN devices on SiC, we obtained several promising results and made progress toward development of the GaN LNA MMIC. In future work, we expect to make further progress toward the project goals, providing the background and technology for the fabrication of the agile radar front-end.

We are refining all of these designs to improve the loss properties and frequency range and give Sandia a differentiating capability in the area of tunable RF MEMS filters.

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Linking Geosciences to Emerging Bioengineering Technologies

R. T. Cygan, C. K. Ho, C. J. Weiss

Geosciences research at Sandia utilizes state-of-the-art techniques to study the fundamental science underlying complex natural physiochemical processes, often spanning time, composition, and length scales well beyond those of the materials and engineering sciences. Until recently, most of this research was limited to applications associated with natural processes occurring within the mantle, crust, and near-surface regions of the Earth. Application of geoscience analytical, experimental, and theoretical methods to biological and human health systems would be beneficial to Sandia's programmatic efforts in these areas. In this effort, we evaluated several cross-over applications of the Geosciences research program at Sandia to bioengineering, biochemistry, and human health areas. This work includes literature research and preliminary computer modeling to explore the potential for cross-over science and technology. One application area involves the chemical reactivity and binding of organic constituents, such as amino acids and oligopeptides (models for proteins), to inorganic substrates such as clay mineral surfaces. These hybrid organic-inorganic materials can be utilized in implants and drug-delivery systems. A second application area examines the transport of pharmaceuticals to human individuals through the skin layers (percutaneous absorption). Concerns about the mechanisms of drug or chemical transport are critical in transdermal drug delivery and in hazardous-chemical exposure assessments. The final application addressed in this study is directed at improving diagnostic imaging of soft tissue through improved interpretation of three-dimensional impedance tomographic imaging. This application is of significance in the diagnosis of cancerous growths.

We completed preliminary molecular simulations to examine the intercalation of amino acids and oligopeptides in the interlayer of a clay mineral. The complex nature of biomolecules within the interlayer or on the surface of clays has significance in our fundamental understanding of such disparate topics as drug-delivery systems, gene therapy, protein function, and the origin of life. We use a hybrid-energy forcefield allowing for the simultaneous simulation of both clay and oligopeptide to determine the general behavior of various amino-acid side chains within the clay interlayer. No atomic or

EIT imaging of upper arm.

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cell parameter constraints are imposed, thereby allowing complete constant-pressure optimization and molecular dynamics (MD) with an NPT (number of particles pressure temperature) ensemble. In general, the molecular mechanics simulations suggest that clay surfaces are effective in creating significant nonbonded interactions between the clay and the oligopeptide. These interactions may be competitive with the nonbonded interactions that exist within the oligopeptide chain and can lead to perturbation of the peptide structure once intercalated. There is evidence of denaturing of the protein structure by the clay surface in our simulations. The polar and charged side chains of the oligopeptide are most likely to interact with the interlayer cations. More sophisticated molecular simulations involving explicit waters of solvation for the protein, hydrated clay interlayers, and different charged distributions in the clay substrates are recommended for future research.

We delivered a transient three-phase model of percutaneous absorption of chemicals. Penetration routes through the skin that were modeled include (1) intercellular diffusion through the stratum corneum, which comprised an immobile sorptive protein phase (keratinocytes) and mobile aqueous (water) and oil (lipid) phases, (2) diffusion through aqueous-phase sweat ducts, and (3) diffusion through oil-phase hair follicles. We assigned uncertainty distributions to model parameters and performed a probabilistic Monte Carlo analysis to simulate mass fluxes through each route. Results yielded a wide distribution of simulated mass fluxes due to the uncertainty in the input variables. At early times (60 s), transport through the sweat ducts provided a significant amount of mass flux into the bloodstream. At longer times (1 hour), diffusion through the stratum corneum became important because of its relatively large surface area. Similarly, diffusion through the hair follicles was more significant than diffusion through the sweat ducts at later times because of the larger porosity of hair follicles. We also performed sensitivity analyses using stepwise linear regression to identify input parameters that were most important to the simulated mass fluxes at different times. This probabilistic analysis of percutaneous absorption (PAPA) method may prove useful to studies of exposure assessment and transdermal drug delivery.

A common goal to both the medical and geoscience communities is the development of noninvasive methods for peering into the interior of an object. The problem of imaging the interior object via some noninvasive method can be broadly lumped into two primary steps: measurement of some physical

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quantity (such as voltage, current, or the electromagnetic fields) on the surface of the body, and utilization of an algorithm that infers the distribution of some physical property (such as electrical conductivity) within the body based solely on these surface measurements. Two imaging methods used by geophysicists for subsurface imaging found utility as methods for imaging the interior of the human body: electrical impedance tomography and magnetic induction tomography. The principles of operation for each method are based on the observation that different biological tissues have varying capacities for sustaining a flow of electric current that is influenced by, for example, the density of vascularization in a given region. The variations in vascularization can, in some cases, be readily correlated to differences in tissue type such as lung, muscle, and bone tissues in the thorax. The variations in the density of vascularization, and hence electrical conductivity, can be attributed to the presence of tumorous growths within the body.

Two imaging methods used by geophysicists for subsurface imaging found utility as methods for imaging the interior of the human body: electrical impedance tomography and magnetic induction tomography.

Refereed

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Energy Storage: Leaving Chemistry in the Dust

B. H. Rose, P. V. Dressendorfer, R. J. Leeper

This project involves examining the interaction between nuclear physics and solid-state physics for possible energy-storage concepts. It is inherently high-risk because it is an area that has not been previously examined extensively. The basic idea is to excite the nuclei or internal tightly bound electrons of atoms or ions arranged in a crystal, whose periodicity impedes the decay of these excited states. The energy could be released by mechanically destroying the crystal structure. The high-energy state can be in the form of an excited nucleus, a radioactive nucleus, or a missing internal orbital electron. The impediment to decaying to lower energy would come from the relationship between the lattice spacing and the wavelength of the resulting gamma, x-ray, or beta particle (forbidden energy levels). One might think the decay product would ignore the lattice, but the Mossbauer effect shows that this is not always true, that a high-energy state can interact with the whole crystal. Energy between 100 and 10,000 eV/atom might be realized if the right combination of energy states and crystal structure can be found. Depending on the characteristic speed of decay, this energy-storage scheme could be used as a battery, rocket fuel, or explosive. Given the complexity of the chart of radioactive nuclides, the many possible energy-level configurations of nuclei and atoms, and the large number of possible lattice structures, investigation of this concept must negotiate many low-probability turns. Therefore, it must be labeled a “one-percenter.” But the payoff could be enormous and would be in the area between nuclear and conventional munitions where Sandia could play a leading role.

This investigation started with a search for (1) an appropriate long-lifetime excited state of the electron orbits or nucleus, and (2) a crystal structure with a periodicity that encouraged the trapping of the photon (gamma or x-ray) that would be emitted by decay to a lower energy state. Our literature search kept running into a reverse problem that was closely related but that made us rethink the true goal.

In short, there has been a 20-year search for isomers that can store million electron volts (MeV) of energy per atom. An isomer is an excited nuclear state that is unusually stable (lasts longer than a millisecond, often many days). Every year universities and other weapons labs have discovered new

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isomers. However, they are troubled with how to create a dense lattice of excited isomeric nuclei, which are hard to excite, and how to trigger their decay quickly. We discovered that the same lattice spacing that would contain a single excited state could also induce a lattice of excited states to complete emission (reduction to ground-state) by repeated internal reflection and stimulation caused by a chance decay.

However, to accomplish this, we continued to search for a regular solid that could be compressed a considerable amount, not the 0.01% with enormous pressure, but 1%–10% with mechanical or explosive pressures. Here we entered the realm of hydrogen-filled solids, aerogels, and biostructures (lipids).

One of the initial motivators was the nuclear/atomic interaction shown by Mossbauer. In this study, we plotted a comparison of the strength of the Mossbauer effect to the lattice spacing and the emission wavelength.

An analogy between the effect we sought and the photonic crystal steered us to face-centered cubic crystals to achieve three-dimensional symmetric bandgaps. In addition, several next-nearest-neighbor effects seem plausible by the analogy.

We showed that the hypothesis held under scrutiny, that many man-years of isomeric studies were making incremental progress, that advances in PhC gave hints around some of the hurdles. However, we may have turned the 1% into 2%, but we did not find the right crystal and the right excitation to store energy at this point.

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38726

Novel Algorithms and Experimental Techniques for Quantitative Spectral Analysis of Particulates

D. M. Haaland, C. M. Wehlburg

Quantitative infrared (IR) spectroscopic measurements of powders are often problematic for a variety of reasons. Current IR technology for analysis of small particles in their natural state as powders generally involves diffuse reflection or attenuated total reflection (ATR) measurements. However, both methods are limited in their quantitative abilities because of variable pathlength effects that cannot be distinguished from concentration changes. Diffuse reflection suffers from particle-size scattering effects that are wavelength-dependent. ATR suffers from variations in packing density and contact with the ATR waveguide that cause wavelength-dependent pathlength variations. Thus, quantitative IR analysis of these materials is greatly limited.

Sandia recently developed new proprietary multivariate algorithms that may be able to solve these longstanding problems in quantitative spectroscopy. The new class of augmented multivariate classical least-squares (CLS) methods can incorporate into the calibration models empirically derived information that must be ignored by the calibration model. Thus, we used these new algorithms to effectively ignore the wavelength-dependent pathlength and instrumental drift effects in quantitative analysis of powders. Success would increase our quantitative spectral-analysis capabilities and allow accurate quantitative analyses of materials such as explosives and propellants, sol-gels, catalysts, coated particles for biosensors, pharmaceuticals, and quantum dots tagged with biomolecules. These novel methods could then be extended to hyperspectral ATR imaging for quantitative analysis of heterogeneous powders, which would have significant impact on the quantitative analysis of aging energetic materials.

The IR spectroscopic study of powders plays an important role in monitoring product in the pharmaceutical industry. A collaborator at GlaxoSmithKline provided ATR IR measurements of a series of two-component mixtures developed for quality control during drug production. To account for variations in the ATR measurements, we varied and recorded the contact pressure with the waveguide for each powder mixture of the two components. Our analysis of this data indicated, however, that there was little correlation of the

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measured spectra with variation in applied pressure to the ATR sample. Theoretically, as the contact pressure is increased, the effective sample contact with the ATR crystal increases and the resulting effective pathlength increases. Therefore, for some concentration mixtures, the spectral response should increase as a function of the applied pressure. However, our analysis pointed out problems in the ATR sampling technique when this correlation was shown not to exist in the data provided to us.

The collaborator made changes in the ATR technique that would improve the contact pressure across the entire sample. To ascertain the efficacy of the new sampling technique, we collected the second set of data at constant pressure, but with multiple repeats of each of the seven concentration profiles. The analysis of the second set of data elucidated a common occurrence in spectroscopic measurements. Over a period of time, an instrument response may drift, causing the predictive ability of the original calibration model to degrade. Our analysis of the second set of data showed a clear correlation with collection time. Previous studies by our group, utilizing proprietary algorithms and novel experimental design, demonstrated improved predictive ability for a calibration model through the use of a repeat sample to extract the instrument-drift spectral response.

We utilized a similar procedure on the second set of data by choosing a mid-concentration sample and its repeats to model instrument drift. Normally, the inclusion of repeats in cross-validation calibration results for a single set of data does not improve the error since the model already includes information about instrument drift from the calibration spectra collected over that day. However, Day 4 data suffered from a higher sampling error than Day 3. The increase in error with the inclusion of repeats from Day 4 indicated that even though the ATR sampling was at a constant applied pressure, there were still variations in pressure that were causing a degradation in the model. Data based on a subsequent experimental design needed to be collected that would separately capture both instrumental drift and pressure variations.

The use of repeat samples improved the predictive ability of both the hybrid classical least-squares/partial least-squares (CLS/PLS) method and the industry standard PLS method. Although the prediction errors do not change, the reduced number of “false” outliers evidences the model improvement. When compared to the standard PLS technique used by industry, the hybrid CLS/PLS algorithm developed by our group also had lower standard errors of prediction for Day 4.

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We recommended a new experimental design to the collaborator at GlaxoSmithKline. A calibration model developed with our proprietary algorithms and the data from this design should be able to separate the pressure effects from instrument drift and further improve the predictive ability of ATR IR measurements utilized for quality control of pharmaceutical products.

38727

Self-Healing Adhesives and Encapsulants: Long-Term, High-Performance Weapon Components

J. A. Emerson, A. M. Morales, R. K. Giunta, S. G. Thoma

The results of this study show that self-healing adhesives may be useful to prolong the lifetime of epoxy-based adhesive bonds in weapon components. In this study, Sandia incorporated a microencapsulated cross-linking agent and a catalyst into epoxy matrices. Based on our experiments, we conclude that the concept of self-healing adhesives and encapsulants may yet be valid for long-term, high-performance weapon components, particularly with respect to slow-growing, age-induced microcracks. However, the chemistry of the self-healing system must be designed around the particular epoxy system used. Specifically, we suggest a concentric microencapsulation approach, whereby the original epoxy resin (two components) is microencapsulated in concentric spheres so that the healing medium is identical to the bulk matrix, and the healing mixture contains both components rather than just the cross-linking agent, as examined in this study.

The results of this study show that self-healing adhesives may be useful to prolong the lifetime of epoxy-based adhesive bonds in weapon components. In this study, we incorporated a microencapsulated cross-linking agent and a catalyst into epoxy matrices. We determined that (1) the cross-linking agent can be microencapsulated into a leak-free shell, and (2) the microcapsules and the catalyst can be prepared and incorporated into the epoxy matrix at concentrations high enough to allow crack healing, but without decreasing the epoxy's strength relative to the virgin system. However, we identified a number of difficulties with this approach. Specifically, (1) epoxy does not heal to original (virgin) conditions—healing often only slightly, (2) healing is a function of contact area and hence crack width and crack-growth rate, (3) healing is a function of compressive force, (4) healing is a function of temperature, and (5) chemistry of the healing system explored is incompatible with War Reserve systems. We concluded that the concept of self-healing adhesives and encapsulants may yet be valid for long-term, high-performance weapon components, particularly with respect to slow-growing, age-induced microcracks. However, the chemistry of the self-healing system must be designed around the particular epoxy system used. Specifically, we suggest a concentric

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38729

Neutron-Only Detector for JTA Tests*J. C. Lund, N. R. Hilton, J. P. Gollnick*

The goal of this project is to develop a neutron detector that is intrinsically sensitive to neutrons alone, but insensitive to x-rays. The proposed device would also be able to score a neutron generator (NG) during a joint test assembly (JTA) flight with better precision and do so in less volume than currently deployed JTA neutron monitors. Such a device would be useful in Sandia's JTA program to measure the reliability of NGs during flight testing. The project consisted of two high-risk experiments that would seek to determine whether either of two physical principles could be used as the basis of a neutron-only detector. The two physical approaches to discriminating neutrons from x-rays will be a time-discrimination technique and a spatial-discrimination method.

The goal of this research is to develop neutron detectors that are insensitive to other types of radiation. We investigated two approaches. The first approach consisted of using the shape and pattern of pulses produced by the neutron detector to discriminate neutrons from other types of radiation. This time-discrimination seemed to work very well and will be used in all of the "far-field" detectors we develop in the foreseeable future. An additional advantage of the time-domain technique is that it not only discriminates neutrons from other particles that strike the detector, but it also is capable of discriminating neutrons that travel directly to the detector from neutrons that have scattered on the way to the detector (to some degree). This additional capability may prove extremely valuable in the development of future far-field neutron detectors.

The second approach to discriminating neutrons from other radiation consisted of a spatial-discrimination method where the pattern of energy deposition in the detector was used to discriminate particles. We built a prototype assembly to test this principle but are awaiting the delivery of a NG to test it in our laboratory.

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39212

MEMS-Based Electromechanical Acoustic-Energy Harvester

K. B. Pfeifer

Sandia analyzed, designed, and microfabricated a circular, piezoelectric-composite membrane for harvesting acoustic energy. The piezoelectric membrane can be coupled to a Helmholtz resonator or used alone in an acoustic field to generate electrical energy that can either be used immediately to power other devices, such as sensors and control systems, or be stored for later use. The compact size of the membrane, afforded by microfabrication, is especially useful for pairing with microfabricated sensors that may have small but finite power requirements. We based theoretical analysis of the piezoelectric-composite membrane on an axisymmetric piezoelectric-composite plate model developed at the University of Florida, leading to an optimized annular ring configuration for the active piezoelectric layer. The resulting structure employs a sol-gel-deposited lead zirconate titanate (PZT) layer for piezoelectric transduction with an underlying silicon structural layer and was fabricated primarily in the Compound Semiconductor Research Laboratory at Sandia.

The goal of this research is to develop an electromechanical acoustic resonator for reclamation of energy using microelectromechanical systems (MEMS) technology. The proposed MEMS device converts acoustical energy to electrical energy, which can then be either stored for later use or utilized directly for a particular circuit application. The relatively small geometries possible in MEMS make such a device useful for pairing with small, low-power sensors to create a self-powered sensor package.

A type of acoustic resonator, known as a Helmholtz resonator, consists of a cavity connected to the environment through a small neck. When excited by an acoustic input, a single resonance is seen whereby the acoustic pressure inside the cavity is much greater than the incident acoustic signal since acoustic energy is stored in the resonator. The large acoustic pressure can be exploited for energy reclamation by converting the acoustic energy to electrical energy. This can be accomplished via acoustical-to-mechanical transduction (i.e., a compliant diaphragm), followed by mechanical-to-electrical transduction. We can achieve electromechanical transduction in a number of ways, including capacitive and piezoelectric techniques. This research focuses on the piezoelectric

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transduction of energy by means of a piezoelectric-composite membrane.

Through the electromechanical transduction, we created a charge that an energy-reclamation circuit can harvest and store. In one implementation, we used a rectifying switched capacitor circuit to efficiently convert the AC signal to DC, which we then stored across a low-loss capacitor [Smalser, 1997]. Another possibility was based on the Kymissis circuit approach [Kymissis *et al.*, 1998]. This approach utilized passive storage elements for impedance matching coupled with a regulated output for improved energy-harvesting performance.

Other Communications

Horowitz, S. B. 2002. Development of a MEMS piezoelectric membrane for acoustic-energy harvesting. Paper presented at the Sandia Student Intern 7th Annual Symposium, 1 August, at the Crowne Plaza Pyramid Hotel, Albuquerque, New Mexico.

Through the electromechanical transduction, we created a charge that an energy-reclamation circuit can harvest and store.

41726

Direct Simulation of Solid-Fluid Systems*B. K. Cook*

Numerous important industrial and natural processes are dominated by the interaction of particles (or a cemented particulate matrix) with neighboring particles and a surrounding fluid. For example, in the petroleum industry, sanding is a billion-dollar problem that results from the erosion of sand from an oil-bearing sandstone formation during production. Sandia's understanding of the discontinuous physics underlying these processes and our associated predictive capabilities have been limited by continuum modeling approaches and difficult-to-perform experimental studies. An alternate approach is to simulate these systems at the grain scale. However, until recently, the direct simulation of these three-dimensional (3-D), dynamic solid-fluid systems has proven computationally intractable.

Rapid increases in parallel-based computational resources, combined with the development of efficient and robust modeling schemes, are marshalling in an exciting era of simulation-based discovery into the behavior and prediction of the dynamics of particle-fluid systems. Leveraging these developments, this project is developing an unprecedented computational capability for the dynamic simulation of the coupled solid and fluid phases, fully resolving the interaction of individual solid particles (and particle assemblages) with other solid particles and the surrounding fluid. The project focuses on the refinement and parallel implementation of a numerical scheme that uses the lattice-Boltzmann and discrete-element methods (DEM) to solve the underlying governing equations for the fluid and solid phases, respectively. We are developing a powerful simulation environment to enable the computational exploration of solid-fluid physics.

Outstanding challenges currently being explored in this research include (1) the formulation and implementation of high-fidelity numerical techniques to better resolve underlying physics, such as the improved representation of irregularly shaped particles, and (2) the software design and implementation of an integrated modeling application.

We are currently developing an efficient discrete-element representation for nonspherical particles. Although commonly used by the modeling community, disc and spherical elements do not capture key behaviors of real particles because they exhibit pathological packing structures, roll when subjected to small perturbations, and cannot interlock. We made significant

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progress on a pseudo-ellipsoidal representation proposed by Wang (1999). The pseudo-ellipsoidal element approximates an ellipsoidal element as the volume enclosed by three arcs rotated about a centerline. This representation has the following important properties:

- Continuous element surface—no singularities to cause contact resolution problems.
- Compact—few variables are needed to describe the geometry of the object.
- Simple analytical representation—allows quick, low-iterative calculation of the contact forces and contact point. Because every surface is the arc of a circle, the curvature is known at every point.

We developed a new analytical-iterative contact-detection method that promises speed increases of between 300% and 600% over the previously proposed contact-detection method for a surface point identification error less than 1° . We will perform further work to incorporate the particle representation and contact-detection algorithm into a 3-D DEM code under development.

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Other Communications

Johnson, S., and J. Williams. 2002. Formation of packing structures in discrete element modeling with disks. *Proc. 3rd International Conference on Discrete Element Methods: Numerical Modeling of Discontinuities* 1 (22–25 September, Santa Fe, New Mexico): 99–103.

42461

Support-Active Site Interactions in Heterogeneous Catalysts

R. A. Kemp, A. G. Hascall

To rationally synthesize heterogeneous catalysts, it is imperative to comprehend the function of the various components of the catalyst. It is of utmost importance to know how a support interacts with the active site of the catalyst. In fact, in the catalysis world this lack of fundamental understanding of the relationship between active site and support is the single largest reason that catalysis is considered an "empirical" or "black box" science rather than a well-understood one. In this study Sandia will look at an industrially important catalyst system with an eye toward explaining the relationship between the support and the active site. Along with the interest in understanding the catalyst in a fundamental sense, we also have the very real possibility of significantly affecting the technology and economics of ethylene oligomer production. In this work we will prepare novel ethylene oligomerization catalysts, which are normally homogeneous, inside the pores of nano- and mesoporous materials. Essentially, we will tailor the size and scale of the catalyst active site and its surrounding environment to match the size of the molecular product(s) we wish to make. The overall purpose of the study will be to understand the effects that steric constraints and pore structures can have on growing oligomer chains. We wish to limit oligomer growth at defined lengths by using the steric constraints imposed by the pore walls of the nano- or mesoporous supports. In the future, understanding the relationship between support and active site should and will certainly lead to faster development and implementation of advanced catalysts. Ultimately, this study should even aid in making catalysts as selective as biological enzymes.

Although we do not yet have catalytic results, we have begun synthesizing main group complexes based on boron, aluminum, and gallium. We are characterizing these species and will adsorb them into the pores of various forms of faujasite. Our previous work showed that these main group compounds are not effective at making polymers; therefore, they should be ideal to make oligomers. We prepared different surfactants to act as templates to prepare various mesoporous silicates and are in the process of learning how to operate equipment to make these materials. We are developing techniques to add these organometallics to porous solids while retaining at least one metal-carbon bond to act as the catalytic site for

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oligomerization. We are also attempting to use the Shell nickel-phosphinocarboxylate catalyst as a templating agent to synthesize it within the pores of a silica-alumina framework. Use of different phosphinocarboxylates as templating agents is also under way, with the goal to determine which water-tolerant ligand can effectively act as a template in this hydrothermal synthesis.

42483

An Analysis of the Automotive Industry as a Source for Weapon Components and Manufacturing Processes

R. J. Steichen

Many of the commercial and captive suppliers who provided nuclear weapons components and manufacturing processes during the Cold War no longer have the capacity or desire to remain suppliers for future systems. For example, radiation-hardened semiconductor suppliers declined from twenty to two from 1985 to 1990. Finding or creating alternative suppliers will depend on Sandia's acquiring in-depth technical and business understanding of both suppliers' industrial capabilities and their cost-management opportunities.

Most suppliers exit because the margins are too low (low volume, few orders) to sustain continued production.

For weapons components, it is important to recognize that each supplier is actually embedded in a value chain that stretches from the supplier's suppliers to the customer's customers. Approaching the "supplier" problem as a value chain provides the opportunity to work with potential suppliers in defining improvement opportunities in (1) linkages with suppliers, (2) linkages with customers, (3) process linkages within the value chain of the nuclear weapons complex, and (4) linkages across lines of business within Sandia, the Department of Energy (DOE), and the federal government. In short, addressing today's defense needs requires more fully engaging the capability of U.S. industry.

Implementing new technologies in weapons systems requires addressing three stages in the technology supply chain: (1) discovery/development engineering, (2) testing/verification engineering, and (3) supply-chain development. The automotive supply chain comprises 6% of the U.S. gross national product (GNP). The technology needs in the automotive industry sector are remarkably similar to those in weapons systems. Automotive components have lifetime, reliability, temperature, thermal-cycle, mechanical shock, and design/manufacturing requirements that are similar to those for weapons components. They also rely heavily on advances in technologies such as metal forging, encapsulated electronics, microelectromechanical systems (MEMS) devices, sensors, power sources, and materials- and computational-based modeling and simulation.

(1) We surveyed Sandia's present relationship with the automotive industry.

...addressing today's defense needs requires more fully engaging the capability of U.S. industry.

(2) We developed a taxonomy of weapons program component and manufacturing process needs aligned with automotive-industry needs. An overall classification scheme of parallel technology requirements has been prepared but must be filled in with weapons-community input.

(3) We evaluated at least five specific needs for technology compatibility, reliability, manufacturability, and cost. We must prioritize technology parallels for weapons and automotive systems according to specific mission-related programs; this priority must be established through input from the weapons groups.

(4) We identified at least four candidate suppliers and their technologies to establish relationships between their capabilities and our needs that demonstrate compatibility. We initiated contacts with Toyota Motor Corporation (fuel cells, batteries), Keystone Powdered Metals (component manufacturing), Kistler Instruments (sensors), and BorgWarner Corporation (system integration). Discussions are currently in the discovery stage.

(5) We conducted an in-depth technical evaluation of the candidate technologies to verify that suppliers' technical capabilities are consistent with Sandia's weapon system stockpile-to-target sequence (STS) requirements. The technical evaluation of potential supplier capabilities is tied to the discovery process being pursued.

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44136

Fluid-Structural Interactions in Wetting and Penetration into Porous Media

P. R. Schunk

Sandia developed a theory for drying a polymer-solution coating on a paper substrate that predicts transport of water into the pores in the paper and removal of water from the coating/paper system. Paper exhibits a dual-scale fibrous porous structure, with small pores in the paper fibers and large pores between the fibers. At low moisture content, water absorbs into the micropores in the fibers, but the macropores contain only vapor. Moisture can transport by diffusion or capillary flow through the fibers and by vapor diffusion in the macropores. At low moisture content, moisture transport in paper can be accurately modeled using a two-phase model. At higher moisture content, the fibers swell and liquid water appears in the macropores; then we need a three-phase model or an unsaturated-flow model to predict moisture transport.

We can predict the degree of swelling and change in porosity of the paper by a microstructural model of fiber deformation. A suitable microstructural model will enable predicting changes in porosity and pore-size distribution due to capillary forces acting within the porous medium. There are several common approaches to modeling moisture transport in porous media that differ in the choice of field variable(s) and in their accuracy at certain ranges of saturation or capillary pressure.

We developed a fluid-structural model of the local deformation near a dynamic contact line on an elastic substrate. The model predicts the effect of several physical properties on the wetting process. We applied this model to predict fluid penetration into a slit pore with deformable walls. If the penetrating fluid is neutrally wetting (contact angle close to 90 degrees), the elasticity of the walls does not significantly affect the rate of fluid penetration. If the penetrating fluid is nonwetting (contact angle greater than 90 degrees), elasticity of the walls increases the rate of fluid penetration, whereas for wetting fluids, elasticity of the walls decreases the rate of fluid penetration. To our knowledge, this is the first model predicting the effect of wall flexibility on fluid penetration into porous media.

We also developed a model of water penetration into silicon-coated paper during drying of an emulsion coating. The model is applicable to drying of paper at low moisture content. The predictions show several stages of drying coatings on

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paper: (1) rapid penetration of water into the paper, (2) drying of the coating, (3) transport of moisture back from the paper into the coating, and (4) drying of the paper. Currently, our model has neglected swelling and deformation of the paper substrate.

Refereed

Madasu, S., and R. A. Cairncross. 2002. Static wetting on flexible substrates: A finite-element formulation. *J. Computational Physics*, accepted.

45279

Macroscopic Rates, Microscopic Observations, and Molecular Models of the Dissolution of Carbonate Phases

R. T. Cygan

Our understanding of the kinetics of dissolution and growth of carbonate phases is critical to a variety of natural, industrial, and environmental processes. Fortunately, the relatively fast dissolution rates of carbonate phases provide a suitable time-scale for the laboratory investigation of these materials compared to the orders-of-magnitude-slower rates for oxide and silicate phases. Sandia will evaluate and combine various macroscopic and microscopic experimental techniques with molecular modeling methods to derive a general mechanistic model for the dissolution of various metal carbonate phases. This work combines real-time morphology observations from the atomic-force microscope (AFM) with dissolution rates from macroscopic flow-through reactors. Etch-pit dissolution mechanisms can be directly linked to molecular models of carbonate surfaces with particular emphasis on the surface structure, surface energy, and formation of dissolution steps. Molecular simulations of the various metal carbonates provide a technically rigorous basis for the intercomparison of bulk and surface structures, surface energies, and relative stabilities of the reacting surfaces.

This research combines the results of experimental dissolution experiments performed at Harvard University with state-of-the-art molecular simulation methods developed at Sandia. The scientific literature of carbonate-phase dissolution is quite large; however, until recently these studies typically provided either independent macroscopic dissolution rates or microscopic observations, usually with an AFM. The unique aspect of the present study is that carbonate dissolution rates are determined through geometry calculations of real-time surface modifications as observed by AFM of single crystals while simultaneously determining macroscopic dissolution rates based on the effluent solution. We perform experiments at a wide range of pH conditions and for various endmember carbonate phases, including calcite (CaCO_3), magnesite (MgCO_3), rhodochrosite (MnCO_3), siderite (FeCO_3), and smithsonite (ZnCO_3).

Results of the microscopic and macroscopic dissolution measurements of the dominant (10–14) cleavage surface as a

Model of rhombohedral pit in carbonate.

The unique aspect of the present study is that carbonate dissolution rates are determined through geometry calculations of real-time surface modifications as observed by AFM of single crystals while simultaneously determining macroscopic dissolution rates based on the effluent solution.

function of solution pH suggest the occurrence of multiple dissolution mechanisms dependent on phase chemistry and pH region. Fast dissolution occurs at the low-pH region, suggesting an acceleration of reaction mediated by the protonation of surface sites and the removal of carbonate material to form a surface covered by shallow pits. Intermediate- to high-pH regimes exhibit a relatively slow dissolution rate, which is interpreted as a crossover to a water-mediated mechanism. Calcite exhibits the most rapid dissolution rate, with the other phases following the general trend in rate, based on water-ligand exchange rates, which are related to metal-ion charge-to-size ratios. Smithsonite behaves contrary to this generalization and dissolves almost as fast as calcite; however, the AFM surfaces exhibit a mixed dissolution morphology of corrosion features with deep pits. The formation of shallow and rhombohedral dissolution pits is quite common for the carbonate materials. Dissolution of rhodochrosite provides an excellent example of pit formation. Pit growth typically occurs at the surface expression of linear defects associated with the bulk material or with minor point defects that congregate at the carbonate surface. Low-pH conditions induce a more asymmetrical development of dissolution pits and results in arrowhead-shaped structures. Crystallographic control of pit growth (carbonate dissolution) is expected and can be directly linked to molecular simulations.

The molecular-simulation component of this study addresses the issue of correlating the observed dissolution rates to the energetics of surface, ledge, and pit formation. We used our previous work on the development of accurate forcefields for carbonate phases as a basis for refining the potentials through parameterization with new data and with converting the more-complex shell model, to represent electronic polarization of oxygen, to a simplified yet accurate rigid ion model. We accomplished this through the simulation and analysis of bulk carbonate structures for the five carbonate structures noted above, plus three transition-element carbonate phases (CdCO_3 , CoCO_3 , and NiCO_3). We derived and tested six different sets of energy parameters for each phase and compared the resulting structures with experiment. We used the optimum parameter set for all subsequent simulations involving surface structures.

We derived surface energies—both unrelaxed and relaxed surfaces—for each carbonate and those that correlate with the observed set of dissolution rates. The correlation is consistent with the energy expected to remove a half-plane of carbonate material and is expected to trend with the formation of surface ledges and pits. Smithsonite is the only phase that fails to follow

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the general trend and may be related to a more-complex dissolution process. We examined the energetics of pit formation by the creation of various-sized rhombohedral pits for each of the relaxed carbonate surface models. We obtained energies as a function of pit size. Computational power and storage limited these calculations to periodic systems having approximately 4200 atoms, although we performed several simulations using up to 16,800 atoms.

Refereed

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geometric models of mineral dissolution
investigated for rhodochrosite. *Geochimica et
Cosmochimica Acta*, New York, New York:
Elsevier Science, submitted.

46070

High-Speed Micro-EDM*G. L. Benavides, S. P. Moylan*

Spark erosion by microelectrodischarge machining (micro-EDM) provides significant opportunities for producing small features and microcomponents such as nozzle holes, slots, shafts, and gears in stainless steels, hard alloys, and advanced ceramic. If the speed and precision of micro-EDM processes can be significantly enhanced, they have the potential to be used for a wide variety of micromachining applications, including fabrication of microelectromechanical systems (MEMS) components. Over the last seven years, a research program on micro-EDM carried out at Purdue University resulted in important advances in the state of micro-EDM technology for the drilling of fuel-injector nozzle holes for diesel-fuel systems. The project addressed various aspects of the micro-EDM system, including power supply, process sensing and monitoring, fast-response servosystems for electrode feed, and the material-removal process. The implementation of the project at a major diesel-engine manufacturing facility resulted in a 40% reduction in drilling cycle time, significant improvement in nozzle-hole quality, and estimated cost savings of \$7 per engine. In collaboration with Purdue University, Sandia seeks to build on these research accomplishments by using our world-class expertise in mesoscale machining processes and to take micro-EDM technology to the next level, namely, high-speed micro-EDM. The main features of high-speed micro-EDM are (1) a twofold increase in material-removal rates over current state-of-the-art micro-EDM systems, and (2) extraordinarily high precision that will enable the machining of high-aspect-ratio features as small as 5 mm in cross-section size in materials that are difficult to fabricate by conventional methods. The development of such a high-speed micro-EDM system is critically dependent on a fundamental understanding of the material-removal process, especially the effect of the "dielectric" fluid and the characteristics of EDM voltage/current pulses on material removal, and of tool wear in micro-EDM.

The objective of the single-discharge study is to determine the relationship between spark energy and feature sizes. This will help realize the minimum feature size attainable and help determine any tradeoff between machining time and minimum feature size.

The results of experiments on steel, tungsten, and copper using spark energies characteristic of micro-EDM showed that

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crater diameter varies linearly with energy and crater volume varies by the cube root of energy. Diameters are on the order of tens of microns, and crater volumes are on the order of tens of cubic microns. An adiabatic heat source appears to provide an upper bound, and a point heat source appears inapplicable.

Additional experiments on zinc, iron, molybdenum, and zirconium led to discussions of dominant material properties and the significance of dielectric type. We have proposed a circular heat-source model.

We developed machine parameter technologies for the Agiecut Excellence 2F wire-EDM system using 0.001 in. tungsten wire tool. We found optimum machine parameters using design of experiments and analysis of means for thin stainless-steel samples. We established the minimum feature size for these technologies.

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Other Communications

Moylan, S. P., G. L. Benavides, B. Jokiel, and M. Saavedra. 2002. Decreasing machining time and minimum feature size attainable with micro-wire electrical-discharge machining. *Proc. American Society for Precision Engineering*, accepted.

46684

Developing Rigid and Compliant Cardiovascular-System Models Using Rapid Prototyping

M. L. Griffith

The objective of this project is to develop techniques to rapidly fabricate anatomically accurate physical models using existing medical imaging data and rapid-prototyping (RP) equipment. These models can then be incorporated into an experimental apparatus for use in biomedical research and evaluation. Our work focused on two goals: (1) identify and investigate the use of alternative RP technologies and polymers for developing accurate cardiovascular-system models, and (2) develop a physiologic flow loop with controllable waveform for use in imaging assessment and hemodynamic experimentation.

- *Manufacture rigid and compliant models using RP.* The number of applications of RP continues to increase as the use of RP becomes more mainstream and RP technologies continue to advance. The researchers at the University of Texas at El Paso utilize four RP technologies, including 3-D Systems SLA 250/50 and ThermoJet machines, and Stratasys Fused Deposition Modeling (FDM) Maxum and 3000 machines. The market advantage provided by Stratasys includes the use of WaterWorks (a water-soluble material) as a support material. The unique properties of WaterWorks, specifically the high melting point of $\sim 230^{\circ}\text{C}$ and 100% water solubility, are intriguing material properties that make WaterWorks a useful material for complex dissolvable molds. The use of WaterWorks as a mold material also allows for manufacturing complex shapes with internal flow passages (that is, flow passages with entrances and exits internal to the model) that do not contain seam lines. The properties of WaterWorks and, in particular, its use in the FDM machine (providing for complex shapes to be manufactured), water solubility, solvent resistance, ability for finishing, and high melting point, make it a very useful material to be used for dissolvable molds. We developed a process based on the WaterWorks modeling technology for manufacturing rigid and compliant models from medical imaging data.

- *Develop a physiologic flow loop with controllable waveform for use in imaging assessment and hemodynamic experimentation.* The physiologically representative flow system is based on a Harvard Apparatus 1423 Pulsatile pump. The pump is designed to simulate the ventricular output of the

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heart. The pump mechanism is based on a variable-speed reciprocating piston and silicone rubber-covered ball valves. Controls include pump rate (motor rpm), phase ratio (%systole/%diastole), and displacement volume (cc per stroke). Although the Pulsatile pump alone delivers physiologically realistic flow, tunable impedance and compliance are incorporated into the system so that any particular waveform can be matched. This further enhances system capabilities because we can simulate individualized flow along with individualized geometry. Resistive and compliant elements are analogous to reactive elements in an electrical circuit. Adjusting the various elements affects the frequency response of the system and the resulting waveform accordingly.

Valve-sealed vacuum jars connected to the main line supply compliance. A three-way valve at the top opens or closes the jar to the atmosphere. When the jar is closed, internal pressure builds during the systolic phase and effectively “springs back” during diastole. Stopcock valves placed in parallel at the outlet to the reservoir provide impedance.

We used this test apparatus to match typical physiological conditions of a human cardiovascular system. Although the components make physiologically representative flow possible, the adjustments to reactive elements in the circuit necessary for duplication of a specific waveform can be difficult to make. Patient contours have structure very specific to cardiovascular function. Compliant elements with more robust control are required to simulate slight modifications to pressure and flow waveforms.

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46685

Nanoscale Hotspots Due to Nonequilibrium Thermal Transport

S. Graham, Jr., E. S. Piekos

In this research, Sandia is investigating the existence of hotspot formation at room temperature and above in silicon (Si), resulting from ballistic phonon transport and far-from-equilibrium phonon distributions. The dimensions of the heat sources will be on the order of the room-temperature phonon mean-free-path in Si (~ 300 nm) and smaller. We will create the experimental samples using electron beam lithography, which will form metal lines deposited on the surface of Si wafers. Linewidths and line separations will vary between 20 nm and 200 nm. The patterned lines will act as both the heat source and the temperature sensor using electrical resistance thermometry. We will measure temperatures in the patterned structures and compare them with Fourier's Law and energy-transport equations based on the Boltzmann transport equation. These experiments and subsequent modeling will determine the relative importance of far-from-equilibrium thermal transport in room-temperature nanoscale devices.

Recent research showed that the temperature rise near nanoscale semiconductor devices can yield dramatically larger temperatures than those predicted using continuum diffusion theory. Such elevated temperatures result from ballistic phonon transport near the heat source and from the large departure from equilibrium of the lattice vibrations (phonons) within the heat source. We experimentally demonstrated these phenomena in micron-scale doped-Si resistors at low temperatures, where the phonon mean-free-path is on the order of 1 μm or greater. While we anticipate that such temperature localization effects will be very important at room temperature, the precise size scale at which this phenomenon occurs and the magnitude of the effect are still unknown. Such data are urgently needed to assist in model development for heat flow in semiconductor and other nanoscale devices.

Research conducted over the past year focused on developing both experimental and modeling tools to study hotspot formation near nanoscale heat sources. To determine these effects experimentally, Si samples containing nano-MOSFETS (metalorganic semiconductor field-effect transistors) were designed by Stanford University and fabricated at Sandia in collaboration with Lawrence Berkeley National Laboratory. Hotspot formation in these devices occurs

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due to the spatial localization of the peak electric field combined with the disparity in the electron and phonon relaxation rates. The spatial confinement of the heat source is achieved in the experiment through electron-beam-fabricated aluminum heaters that are 100–200 nm wide. We achieved the pump conditions by designing the heaters to sustain current densities of around 10^{11} A/m². The heaters double as temperature sensors using four-point-probe electrical-resistance thermometry.

Experimental progress was slowed by the fabrication process, which initially resulted in very low yields. Thus, we put much effort into sample process development and resolved sample fabrication issues. However, experimental measurements of the nano-MOSFET devices at Stanford showed poor electrical isolation of the sensors from the Si substrate, which prevented any thermal measurements. The poor isolation in the nanoscale devices was an unanticipated sample design flaw. We redesigned the samples to alleviate this problem by using reverse-biased metal-semiconductor junctions to achieve electrical isolation. We currently are fabricating the samples with three junctions instead of one, as used in the original design. We introduced a doping step to create a *p-n* junction under the heater/sensor that will separate two metal-semiconductor Schottky diodes. This sample design is unique in that no dielectric isolation is required that has been used in all other electrical-resistance thermometry experiments utilizing metal heaters and sensors in the literature. By eliminating the need for a dielectric layer, we will achieve the measurement sensitivity that is required for these experiments. Experiments are currently under way on these newly fabricated devices.

To simulate heat transport from the hotspot, we explored solving the phonon Boltzmann transport equation using the Monte Carlo (MC) method as well as atomistic simulations. In research parallel to this effort, we demonstrated the development of a phonon MC simulation tool this year as effective for calculating the thermal conductivity of thin Si films by Sandia. However, we identified key areas of refinement for the MC model that must be addressed before it can be applied to the hotspot problem. A major problem is the unavailability of anharmonic phonon-scattering rates or probabilities for high phonon energy densities. We are currently exploring atomistic simulations to generate the scattering rates required for an MC simulator. We will use these scattering rates as input to the current MC simulation tool to model the nano-MOSFET device in upcoming work.

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We completed a thermal and electrical design of heaters/sensors for hotspot experiments, developed a fabrication process for and manufactured electron-beam-patterned 100 and 200 nm-wide heaters/sensors, and began preliminary work on MC and atomistic simulations, including nonequilibrium optical phonon wavepackets.

46686

Micro External Combustion Engine: The P3 Engine Prototype

C. A. Applett

In this project, Sandia focuses on the development and low-frequency testing of a microheat engine and demonstrates the production of electrical power by a dynamic microheat engine. The prototype microheat engine is an external combustion engine in which thermal power is converted to mechanical power through a novel thermodynamic cycle. Mechanical power is converted into electrical power through the use of a thin-film piezoelectric membrane generator. This design is well suited to photolithography-based batch-fabrication methods and is unlike any conventionally manufactured macroscale engine. We realized a peak-to-peak voltage of .84 V and power output of 1.5 mW at operating speeds of 10 Hz. We also achieved measurements for the engine operating at resonant conditions. We obtained cycle speeds up to 240 Hz, with peak-to-peak voltages of 70 mV.

Based on previous work at Washington State University, we directed work toward the development of a microelectromechanical systems (MEMS) power system based on a dynamic heat engine that is driven by an external heat source, the P3 microheat engine. The P3 microengine produces electrical power by employing a three-part strategy. First, we conducted thermal power into the P3 engine from an external heat source. Second, we converted thermal power to mechanical power through the expansion and compression of a two-phase working fluid by the oscillation of a flexible membrane. Third, we converted mechanical power into electrical power using a thin-film piezoelectric generator. We designed and fabricated a prototype P3 microheat engine and fabricated prototypes. We designed and built facilities developed to characterize the performance of the piezoelectric membrane generators and the microheat engines. Finally, we presented the results of a study to characterize the operation of the microheat engine at low frequencies and its membrane generator at the American Society of Mechanical Engineering (ASME) Conference.

We based the design of the P3 microheat engine on a two-dimensional modular architecture. An individual module or unit-cell engine consists of a cavity filled with a saturated two-phase working fluid bounded on the top and bottom by thin membranes. The top membrane of the cavity is a thin-film

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piezoelectric membrane generator. The bottom membrane contains an electrical-resistance heater. Heat is alternately conducted in and out of the two-phase working fluid through the thin membranes capping the top and bottom of the cavity. As heat is conducted first into and then out of the working fluid, the quality and volume of the saturated mixture first increase and then decrease. As a consequence, the top membrane acts like a piston in a conventional large-scale engine. However, rather than sliding in the cavity cylinder, the piezoelectric thin-film membrane flexes in and out. In this way, the piezoelectric membrane acts alternately as a generator/expander and as an actuator/compressor during the engine cycle. The useful output of a unit cell engine is the electrical power generated by the piezoelectric membrane as it is strained during expansion of the two-phase working fluid, minus the power consumed by the membrane during the compression of the working fluid.

Refereed

Whalen, S. A., M. R. Thompson, C. D. Richards, D. F. Bahr, and R. F. Richards. 2002. Low-frequency operation of the P3 microheat engine. *Proc. International Mechanical Engineering Congress and Exposition 1* (17–22 November, New Orleans, Louisiana): 1–8.

...rather than sliding in the cavity cylinder, the piezoelectric thin-film membrane flexes in and out. In this way, the piezoelectric membrane acts alternately as a generator/expander and as an actuator/compressor during the engine cycle. The useful output of a unit cell engine is the electrical power generated by the piezoelectric membrane as it is strained during expansion of the two-phase working fluid, ...

47516

Effectiveness of Dielectrophoretic and Electrokinetic Filters/Concentrators for Collecting Smallpox and Anthrax Surrogates from Raw Samples

M. S. Derzon, A. K. Singh, E. B. Cummings

The goal of this project is to develop a general-purpose sample-preparation system that selectively filters and concentrates suspended particles having a selected range of surface-charge density, size, and polarizability. This device is intended to interface with hand-held analytical devices and sensors also under development at Sandia. We built and began testing prototype devices to evaluate how effective this filter concept will be for trapping bacteria and small molecules in raw samples, including (1) the liquid effluent of an aerosol collector, (2) saliva, (3) mucus, and (4) blood. We successfully trapped and released molecules and bacteria in distilled water, tap water, and phosphate-buffered saline (PBS, an initial surrogate for blood). This has application in pathogen detection as well as environmental monitoring.

We (1) designed and fabricated a low-flow and a high-flow version of the concentrator/separator, (2) performed testing in deionized water, tap water, and PBS with *Staphylococcus aureus*, *Escherichia coli*, and fluorescein, and (3) demonstrated differential trapping and release of bacteria and fluorescein.

We successfully trapped both fluorescein dye and bacterial particles with the low-flow concentrator. We also successfully released both fluorescein and bacteria from the low-flow concentrator substrate. We demonstrated that the low-flow concentrator can process microliter-scale samples suspended in either water or PBS. We also demonstrated that the high-flow concentrator can trap fluorescein dye out of solution at 10 ml/min flowrate.

We find these results quite exciting, although somewhat crude compared to what we hope to get. Based on the preliminary data, we are confident that we have a high probability of demonstrating trapping and release of particles in aqueous solution, such as small peptides, viruses, and bacteria (living or dead) in biological fluids.

We filed a technical advance (TA) and one provisional patent and are preparing additional TAs.

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47517

Mathematical and Algorithmic Issues in Multiphysics Couplings

C. M. Stone

One may have different physical processes (e.g., flow, transport, reactions) occurring within the same physical domain, or one may have different physical regimes (e.g., surface/subsurface environments, fluid/structure interactions) interacting through interfaces. Sandia is investigating both of these types of multiphysics couplings during the course of this research.

We will investigate issues related to the determination of appropriate matching or transmission conditions (e.g., flux balance, conservation of mass, energy, momentum, etc.) across multiphysics interfaces. Specific energy and environmental Department of Energy examples include the matching of different multiphase-flow regimes, coupling of geomechanics and geophysics codes with reservoir flow, and the coupling of surface water to groundwater.

When coupling multiple physics and/or multiple domains through interfaces, one must account for the coupling through discretization strategies. Mortar finite-element methods (FEMs) can be used for coupling different physical domains and also for multiscale resolution, as one can couple highly refined regions with more coarsely refined regions through the use of a mortar space. Also of interest will be the development of coupling approaches that do not require mortar spaces, e.g., the coupling of discontinuous Galerkin (DG) methods with continuous and mixed FEMs for treating different physical phenomena and/or different grids.

We plan to explore effective time-stepping schemes for solving general partial differential equations (PDEs) arising in multiphysics applications. We will study theoretical as well as practical issues related to the time-stepping in the individual domains and in the coupled multiphysics applications. In particular, we will develop fully implicit and time-split approaches for systems of coupled PDEs. Depending on the nature of these equations and the feedback between them, the couplings can be “loose” or “tight” in time. There is a need to develop an adaptive time-implicit/time-split technique, whereby certain terms are adaptively modeled either fully implicit or through a split step.

The modeling of fluid/structure interaction is of growing importance in both energy and environmental applications. Because of the inherent complexity, these problems must be

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simulated on parallel machines to achieve high resolution. The purpose of this research is to investigate techniques for coupling flow and geomechanics in porous media that are suitable for parallel computation. In particular, our main objective is to develop an iterative technique that can be as accurate as a fully coupled model, but that allows for robust and efficient coupling of existing complex models (software).

We developed a parallel linear elastic module that we coupled to a three-phase, three-component, black oil model in IPARS (Integrated Parallel Accurate Reservoir Simulator). We introduced an iterative decoupling technique at each time-step. The resulting nonlinear iteration involved solving for displacements and flow sequentially. We used rock compressibility in the flow model to account for the effect of deformation on the pore volume. We achieved convergence when the mass balance for each component satisfied a given tolerance. We validated this approach by comparing it with a fully coupled approach implemented in the British Petroleum/Amoco ACRES simulator.

A second objective of this work is to develop an efficient parallel solver for the elasticity equations. We implemented a preconditioned conjugate gradient solver to solve the algebraic system arising from tensor product linear Galerkin approximations for the displacements. We developed three preconditioners: LSOR (line successive over-relaxation), block Jacobi, and agglomeration multigrid. The latter approach involved coarsening the 3-D system to 2-D and using LSOR as a smoother that is followed by applying geometric multigrid with SOR (successive over-relaxation) as a smoother. Preliminary tests on a 64-node Beowulf cluster indicate that the agglomeration multigrid approach is robust and efficient.

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47687

MEMS Adaptive Optics Devices

J. J. Allen, D. J. Dagel

This project leverages the surface-micromachining (SMM) capability embodied in Sandia's Ultraplanar Multilevel MEMS (microelectromechanical systems) Technology (SUMMiT™) to develop optical mirror arrays for spectroscopic remote-sensing systems. The research consists of two parts: (1) the development of a programmable diffraction grating for use in a correlation spectrometer, and (2) the development of a programmable mask for use in a hyperspectral imager (HSI). From a design perspective, these efforts overlap considerably in terms of array geometry, layout, and optical tolerances and differ mainly with regard to the degrees of freedom (DOFs) of the mirror elements. Similarities exist on a functional level as well; both devices select a subset of the source spectrum for analysis. The first device, referred to as the Polychromator, reproduces the characteristic spectra of substances by changing the diffraction pattern reflected from its mirror array, while the second device, the Hadamard transform spectral imager (HTSI), identifies the spectra of objects by sampling the different wavelength bands generated by a conventional grating.

The objective of the first part of this project is to develop a variable programmable grating structure within the SUMMiT™ SMM fabrication process that will be used in an optical chemical-detection system, the Polychromator. The grating consists of an array of vertically actuated mirror “slats,” which can be configured to mimic the spectrum of a particular chemical. This array will be used as the reference cell in a correlation spectrometer.

The status of work on the SUMMiT™ Polychromator is as follows:

- Developed design concepts for programmable grating structures that have a combination of vertical, rotational, and horizontal DOFs.
- Designed four sets of modules based on these concepts (RS-331, RS-335, RS-353, RS 372).
- Completed fabrication of two reticle sets (RS-331, RS-335).
- Evaluated designs of structures that minimize residual stress effect.

Preliminary design evaluation results on the mirror arrays showed the following:

- Vertical DOF slats with up to 2.5 μm of stroke.

SUMMiT prototype Polychromator structure.

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- Functionally tested operational rotational DOF slats.
- Developed and successfully actuated structure (“ToadStool”) that minimizes residual stress effects.

The goal of the second part of the project is to develop an encoding mask using the SUMMiT™ process that largely overcomes the limitations and drawbacks of the MEMS mirror array (the Texas Instruments Digital Micromirror Device, or DMD™) currently being used in the Sandia-developed Hadamard HTSI. As above, the mask consists of an array of reflective slats, so-called *venetian blind mirrors* (VBMs). Wavelength selection occurs through the rotation of individual mirrors so as to reflect or reject the light from a dispersed source.

The advantages of the VBMs are optical in nature: better match to the diffracted light, fewer gaps between mirrors, smoother surface profile, and higher reflectivity. Taken together they will translate into improved signal-to-noise and sensitivity in the HSI.

The status of work on the SUMMiT™ encoding mask is as follows:

- We designed VBMs of varying width, torsional stiffness, and angular states.
- We fabricated first-generation arrays (RS-331).
- Thorough characterization is currently under way.
- Second-generation designs are under development.

Preliminary design-evaluation results on the mirror arrays show the following:

- Simulated voltage response agrees with experimental data when adjusted for the larger-than-expected air gap.
- Interferometry indicates that stress-induced curvature is acceptable.
- We observe electrostatic discharge failure mechanism at full mirror tilt.

Venetian blind micromirror array.

The goal of the second part of the project is to develop an encoding mask using the SUMMiT™ process that largely overcomes the limitations and drawbacks of the MEMS mirror array...currently being used in the Sandia-developed Hadamard HTSI.

47688

Securing the U.S. Mail Distribution System Against the Threat of Biological and Chemical Agents

T. R. Lockner, R. J. Kaye, D. W. Vehar, L. E. Martinez, J. M. Jojola, J. A. Jacobs, L. M. Zurzolo, R. A. Deola, M. M. Archuleta

This project investigated some of the effects that irradiation of the U.S. mail may produce. Sandia addressed three areas with both theoretical and experimental efforts, including an assessment of the volatile organic compounds (VOCs) and surface compounds generated during the irradiation process, the effect of large radiation doses on common information-storage media, and the effect of shielding on the irradiation process. After a literature search, we performed experimental work using RHEPP II (repetitive high-energy pulse power) (the world's highest average power electron-beam source), a 300 kW, 2.2 MeV, 2.5 kJ/pulse repetitive pulsed electron-beam accelerator system, to study the radiation effects.

VOC results were largely in agreement with previous measurements taken at other irradiation facilities. Our measurements differed from previous ones in that the measurement was taken in the bag containing the samples, as opposed to the ambient atmosphere in the handling area. Results indicated only benzene, acetaldehyde, ethane, and methanol at significantly elevated levels. Of these, only benzene was above the threshold limit value (TLV), but benzene would not cause the symptoms described by mail workers. It was also not high enough to pose a reasonable health risk in a well-ventilated room. The surface chemical measurements indicated a general decrease in surface chemicals with increasing dose (from zero dose).

- *Experimental measurements of VOC released during irradiation of mail at dose levels from 50 to 240 kGy (kilo Grey). We performed measurements from plastic bags sealed as in the USPS mail-irradiation process. We removed the air sample from inside the bag approximately 10 minutes after irradiation.*

- *Experimental measurements of surface chemicals released during irradiation of mail at dose levels from 50 to 240 kGy. These measurements were made immediately after the VOC air samples were taken.*

- *Simulations of shielding in USPS irradiation process at electron kinetic energy of 10 MeV. We determined the plausible shielding scenarios and areal density necessary to subvert the*

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irradiation process and found the mail-irradiation process to be quite robust.

- *Experimental measurements on commercial radiation shielding packages to benchmark simulations.* We performed measurements at an electron energy of 2 MeV on the RHEPP II accelerator and compared them with 2 MeV simulations.

- *Experimental measurements on mass electronic storage media response to high radiation doses (240 kGy).* Media tested included 3.5 in. floppies, CD-R, CD-R/W, and DVD-R.

*We performed measurements
at an electron energy of 2 MeV
on the RHEPP II accelerator
and compared them with
2 MeV simulations.*

47795

Lipid Membranes on Nanostructured Silicon

D. Y. Sasaki

Sandia seeks to develop unique hybrid nanostructures that interface nanolithographically defined silicon (Si) surfaces with molecularly dynamic, self-assembled materials. Our goals are to (1) develop a mechanistic understanding of how the self-assembled materials interface with the structured substrate, (2) examine how the nanostructure influences the mobility of the molecular assemblies, and (3) develop an understanding of how to manipulate the interfacial interactions and mobility of the molecular assemblies to tailor features in the material from the microscale to nanoscale. The hybrid structures will be composed of a nanolithographically defined Si substrate patterned with lines or posts with a pitch of ~ 360 nm and feature widths of tens to hundreds of nanometers. The self-assembled material will be a lipid-bilayer membrane composed of fluorescent-labeled and/or functionalized lipids. Coupling of the bilayer to the Si wafer could be achieved by either the vesicle-fusion or membrane-stamping techniques. We will characterize the hybrid structure by atomic-force microscopy (AFM), fluorescence recovery after photobleaching (FRAP), and confocal microscopy. AFM and confocal microscopy will evaluate whether the lipid membrane is spanning the top pillars of the structure or conformally coating the surface. We can use all three methods to monitor the dynamic motion of lipids in the membrane and to determine the effect of the underlying nanostructured surface on asymmetric motion of the lipids. The results of this project will impact numerous areas, in particular nanoarchitecture, biosensors, and biocompatible surfaces for bio-MEMS (microelectromechanical systems). This work will be the first to interface a precise, regular, nanostructured semiconductor substrate with a molecularly dynamic self-assembled material. This research will lay the groundwork for understanding how structured substrates influence the macroscopic structure of a coupled lipid membrane and the molecular dynamics within the membrane.

We prepared nanostructured Si substrates, formed vesicles from single-lipid films, investigated solution conditions that promote vesicle fusion to the nanostructured Si surfaces, and obtained images of the hybrid structures with AFM. We prepared structured Si wafers with the help of the Center for High-Technology Materials at the University of New Mexico, with nanolithography forming line patterns with a pitch of

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~ 360 nm, depths of 200 nm, and linewidths of about 100 nm. We cleaned the wafers with ultraviolet/ozone to remove any hydrocarbon contamination, then placed them in the AFM solution cell. We prepared liposomes of dipalmitoylphosphatidylcholine by extrusion through two stacked filters with 200 nm to yield 200 nm-diameter unilamellar vesicles. We then added the liposomes to the solution cell and allowed them to fuse with the Si substrate at room temperature. Scanning of the surface with tapping-mode AFM provided images that revealed partial coverage of the surface with lipid membrane. The membrane also appeared to span the gaps of the nanostructured Si. We are currently repeating those experiments to see if the vesicle fusion is reproducible and if we can improve surface coverage.

Scanning of the surface with tapping-mode AFM provided images that revealed partial coverage of the surface with lipid membrane. The membrane also appeared to span the gaps of the nanostructured Si.

48339

Combating the Chem-Bio Threat Using Sandia Assets: Need for a Technology Roadmap

R. O. Griffith, J. E. Brockmann, L. D. Brandt

Sandia has a number of technologies that address chemical, biological, and radiological weapons-of-mass-destruction (WMD) threats to national security, including sensor-development activities, agent transport and fate modeling and simulation activities, decontamination technologies, robotics and remote-sensing platforms, collective behavior modeling, physical security assessments, and others. Little effort has been made to coordinate the work or to understand how the combined set of capabilities might be used to address the broad security needs of the nation. We seek to develop a technology roadmap that would identify existing relevant Sandia technologies and guide the development of new capabilities to fill the identified gaps. It should be noted that the diverse sets of needs and technologies make this an extremely challenging exercise with no perfect solution, but it is one that we believe must be attempted.

We identified a number of specific modeling and simulation technology needs and divided them into distinct functional units or modules. The specific information and algorithm needs included methods to extract geometry and physical feature data describing large complicated facilities from AutoCAD facility representations, models for predicting gas and aerosol transport, algorithms to determine optimal sensor-placement locations in facilities, algorithms to interpret information from a sparse distributed-sensor network, algorithms to determine dose response and human health effects to chemical-/biological-agent exposures, algorithms to predict demographics and evacuation routes in large facilities, and decision-making algorithms to choose between various response strategies to minimize consequences.

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48340

Numerical Methods for the Study of Hydrocarbon Combustion

L. A. Rahn

Sandia seeks to develop implicit, adaptive numerical methods for the study of hydrocarbon-air coflow flames for both nonpremixed and partially premixed systems on serial and parallel machines. The work focuses on both steady-state and time-dependent systems. These studies will provide valuable information on the applicability of implicit methods in the direct numerical simulation (DNS) of transitional and turbulent flames. Multiprocessor computations will be on both shared-memory and message-passing machines. Specifically, time-dependent problems with moving flame fronts necessitate a sophisticated grid-refinement method in which points move as the calculation advances in time. We intend to incorporate the local mesh-refinement procedure developed for steady-state systems into the time-dependent velocity-vorticity model. The local refinement method will maintain orthogonality at grid-line intersections, but it will lift the tensor product restriction common to traditional grids, thus producing an unstructured grid. The grid will be refined through cell division, which occurs without the introduction of many unnecessary points. Although few points may be added during adaptation and the derivatives do not require transformation to a computational space, the loss of the tensor product data structure increases the difficulty of finding neighboring points. We will test the method on both methane-air and ethylene-air flames. This work is being performed in collaboration with researchers at Yale University.

We studied laminar, sooting, ethylene-fueled, coflow diffusion flames at atmospheric pressure experimentally and computationally as a function of fuel dilution by inert N. We diagnosed the flames using a combination of laser diagnostics and thermocouple gas-sampling probe measurements. We based numerical simulations on a fully coupled solution of the flow conservation equations, gas-phase species conservation equations with complex chemistry, and the dynamical equations for soot spheroid growth.

Predicted flame heights, temperatures, and the important soot-growth species, acetylene, are in good agreement with experiment. Benzene simulations are less satisfactory and are significantly under-predicted at low dilution levels of ethylene. As ethylene dilution decreases and soot levels increase, the experimental maxima in soot moves from the flame centerline

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toward the wings of the flame. Simulations of the soot field show similar trends with decreasing dilution of the fuel, and predicted peak soot levels are in reasonable agreement with the data.

Modifications to a prior soot model include (1) the use of a more comprehensive chemical kinetics model, (2) a revised inception model, and (3) a maximum size limit to primary particle size. We made estimates of the importance of radiative optical thickness corrections to computed flame temperatures. We need additional work on assessing the importance of various ring chemistry submodels on both benzene and soot production.

49170

Assessment of the Potential Impact of Disruptions in Manufacturing Supply Chains

J. A. Ruffner

The terrorist attacks of September 11 revealed for the first time the vulnerability of the nuclear weapons (NW) complex and U.S. manufacturing to disruptions in manufacturing supply chains. In the immediate aftermath of the attacks, ground, sea, and air transportation systems were nearly halted, leaving many companies that utilize just-in-time (JIT) management for their supply chains dangerously low on critical inputs.

The NW complex and the nation's manufacturers are dependent on critical infrastructures, as defined in Presidential Decision Directive (PDD-63) to include telecommunications, electrical-power systems, gas and oil, banking and finance, transportation, water-supply systems, government services, and emergency services. To date, we have not developed an integrated view of the dependency of manufacturers on these infrastructures in light of their potential for disruption. Sandia did a feasibility study to build on our present understanding of how supply chains operate to explore their dependency on critical infrastructures, their vulnerabilities to disruption, and the economic, social, and national security impacts of supply-chain disruption. The results of this report will be presented to our leading federal policy makers and industry leaders and could be instrumental in helping to establish policy and business practices that minimize these vulnerabilities and risks.

Sandia collaborated with the National Coalition for Advanced Manufacturing (NACFAM) and Arizona State University (ASU) to evaluate the effects of disruptions in the supply chain to U.S. manufacturing and the NW complex. We chose the electronics industry as the focus group because it is a major contributor to the gross domestic product and is a fundamental element of all aspects of national manufacturing (e.g., automobiles, aerospace and defense, and consumer electronics). With ASU, we developed a model of the electronics-supply network, established the dimensions of risk and a means to measure it, and estimated the risk. The supply-chain network model takes into account flow of product (material), information (orders), knowledge (schematics, "recipes," etc.), and cash from the first supplier to the ultimate customer. Next, the team identified dependencies and susceptibilities to disruptions (qualitatively and quantitatively, in some cases). The team is presently meeting with focus

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groups of electronic manufacturers and end-users to validate the model, infrastructure dependencies, vulnerabilities, and potential impacts. Our final report will outline the structure of the semiconductor supply chain, its points of greatest vulnerability to disruptions in the national infrastructure, strategies to mitigate those effects, government policy implications, and recommendations for future research.

Other Communications

Gramsch, P., and J. A. Ruffner. *Assessment of the potential impact of disruptions in manufacturing supply chains*. Sandia Technical Report SAND2002-4109P. Sandia National Laboratories, Albuquerque, New Mexico (November).

49769

Resin Infusion Between Double Flexible Tooling

J. A. Ruffner

The potential for cost savings is a motivating factor behind the development and construction of a novel composite manufacturing technique known as Resin Infusion Between Double Flexible Tooling (RIDFT). It is a two-stage process—resin infusion and wetting followed by vacuum forming. Sandia places dry reinforcement between the two membranes, then secures the membranes and infuses resin under a vacuum. After infusion, we draw the membranes over a male mold (the desired final product shape) by applying a vacuum. The use of a one-sided mold provides huge cost benefits when compared to the conventional resin transfer molding (RTM) processes. In addition, molds are not subjected to high pressures and consequently can be fabricated using less-expensive materials and processing techniques. This further reduces the cost and time for processing. The potential for savings is even more evident in the production of large component parts. The RIDFT process lends itself to the incorporation of reconfigurable tools that can conform to different geometries, thus reducing tooling requirements and the development of cycle times. Since infusion of resin is done between translucent silicon diaphragms, we can utilize ultraviolet (UV)-curing techniques in the RIDFT process. However, the RIDFT process is limited to “line-of-sight” geometric shapes.

The successful development of this technology could provide Sandia with a better understanding of in-mold painting techniques and coating processes that are important for a variety of Defense Programs (DP) and commercial applications. Potential DP applications include robotic-vehicle bodies, target/decoy shells, and re-entry bodies. Potential military and commercial applications include structural members for satellites, hatch covers, doors, panels, and lightweight members for robot arms.

In collaboration with FSU, we laid the groundwork for developing the prototype equipment for use in large-component manufacture. We started to modify the RIDFT system and determined suitable organic materials for the resin-infusion process.

We are preparing for the following tasks:

- Prototype equipment for large-component manufacture.

The successful development of this technology could provide Sandia with a better understanding of in-mold painting techniques and coating processes that are important for a variety of Defense Programs (DP) and commercial applications.

- Incorporate UV-cure equipment and component production.

- Investigate incorporation of gel coats and thin films.
- Write report and make recommendations.

We continue to explore opportunities for implementing this technology into DP and commercial applications. For example, we may be able to utilize this technology for stateside communications module/power module packaging with enhanced security features. This process would reduce costs, reduce processing time, and be readily transferable to Kansas City or other outside manufacturers.

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49772

Studies on the Disbonding Initiation of Interfacial Cracks

E. D. Reedy, Jr.

Difficulties in rigorously applying interfacial fracture mechanics to small-scale delamination problems in microelectronic packaging encouraged a shift from the study of disbond propagation to the study of the nucleation of a disbond. The region around a bimaterial interface edge is highly stressed, and delaminations are believed to nucleate once a critical interface-edge stress state is attained. The critical stress state is characterized by a critical value of the interface-edge stress-intensity factor. The approach Sandia is using is similar to linear elastic fracture mechanics, but here we consider discontinuities other than a crack. We are applying this approach to an adhesively bonded, butt tensile joint geometry to evaluate underfill adhesives used in flip-chip assemblies. We are also developing new test geometries to characterize debonding at edge discontinuities more like those found in flip-chip assemblies.

We are evaluating a novel stress singularity approach for assessing the propensity for a disbond to develop in an adhesive joint. An accepted methodology for predicting the nucleation of a disbond currently does not exist. Disbond nucleation is believed to first occur at bimaterial edges and corners, which act as high-stress concentration sites. We based our research on the use of a critical edge-stress singularity factor to quantify the formation of disbonds. The advantage of this technique is that no pre-existing flaws need to be measured, nor does the failure process need to be known in full detail. Previous results indicate a good correlation between critical edge-stress singularity factors and critical interfacial-strain energy-release rate for several types of epoxy/aluminum interfaces. Presently, we are attempting to use edge-stress singularity factors to predict the fatigue behavior of butt tensile joints. We generated preliminary low-cycle fatigue data; these early results appear promising. This work is being performed in collaboration with Lehigh University.

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49914

Effect of Machining Parameters on Tool Life

B. Jokiel, Jr.

Sandia collaborated with the University of Texas at El Paso (UTEP) on this project. The focus of the research was in the area of improved machining of stainless steel (SS). Machining is a complex process involving the interaction of a cutting tool with the workpiece and influenced by the machine tool and fixtures selected. The efficiency of the material-removal process depends on numerous factors. Among them are the machine-tool and cutting-tool system, cutting speeds, cutting-tool geometry and material, and the coolant/lubricant that is used in the process. Currently most machining processes are accomplished with cemented carbide cutting tools (inserts), and there are numerous variations and manufacturers of these tools. The main differences lie in the carbide microstructures, coatings utilized, cutting-edge design, and chip-breaker design. The introduction of very hard coatings on cutting-tool inserts is given credit for greatly improving these inserts. Claimed improvements in insert design are accompanied by claims of faster, more-efficient removal rates. This study is determining maximum cutting rates that can be achieved with state-of-the-art cutting-tool inserts.

This study focused on evaluating six commercial insert types. Sandia is testing these cutting inserts in a turning process. The workpiece material is 15-5 PH SS. UTEP selected the heat-treat condition in consultation with Sandia (Rockwell C numbers [a Rockwell hardness test] may vary from about 34 to 44). We are testing the six cutting tools selected to their limits by varying the surface speed and feed rate while observing the cutting forces generated and the quality of the surface finish. We are conducting the machining experiments dry, as the trend is to do away with coolants.

We obtained all materials, created the test setup, developed the instrumentation, and set up a procedure for weighing the inserts and examining them with a scanning electron microscope (SEM). We also ran tests on one of the inserts at three machining speeds.

We prepared 20 precipitation-hardened 15-5 SS specimens for testing and tested three of them with the following results.

We machined the first sample at an average surface speed of 141 ft/min, which is the lowest speed at which we are testing. This is also in the area of the commonly recommended speed for machining SS. At this speed, the insert went through the test

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with minimum wear, and the test was run to completion. The volume of material removed in a complete test is 61.1 cu in.

We machined the second sample at an average speed of 343 ft/min, and the insert failed after 14 passes, having removed 57 cu in. of material. The nature of the failure was a fractured tip.

We machined the third sample at an average speed of about 831 ft/min. It failed due to a large fracture of the tip after we removed 31.2 cu in. of material.

The tests on these three samples included in-process and post-machining examination of the cutting inserts. We did the in-process examination with a digital camera equipped with a magnifying lens and monitored machining forces during the process. Post-machining examination includes weight loss and SEM analysis of the insert.

We experienced a severe problem with our instrumented tool holder. We initially instrumented the tool holder with gages installed and cured on the surface. We sealed the gages with room-temperature vulcanizing (RTV) and covered them with sheet metal. However, this system did not survive the harsh environment caused by chips scraping the surface of the tool holder. Some chips forced their way under the sheet metal and shorted the gages. We are resolving this problem by mounting the gages in 0.075 in.-deep pockets, which we are machining into the tool holder using sinker electrical-discharge machining (EDM). We will then recess the gages and cover them with silicon and thin steel plates that will be epoxied to the tool holder. We are also machining small slots where the wires can also be recessed and run to the back of the tool holder. In this manner, the gages and the wiring will be internal to the tool and survive the harsh environment. We are in the process of completing this work and calibrating the tool in a special fixture that we fabricated for this purpose.

We also experienced failure of the chip breaker to break up the SS chips. This results in long, stringy chips that can quickly wrap around the spindle, which is especially severe at the higher speeds. We are averting this by being alert not to let chips build up. This requires that the experiment be momentarily interrupted to clear long chips. This may not be necessary with all of the inserts if the other chip-breaker designs turn out to be more effective than the first one tested.

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50396

Compliant Membranes for MEMS Microphones

D. R. Sandison

The goal of this project is to develop compliant diaphragms using microelectromechanical systems (MEMS) technology for acoustic and pressure sensors. The mechanical sensitivity, bandwidth, and linearity of a MEMS microphone are directly related to the structural behavior of the diaphragm. Scaling analysis indicates that the presence of residual tensile stress in the diaphragm will reduce the mechanical sensitivity of the microphone through a stiffening effect. One method to reduce the effect of residual and extrinsic stresses on a MEMS microphone is to increase the compliance of the diaphragm through corrugations.

The use of corrugations reduces the initial stress, thus increasing the mechanical sensitivity. A diaphragm with a circular corrugation pattern exhibits smaller tensile rigidity in the radial direction compared with a flat diaphragm and improves the mechanical sensitivity over a range of corrugation depths. Sandia employed corrugation in the design and fabrication of single-backplate MEMS condenser microphones to yield a higher mechanical sensitivity. However, these designs were limited by material and process variations and pull-in voltage instability.

Compliant diaphragms using the chemical-mechanical polishing (CMP)–planarized, low-residual-stress SUMMiT-VTM (Sandia Ultraplanar Multilevel MEMS Technology) process at Sandia will be designed, analyzed, and fabricated to provide a critical component for MEMS acoustic and pressure transducers, in particular for a dual-backplate force-feedback MEMS capacitive microphone that alleviates the pull-in voltage instability of single-backplate designs.

The goal of this project is to develop compliant diaphragms using microelectromechanical systems (MEMS) technology for acoustic and pressure sensors. ...Compliant diaphragms using the chemical-mechanical polishing (CMP)–planarized, low-residual-stress SUMMiT-VTM...process at Sandia will be designed, analyzed, and fabricated to provide a critical component for MEMS acoustic and pressure transducers, ...

50717

Multiscale Experimental/Numerical Study*N. Y. C. Yang*

Sandia made in situ scanning electron microscopy (SEM) observations of the formation and propagation of small fatigue cracks in cast AM60B magnesium (Mg). Using an environmental SEM, we made observations in vacuum and in the presence of water vapor at 20 Torr. In the vacuum environment, fatigue cracks in the Mg formed preferentially at pores, sometimes precluded by observable cyclic slip accumulation. At higher cycle numbers in the vacuum environment, we discovered additional cracks to initiate at persistent slip bands within relatively large Mg dendrite cells. We discovered that small fatigue cracks in the Mg cycled under vacuum propagate along interdendritic regions in the presence of microporosity and along crystallographic planes in the presence of persistent slip bands ahead of the crack tip. When these relatively weak microstructural paths were not available, the small cracks would propagate straight through the dendrite cells in a Mode I manner. Fatigue cracks in the Mg formed more rapidly both at pores and within the dendrite cells in the water-vapor environment compared to the vacuum environment. The majority of small cracks in Mg cycled in the water-vapor environment propagated straight through the dendrite cells in a Mode I manner at a rate faster than the cracks in the vacuum. Cracks in the water-vapor environment were not observed to grow through persistent slip bands in dendrite cells or through interdendritic regions, even in the presence of some microporosity. Small fatigue cracks in the Mg propagated around second-phase particles and were perturbed by interdendritic regions in both vacuum and water-vapor environments.

We will use the structure-property relations from simulations and experiments to develop models used in design. In particular, we plan the following tasks:

- Fabricate test specimens and experimental fixtures.
- Determine resolution limits and specimen preparation constraints for the various materials using the high-voltage transmission electron microscope (TEM), *in situ* SEM, and atomic-force microscope (AFM).
- Characterize the initial structure in LIGA (the German term *Lithographie, Galvanoformung, und Abformung*, for lithography, electroforming, and molding) nickel (Ni), aluminum silicon (Al-Si) thin films, and cast Mg as a function of extreme and typical processing routes.

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- Experimentally characterize the effect of boundary conditions (BCs) and environments on damage evolution at nano- and micro-scales.
- Determine potentials for hexagonal close-packed (HCP) Mg modified embedded atom method (MEAM) simulations; conduct baseline MEAM simulations to understand geometry effects (periodicity and size) under simple BCs for Mg and Al-Si systems.
- Incorporate crystal plasticity constitutive relationships into finite-element (FE) simulations.
- Conduct benchmark FE simulations to examine mesh-size effects and interaction between damage and basic crystal plasticity parameters.

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50772

Cellular Observatory: Simultaneous Time- and Frequency-Resolved Microscopy

D. W. Chandler, C. C. Hayden, A. K. Luong

The goal of this project is to develop methods for measuring the dynamics of cellular constituents in real time. In particular, Sandia is developing a confocal microscope and detection system with the capability to record simultaneously the fluorescence lifetime and spectrum of each pixel that comprises the scanned image of the microscope. The fluorescence carries information about the local environment within each pixel. Thus, the microscope will be able to continuously monitor very small-scale chemical changes around fluorescent chromophores tagging biological structures. This apparatus should also increase the applicability of fluorescence energy-transfer techniques (FRET) to studies of cellular dynamics.

We made substantial progress toward assembling the microscope and detection system. We interfaced a high-repetition-rate pulsed laser system, necessary for lifetime measurements, with the optics of the microscope. We are currently performing calibration and resolution tests to ensure that the performance of the microscope meets our needs. The detection system is intended to detect individual fluorescence photons emitted from the sample. We will image photons through a dispersive optical system onto a time- and position-sensitive detector. The output of this detector will be a measurement of the wavelength and emission time of each photon. Measurements on many photons will reveal the frequency spectrum of the excited species and the lifetime of the emission. We designed and fabricated the detectors. Prototype electronics are almost complete for the fast processing of the detector signals needed for initial testing of the detectors and for the first experiments. We are also collaborating with Sandia researchers to grow tagged cells for observations of cellular structures and to produce tagged, simulated cell membranes to begin controlled experiments on membrane proteins.

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50858

Near-Real-Time Site Characterization for Assured HDBT Defeat

P. Yarrington, K. T. Stalker, M. C. Walck, D. L. Keese, K. D. Meeks

This project explored the technical challenges associated with developing a system to provide near-real-time (NRT) site characterization for hard and deeply buried target (HDBT) defeat. Potential system performance objectives included (1) rapid characterization of the near-surface geology at the site, to locate penetration obstacles and guide aimpoint selection for assured survival of a follow-on earth-penetrating weapon (EPW) attack, (2) target-facility depth localization, to assist in tailoring the weapon attack (number, yield, fuzing, timing, etc.) for assured target defeat, (3) a sensor and signal-generating array-based system for remote missile/aircraft delivery capable of penetrating a short distance below the surface of the target site, and (4) rapid data analysis, through telemetry reachback coupled to high-performance computing platforms and high-fidelity models of the seismic and weapons effects phenomenology.

The motivation for this study is the national security need for capabilities to quickly and accurately characterize geologic features at an HDBT site to ensure the success of any planned attack on such locations. Specifically, the present project explored the technology challenges for developing NRT characterization of key geologic features at an HDBT site using a system of air-deployable, earth-penetrating sensors and active sources. Guidance to the targeting community for tailoring the attack (aimpoints, number of weapons, etc.) on an HDBT site is the goal of the system.

Improved localization and definition of key features of the target facility would be one of the primary objectives of the system. Since attack on an HDBT site will likely involve an EPW, another objective for the system is to provide near-surface site characterization to ensure EPW survival.

The present study included subject-matter experts from the major technical areas involved in the proposed concept. The study identified the major technical challenges for the proposed concept and assessed the feasibility of meeting those challenges.

The technical challenges identified in the study are listed here; the asterisk indicates the areas that present the greatest challenges:

- Source/sensor specifications*

This project explored the technical challenges associated with developing a system to provide near-real-time (NRT) site characterization for hard and deeply buried target (HDBT) defeat. ...The motivation for this study is the national security need for capabilities to quickly and accurately characterize geologic features at an HDBT site to ensure the success of any planned attack on such locations.

- Near-surface mapping technology*
- Sensor coupling*
- Faster algorithms*
- Data interpretation*
- ConOps
- Signal processing and communications
- Data integration
- Sensor placement
- Source/sensor penetrator design

Source/sensor specifications. Specifications have to be established for the characteristics of target material features that the system must be able to resolve. The parameter space is quite large, and the task would be arguably infeasible if experimental methods alone were the only means to address these issues.

However, recently developed modeling techniques demonstrated capability for simulating the three-dimensional (3-D) phenomenology involved in penetration of highly heterogeneous target media, such as boulder fields.

- *Near-surface mapping technology.* A seismic imaging technique called *surface-wave tomography* is well suited for application to the near-surface imaging problem. The fact that locations of both the sources and receivers would be known will expedite the process of inverting surface-wave travel times to map the near-surface velocity structure.

- *Sensor coupling.* The sensor delivery package must ensure that seismic data can be transmitted with high fidelity across the interface to the onboard instrumentation. Sandia developed multiple unattended systems (e.g., Steel Eagle) for remote air insertion into a range of geologies, and the present project could build on that technology.

- *Faster algorithms.* To support the anticipated tempo of operations, analysis of the sensor data must be accomplished within several hours. This process now takes days to weeks on serial processors. Accordingly, new analysis methods and parallel versions of current seismic processing algorithms would be needed. The SALVO 3-D massively parallel seismic imaging code is an example of where similar parallel software has been developed.

- *Data interpretation.* A methodology will be needed to compare the seismic velocity data to the parameters needed for predicting weapon survivability and effectiveness. One approach would be to combine penetration and seismic data to produce the composite characterization. We would construct a composite material-response model by linking the low-stress (seismic) and high-stress (penetration) regimes at sensor-impact points in the target site.

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- *ConOps—concept of operations.* The information product would need to be usable by U.S. Strategic Command (USSTRATCOM) in its mission planning and execution processes. Sandia has had a continuing staff presence in the USSTRATCOM planning organization; thus, a communication channel exists for obtaining the information that will help meet this goal.

51537

Ironless Permanent Magnet Actuator

K. I. Diaz

A characteristic common to most permanent magnet actuators, also referred to as electromagnetic (EM) actuators, is the iron (Fe) content that resides within the materials of the actuator. The Fe content can be in either the permanent magnet itself or in one of the components comprising the actuator, or both. Fe provides many advantages when it comes to the functional performance, such as output torque of EM devices—in both linear and rotary motion. There are, however, certain applications that cannot tolerate the presence of Fe. This report shows how a preliminary concept for an ironless permanent magnet actuator came about by understanding the EM and magnetic properties of materials and their inherent systems.

The ironless permanent magnet actuator was to operate a 50-tooth ratchet wheel 360 degrees in less than 800 ms. Initial methods planned to accomplish the task were electromagnetically or magnetically by a separate actuator wheel; we referred to this as a “leader/follower system.” This initial concept required very extensive calculations and analyses to obtain a first run of its mechanical output capacity; however, it did not show promise in terms of other requirements set forth, such as volume restriction. We pursued a second concept that is very similar to a common rotary solenoid or direct-current (DC) motor. We pursued two derivatives of this common rotary actuator design: (1) the actuator attached to a lever or gear would actuate the ratchet wheel, and (2) the actuator would drive the shaft to which the ratchet wheel is connected. The latter concept seemed the most promising; we pursued it and made initial calculations. However, we did not complete the more extensive calculations and analyses of models using EM modeling simulation software.

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52174

Inelastic Deformation Mechanism in Shocked Sapphire Single Crystals

M. D. Knudson

Sandia collaborated with Washington State University (WSU) to understand the deformation mechanisms in shocked sapphire single crystals. In particular, the work focused on understanding the inelastic behavior of sapphire shocked along different crystallographic axes; previous work at WSU showed that the inelastic behavior varies with orientation. The long-term goal is to develop a good material model for this nonisotropic material. We will perform experiments both at WSU (gas-gun, shock-wave experiments) and at the Sandia Z accelerator (quasi-isentropic experiments). Detailed comparisons of the mechanical response under these distinctly different loading conditions (shock and quasi-isentropic) should provide insight into the failure mechanism. Further, these experiments will provide needed information regarding the index of refraction changes of sapphire under quasi-isentropic compression. Knowledge of the inelastic behavior and the change in the index of refraction is needed to use this material as an interferometer window in quasi-isentropic experiments; this will directly benefit material dynamics studies at Sandia, directly benefiting pulsed-power sciences.

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52796

Portable Endospore Detection System for Real-Time Anthrax Screening

P. L. Gourley, J. K. Hendricks, A. E. McDonald

Sandia is developing novel micro-/nanotechnology platforms for high-speed characterization of cells and biomolecules using high-efficiency, light-emitting semiconductors tailored with biocompatible surfaces. These new tools have potential as the ideal probe of proteins within living cells to elucidate protein structure and function in their physiological condition with minimal perturbation. Recently, we investigated coherent nanolaser techniques for rapidly assessing protein in bacterial spores flowing through an integrated nanolaser/microfluidic chip. Signal transduction occurs by coupling spontaneous light from a semiconductor surface through a cell flowing in the laser microcavity. Concentrated intracellular proteins induce stimulated emission spectra that are projected into an analyzer. The laser light is spatially/temporally resolved, recorded by high-speed digital video imaging, and analyzed within seconds using efficient pattern-recognition algorithms. The laser hyperspectra are sensitive to scattering from the distribution of protein molecules and organelle structures in the cell. We used this technique to distinguish anthrax endospore simulants.

We analyzed spores and other common microparticulates (sugar, talc, protein powder) that might be mistaken for bacterial spores by the simple method of biolaser counting. Because *Bacillus anthracis* (anthrax) spores can cause death in mammals when inhaled, we used other spore-forming bacteria that are similar to *B. anthracis* but are not pathogenic. We tested *B. subtilis* and *B. pumilus*, spores often used for routine testing, in addition to the common powders. We began analysis by simply suspending the particles in solution and immediately flowing them through the biolaser to count light pulses.

The results for bacterial spore and microparticulate counting are recorded in the form of histograms for different water suspensions of particles flown through the biolaser. The histogram reveals that only bacillus spores were detected in the laser counter. To produce a measurable count, a flowing cell must be present in the biolaser. The membrane-confined proteins of both bacterial cells (prokaryotes) and animal cells (eucaryotes) trigger the lasing process. In contrast, the detector registered no counts when suspensions of other white powders (talc and sugar) flowed through the detector. Substances that might be mistaken for anthrax spores such as talcum powder do

Sandia is developing novel micro-/nanotechnology platforms for high-speed characterization of cells and biomolecules using high-efficiency, light-emitting semiconductors tailored with biocompatible surfaces. These new tools have potential as the ideal probe of proteins within living cells to elucidate protein structure and function in their physiological condition with minimal perturbation.

not support lasing; thus, no counts are registered by the biolaser. These results demonstrate the feasibility of using the biolaser for near-instantaneous detection of bacillus spores in an unknown powder.

In the second, more-detailed mode of operation, the biolaser performed differential analysis of spore strains on the basis of their lasing phenotypes. This method extracts critical biological information from the biolaser hyperspectra, including spore size (angular divergence), protein density (wavelength shift), protein-density fluctuations (spectral linewidth), and spore translucence (lasing intensity). The analyzer creates three-dimensional (3-D) cluster plots comprising three 2-D planar projections that correlate hyperspectra parameters. By overlaying data from different spore types, the analyzer can distinguish spore signatures for identification. Testing of *B. subtilis* and *B. pumilus*, which appear identical under the microscope (oval spores of approximately 1 μm diameter), produced significantly different hyperspectra. The *B. pumilus* spores are more dispersed in their protein density and translucence. In contrast, the *B. subtilis* spores produced two tightly clustered peaks in protein density. Also, the latter spore produces intensities that are more correlated with protein-density fluctuation than the former. These differences in spores lasing phenotypes arise from differences in physical phenotype such as the protein coat morphology, intracellular granularity, spore shape, and intracellular protein density and uniformity.

These results demonstrate the feasibility of using the biolaser for near-instantaneous detection of bacillus spores in an unknown powder.

52797

Design and Control of the Magnetic Properties of Nanoparticles

B. A. Simmons

The magnetic properties of materials are closely related to the quantum couplings at an atomic level, including electron spin-spin (S-S) and electron spin-orbital angular momentum (L-S) couplings at crystal lattices. Since these couplings are determined by atomic placement on crystal sublattice sites, the magnetic properties of materials can be designed by controlling crystal chemistry. Spinel ferrites, MFe_2O_4 ($M = Mn$ [manganese], Mg [magnesium], Zn [zinc], Co [cobalt], iron [Fe], etc.) are among the most important magnetic materials and have a rich crystal chemistry. By utilizing the high compositional and structural flexibility of spinel ferrites, Sandia's current research focuses on designing and fine-tuning the magnetic properties of spinel ferrite nanoparticles by changing their chemical composition and particle size.

We can use our specially designed magnetic nanoparticles to form magnetic fluids. The properties of such fluids can be designed following the requirements of their applications. The design will be based mainly on two variable parameters. The first one is the intrinsic magnetic properties of the nanoparticles since the magnetic properties of these nanoparticles can be fine-tuned. The second one is the surface chemistry of the nanoparticles. We are working on linking a variety of organic and biological molecules covalently to the surface of the nanoparticles. By using atom-transfer radical polymerization (ATRP), we also added a polystyrene shell to the nanoparticle. The chemical control of the nanoparticle surfaces will enable us to control the internanoparticle interactions in the fluids and the interactions between the nanoparticles and the liquid matrices.

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52825

Aerospace Vehicle Trajectory Optimization System by Primer Vector Methods

W. P. Wolfe

As aerospace vehicles are expected to do more and more with less and less, the need for performance in an absolutely optimal manner becomes imperative. This is especially true in space applications and, more specifically, in spacecraft trajectory design, where an extremely high cost is paid for every bit of propellant on board. Being able to perform maneuvers at the smallest possible cost enables certain applications to be done that could not possibly be performed in a nonoptimal way. This alone has prompted a growing need for optimization methods. The culmination of this project is expected to be a trajectory optimization method that will address this growing need. Sandia will perform this work in collaboration with researchers at the University of Texas.

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52826

Algorithm Development for Smart Antennas*R. J. Franco, L. H. Marshall, M. A. Forman*

Smart antennas have received much interest in recent years in connection with a wide variety of commercial, military, and intelligence applications. These applications require sophistication in antenna development to overcome multipath, clutter, and jamming concerns in very complex physical environments. There is great interest in the intelligence community to enhance the low probability of detection (LPD) properties of communication links. Work in this area has often led to architectures that consist of an array of elements connected to a digital signal processor. This configuration provides the potential to improve the capacity and versatility of a wireless communication link through a combination of diversity gain, array gain, and interference suppression. These improvements allow for higher link capacity and the opportunity to improve link utility in complex environments and geometries. The research proposed here will address the development of analytic tools to facilitate the design of smart antennas for applications that include the challenging constraints in modern wireless communication links. Sandia will perform this research in collaboration with researchers at New Mexico State University.

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52976

Failure Analysis and Surety Design of Composite Patching Systems

D. C. Hammerand

In this project, Sandia will conduct an in-depth study of acute and chronic damage mechanisms threatening composite materials used in patching systems to repair deficient aircraft components. We know that disbonding and delamination are the primary defects in composite repair of aircraft components. These may be caused by poor surface preparation, thermal mismatch, moisture, and other chemical contamination, etc. The defects can occur during the repair or after prolonged exposure. Because composite patching for aircraft is a relatively new technology, supplanting traditional riveted patches, several reliability and surety issues remain uncertain. Composite patching systems are attractive, in part because the lay-up of the reinforcing fibers can be optimized to handle the service conditions of the aircraft. However, the design must also anticipate the occasional unexpectedly large loading conditions that can occur in rough weather or during emergency evasive maneuvers. To ensure safety of the aircraft on which the repairs are deployed, it is essential to proactively appraise the performance of composite patching systems under long-term normal service conditions and short-term abnormal environments, as well as to develop protocols for preventive maintenance. Sandia will perform this work in collaboration with researchers from North Carolina A&T University.

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52977

Flow Control and Mixing in Microfluidic Devices

A. C. Sun

Sandia is focusing on two important considerations for microfluidic devices: flow control and mixing. These research topics will significantly impact the efficiency of microfluidic devices used for delivering buffer, reagents, and cells. This work will first focus on flow control and subsequently shift to mixing.

- Flow control in microfluidic polymeric devices. We will consider two approaches for controlling flow in microfluidic devices: electrokinetic (EK) transport and varying channel dimensions. First, this work will investigate EK phenomena for pumping as well as flow control. Manipulation of the flow in microchannels is achieved by varying the electric fields and the surface charge. We will consider both approaches. We can use electric fields to direct the flow throughout the device and surface charge to increase the effectiveness of EKs, as well as manipulate the velocity profile of the fluid by patterning the surface charge. This work will also investigate manipulation of channel dimensions to better understand microflow and influence its behavior.*

- Mixing in microfluidic devices. In microfluidic devices that utilize chemical reactions, mixing is a major concern. A possible solution involves porous polymeric plugs. These plugs promote mixing by forcing the two liquids to take tortuous paths through the plug, which shortens the mixing length and disturbs the laminar nature of the flow. Extensive experimentation and modeling will be necessary to fully understand the use of porous polymer plugs. We will then take the next step to use this understanding and help develop mixing plugs that are even more effective.*

Sandia is doing this work in collaboration with the University of Colorado.

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53339

Wire-Initiation Dynamics and Monochromatic Imaging

D. B. Sinars, M. E. Cuneo, M. G. Mazarakis, C. A. Coverdale

Z-pinches are proving to be a critical technology to provide intense radiation fluxes to support Sandia and the other Department of Energy stewardship programs. Examples are in the areas of radiation-material interactions and radiation-driven hydrodynamics, and as an enabling technology for inertial confinement fusion (ICF). To continue to develop these radiation sources, Sandia needs advanced diagnostics plus a thorough understanding of Z-pinch implosion physics, i.e., ultimately, three-dimensional magnetohydrodynamic (MHD) calculations. In collaboration with Cornell University, we will explore the early time dynamics of wires exploding in the array, provide fundamental data to incorporate into our MHD codes, and consult on advanced monochromatic imaging diagnostics.

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53342

Investigations into the Transient Analysis of System Reliability/Availability Via Cumulant Functions

L. P. Swiler, J. E. Campbell

This research involves the development of cumulant-based procedures for the analysis of the reliability/availability of systems and components over a finite time horizon. This analytical approach would apply to a large number of systems and components whose failure and/or repair times are either assumed Markovian or approximated through a phase-type distribution. These types of systems are typically encountered in “real-world” applications and are typified by a large collection of systems with dependent failures and/or nonideal repairs. The use of cumulant functions in stochastic modeling was previously applied to the analysis of compartmental models and queueing systems, but not to the areas of reliability and quality control. Due to the high degree of theoretical merit and practical applicability of this work, this technology would be of interest to both industry and Sandia. The work supports our Enhanced Stockpile Surveillance Program and many of the Department of Defense initiatives.

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53372

Topological Layout for the Optimal Design of Electrostatically Actuated MEMS

J. J. Allen

In recent years, the potential of topology optimization has been studied intensively and successfully applied to the design of microelectromechanical systems (MEMS) structures. The main advantage of this computer-based design-optimization methodology is the capability to generate conceptually novel layouts without requiring close-to-optimal initial designs.

This work will use the media of MEMS to fully exploit the potential of topology optimization, as well as advance the state of the art of MEMS design. The following aspects of this work will be unique from heretofore-published research:

- Topology optimization has not been used in the context of a full two-way-coupled problem. The proposed work will focus on electrostatic mechanical coupling since this is relevant to the design of MEMS.*

- The layout of the entire structure is subject to topology optimization. This includes internal structural elements and also the shape of the interface between the electrostatic field and the structure. Of particular interest from a theoretical and a design point of view is the generation of this interface, which is flexible throughout the process, therefore avoiding rigid structural boundary topology, as is standard in topology optimization.*

The collaborating parties on this research bring expertise on topology optimization and MEMS design. This collaboration will have the unique opportunity of verifying numerical results with experimental results, since optimal MEMS structures designed will actually be built and tested. This close work with the device side of MEMS technology will ensure continuity between theoretical numerics and actual performance.

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53464

Atomic-Scale Scanning-Tunneling Microscopy Measurements of Nucleation and Growth of Ge/Si Alloy Structures

B. S. Swartzentruber

One of the key issues in the development of nanoscale technology is the fundamental understanding of the kinetics involved in their formation and stability. Often self-assembly (or self-organization) is the proposed route to forming desirable nanoscale structures in parallel. Self-assembly is driven by a system's desire to reach equilibrium, tempered by activation barriers that control the kinetics or time-scale of pattern formation. Once understood, the tradeoff between kinetics and thermodynamics can be used to control the nanostructure morphology.

Sandia's goal in this work is to determine and measure the fundamental atomic-scale processes responsible for the formation and stability of germanium/silicon (Ge/Si) alloy structures on Si(001). The Ge/Si(001) material system is of technical interest because its electronic properties make it useful for optoelectronic devices. In addition, it is a model system for the self-assembly of quantum-dot structures with a length scale that is tunable through the atomic-percent of Ge in the alloy. Because of the size mismatch between Ge and Si (Ge is 4% larger than Si), lattice strain relief provides much of the driving force for pattern formation. However, little is known about how the strain affects the kinetics of mass transport and Ge incorporation into the Si lattice. Our atom-tracking scanning-tunneling microscope is an ideal tool with which to study this problem. We will perform this work in collaboration with researchers at Arizona State University.

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53465

Micro-/Nanoscale Thermomechanical Manufacturing

A. C. Sun, A. M. Grillet

A wide variety of engineered organic materials have the ability to conduct electricity, emit light, and demonstrate biochemical reactivity. The functionality and inexpensive nature of these materials make them appealing candidates for materials in micro-/nanodevices and -systems.

Hot embossing offers the opportunity for large-area stamping with nanometer-scale features. In embossing for micro-/nanoscale patterning, a relief mold is pressed into a soft polymer medium. Typically the stamp is heated such that the polymer melts beneath the stamp. Feature sizes are possible as small as 10 nm over several square centimeters. Elsewhere, atomic-force microscopy (AFM) thermal-indentation writing can form pixels as small as 10 nm with a pitch of 3 nm. While much progress has been made by the materials science and microelectromechanical systems (MEMS) communities on developing micro-embossing technology, hot-embossing processes remain almost entirely recipe-based. There is at present little published work to predict from first principles the relation between the stamp size, stamping features, time, temperature, and loading force of the stamping process, and the size and shape of the resulting features. Additionally, at nanometer-length scales, materials properties such as viscosity and thermal conductivity can be substantially different from those of the bulk.

This work investigates the design of embossing masters and processes for the purpose of micro-/nanoscale patterning of functional organic materials. Experimental and numerical work determines the relation between stamp size, process parameters, and resulting feature sizes. The ultimate goals of this work are to develop design rules for manufacturing nanometer-scale devices from advanced organic materials and to fabricate several working devices with a manufacturing approach derived from these rules. Sandia will perform this work in collaboration with researchers at Georgia Tech.

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53681

Design of Biospecific Surfaces to Control Specific Cellular Responses

S. M. Brozik

Many biological systems exhibit unique properties and functionalities arising from the nanoscale of operation. Sandia is pursuing several biomimetic and self-assembly strategies to engineer bio-inspired surfaces to elicit specific cellular responses for biomaterials, tissue engineering, and biotechnological applications. This project focuses on engineering robust surfaces that present controlled biomimetic ligands whose nanoscale structure governs specific cell-receptor binding and activates diverse signaling pathways. Sandia will perform this work in collaboration with researchers from Georgia Tech.

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53682

High Field Effects of GaN HEMTs

R. J. Shul

Transport measurements are of vital importance to electronic semiconductor devices. While low field-mobility measurements are a routine measurement for evaluating semiconductor materials, high field measurements have been more problematic and less commonly used. A new technique developed by Arizona State University (ASU) was recently applied to bulk gallium nitride (GaN) and is currently being evaluated for aluminum gallium nitride (AlGaN)/GaN high-electron mobility transistors (HEMTs). The technique uses specially developed test structures with an etch constriction and high-voltage pulsed measurements. The methodology developed at ASU for testing and modeling was aided by the GaN processing capabilities at Sandia. Now that the new method for high field transport has been developed, we can evaluate new GaN materials and transistor device structures for their impact on saturated velocity. These measurements can also be correlated to the performance metrics available from transistor characterization. We seek to create structures from bulk GaN and AlGaN/GaN structures with intentional variation of defect density (through cantilever epitaxy), interface roughness, and intentional variations of the transistor structure, and to evaluate the high field-electron velocity of these structures.

Now that the new method for high field transport has been developed, we can evaluate new GaN materials and transistor device structures for their impact on saturated velocity.

54210

Cognitive Models Applied to Human Effectiveness in National Security Environments

A. B. Doser

Machine perception and cognitive modeling are emerging fields with broad applicability to improving human effectiveness, intelligent systems, and large-scale simulations involving humans and systems of systems. From a human effectiveness standpoint, cognitive modeling is also an enabling technology that will improve visualizations, situational awareness, and critical decision making. This project will explore the use of cognitive models in systems applications from the standpoints of human and systems performance, as well as validation requirements for the use of cognitive models in engineered systems. Sandia will perform this work in collaboration with North Carolina A&T University.

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54211

Nanomagnetic Films*M. W. Jenkins*

Recent advances in chemical synthesis allow the fabrication of molecular nanomagnets. Micro- and nanodevices that could be enabled by nanomagnets will require a reproducible process for creating films. The first goal of this project is the nontrivial challenge of producing two-dimensional (2-D) nanomagnetic structures. These molecules disintegrate at high temperatures and in vacuum, so new approaches like evaporation, aerosol deposition, and precipitation from suspension will be investigated.

A second goal is to integrate patterned molecular magnetic films onto surfaces that contain other functional elements like miniature superconducting quantum interference devices (SQUIDS). Patterned molecular nanomagnetic films make possible 2-D patterned molecular nanomagnets by which controlled studies of shape anisotropy and magnetic properties can be made.

This work directly supports both Sandia's nanotechnologies and microsystems efforts. Developing the science and process associated with nanomagnetic film deposition will allow such novel materials to migrate into microsystems that directly support Sandia's national security missions.

This research will be performed in collaboration with Texas A&M University.

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54213

A Multiscale Approach to Modeling Carbon Nanotubes

J. W. Foulk, III

In collaboration with Texas A&M University, Sandia will focus on ascertaining the feasibility of modeling individual as well as networks of carbon nanotubes (CNTs) using multiscale techniques to relate atomic, micro, and macro continuum length scales. We will address applications for cohesive zones in modeling fracture in nanotube chain connections and in CNT bundles.

We will develop computational tools to model specific applications of CNTs in spacecraft, bulletproof vests, and nanomachines where mechanical as well as electrical properties may be of interest.

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<i>Project Number</i>	<i>Title</i>	<i>Page Number</i>	<i>Project Number</i>	<i>Title</i>	<i>Page Number</i>
28763	Use of Intense Ion Beams for Surface Modification and Creation of New Materials	661	32913	Aging Mechanisms in Dormant MEMS Structures	186
28764	Low-Intensity Laser Triggering of Spark Gaps	663	32914	Biomimetic Chloroplasts: An Integrated Microdevice Power Source	99
28769	Z-Pinch Power-Plant System Development	664	32915	Study of Polymer Spin-Coating for Photolithographic Semiconductors in Near-Zero-Gravity Environment	494
28770	Recyclable Transmission Line Concept for Z-Pinch IFE	666	32923	MEMS in μ Fluid Channels	188
28771	Suppression of Electron Emission from Conductors	669	33602	Dispersive Photonics for Next-Generation Sensors and Microsystems	191
28772	Solid-State Switch for Advanced Pulsed Power	671	34465	Understanding Metal Vaporization from Transient High-Fluence Laser Irradiation	496
28775	Laboratory-Scale Coherent Multikilovolt X-Ray Sources for Advanced Imaging Applications	257	34466	Mechanics and Tribology of MEMS Materials	498
28776	Interfacial Bioscience Grand Challenge (IBIG)	447	34467	Dynamics of Metal/Ceramic Interfaces	502
32574	High-Throughput Instruments, Methods, and Informatics for Systems Biology	95	34468	<i>In Situ</i> Characterization of Soft Solution Processes for Nanoscale Growth	504
32807	Low-Work-Function Material Development for the Microminiature Thermionic Converter	343	34469	Determination of Critical Length Scales for Corrosion Processes Using Microelectroanalytical Techniques	506
32809	Autonomous Microexplosive Subsurface Tracing System	346	34478	LIGA Microsystems Aging: Evaluation and Mitigation	508
32815	Security Models of Agent-Based Coalitions	349	34485	Science-Based Processing of Field-Structured Composites	511
32816	Vulnerability Assessment of National Power Grid	351	34692	Self-Assembly of Polymers in Confined Geometries	693
32817	Molecular Simulations of MEMS and Membrane Coatings (PECASE)	691	34693	Building Conscious Machines Based on the Architecture of Visual Cortex in the Primate Brain	695
			34698	Microfuze	258

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<i>Project Number</i>	<i>Title</i>	<i>Page Number</i>	<i>Project Number</i>	<i>Title</i>	<i>Page Number</i>
34699	Exploration of New Multivariate Spectral Calibration Algorithms	514	38615	Sensitivities for Large-Scale Simulation Codes	142
35376	Development of Experimental Verification Techniques for Nonlinear Deformation and Fracture	696	38616	Engineered Superconductivity in Electron-Hole Bilayers	193
36901	Microcontact Printing of Nanoparticle Arrays	699	38617	Silicon-Based RF MEMS Components	195
36902	Mathematical Analysis of Deception	703	38618	2-D Arrayed Resonant Subwavelength Gratings	197
36904	A System-Dynamics Approach to Modeling Water Demand	704	38619	Nanoelectromechanical Oscillators (NEMOs) for RF Filtering	200
38605	Microfabrication with Femtosecond-Laser Processing	69	38620	Continuous-Wave Intersubband Terahertz Sources	203
38606	Mesoscale Controlled Motion for a Microfluidic Drop Ejector	71	38621	Microsystems for Chemical Signature and Reagent Delivery	205
38608	Science-Based Sensing of Phase Transformations in Steels	73	38622	Microfluidic Cellular Sample Pretreatment	207
38609	Physical and Electronic Changes Caused by Membrane Signaling as a Transduction Pathway in Affinity-Based Biosensors	101	38623	Automated Visual Direction of Mobile Manipulation	261
38610	Graduated Embodiment for Sophisticated Agent Evolution and Optimization	130	38624	Miniature Fourier-Transform Ion-Mobility Spectrometer for Real-Time Detection and Identification of Explosives and Chemical Agents	263
38611	Stochastic Programming for Enterprise Modeling—Optimization for Nondeterministic Simulation	133	38625	CONOPS Development for Automated Systems	266
38612	Robust Message Routing for Mobile (Wireless) <i>Ad Hoc</i> Networks	136	38626	Rapid Mitigation and Decontamination of Toxic Industrial Chemicals	268
38613	Scalable Fault-Tolerant Algorithms for Linear-Scaling Coupled-Cluster Electronic Structure Methods	138	38627	EM Interactions with Systems to Enhance Security	270
38614	Micromagnetic Suspension	140	38628	Adaptive Awareness for Personal and Small-Group Decision Making	272

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<i>Project Number</i>	<i>Title</i>	<i>Page Number</i>	<i>Project Number</i>	<i>Title</i>	<i>Page Number</i>
38629	Use of Seismic and Acoustic Responses to Assess Bomb Damage to Underground Facilities	274	38672	Validated Modeling of Distributed-Energy Resources at Distribution Voltages	369
38655	Free-Space Electrooptic Sampling and Remote Mapping of Electromagnetic Fields from Emitting Structures Using Femtosecond Terahertz Transceivers	277	38673	Water Desalination	370
38658	Kinematics-Based Video Compression Using a Foveated-Imaging Sensor for Remote Telepresence Applications	279	38674	Revolutionary Systems for Catalytic Combustion and Diesel Catalytic Particulate Traps	373
38659	Information Assurance for Wireless <i>Ad Hoc</i> Networks	281	38677	Potential Application of Microsensor Technology in Radioactive-Waste Management—with Emphasis on Headspace Gas Detection	376
38661	Low-Toxicity Hypergolic Propellant System Using H ₂ O ₂ Oxidizer	283	38678	Surety Enhancement for Wireless Automated-Control Networks	378
38662	Natural-Gas Production Problems: Solutions, Methodologies, and Modeling	354	38679	Advanced Nuclear-Engineering Analysis Technology	380
38664	High-Efficiency Turbine Blade Coatings	356	38681	Identification of Chemical Plumes: Range-Resolved IR Lidar Enabled by New Photonic Technologies	383
38665	Time-Domain Reflectometry for Remote, Real-Time Water Quantity/Quality Monitoring of Ephemeral Streams	358	38682	Multiscale Thermal Modeling	422
38667	Research and Development of Mathematical Algorithms to Define and Quantify Critical Infrastructure Interdependencies	361	38684	A Robust, Coupled Approach for Atomistic-Continuum Simulation	424
38668	Functionalized Nanoelectrode Arrays for <i>In Situ</i> Identification and Quantification of Regulated Chemicals in Water	364	38685	Microscale Rarefied-Gas Dynamics and Surface Interactions for EUVL and MEMS Applications	427
38669	Hybrid Infrastructure Cryptography	367	38686	High-Fidelity Frictional Models for MEMS	430
			38687	Soot Formation, Transport, and Radiation in Unsteady Diffusion Flames	433
			38688	The Basics of Aqueous Nanofluidics: “Interphase” Structure and Surface Forces	518

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<i>Project Number</i>	<i>Title</i>	<i>Page Number</i>	<i>Project Number</i>	<i>Title</i>	<i>Page Number</i>
38689	Design, Synthesis, and Characterization of Soft-Matter Nanolayer Superlattices	521	38705	The Effects of Varying Humidity on Copper-Sulfide Film Formation	532
38690	Photocontrol of Nanointeractions in Microsystems	523	38706	Detecting and Tracking the Active Insider Using 3-D Detection Technology	618
38691	Electrochemically Deposited Alloys with Tailored Nanostructures for LIGA Micromachines	526	38707	Microfabricated Dielectrophoretic Sample Preparation System	620
38692	Nanostructured Materials for Directed Transport of Excitation Energy	528	38708	Automation of Microelectronic Physical Analysis	623
38693	Modeling Local Chemistry in the Presence of Collective Phenomena	530	38712	Nonlinear Optical Limiters Using Photonic-Bandgap Structures for Sensor Protection	624
38695	Passive-Legged, Multisegmented Robotic Vehicle	601	38713	Secure MPLS Control Plane for Internet Connectivity	626
38696	Low-Cost Photonic Lattice Structures for Remote Sensing	603	38714	Integrated-Sensor Network Chip	628
38698	Security Monitoring and Management with Information Technology (SUMMIT)	605	38716	Self-Organization of Software	706
38699	Novel Methods for Ultracompact, Ultralow-Power Communications	607	38717	Nanoscale Energetic Materials by Inverse Micellar Synthesis	707
38700	Collaborative Approach in System Design and Protection	609	38718	Modeling of Rock Penetration	709
38701	Novel Tagging Technologies for the Tracking and Authentication of Documents, Property, and Other Items	610	38719	Nanoconverter	712
38702	A Revolutionary Long-Lived Power Supply: The Icosahedral Boride Semiconductor (IBS) Beta-Cell	612	38720	Novel Proton-Exchange Membrane Materials for the Advancement of Direct Methanol Fuel-Cell Technology	713
38703	Remote-Sensing Data Exploitation for Geologic Characterization of Difficult Targets	615	38721	Communicating with the <i>In Vivo</i> Sensor	715
			38722	Agile, Microsystems-Enabled Receiver	718
			38723	Linking Geosciences to Emerging Bioengineering Technologies	721
			38724	Energy Storage: Leaving Chemistry in the Dust	724

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<i>Project Number</i>	<i>Title</i>	<i>Page Number</i>	<i>Project Number</i>	<i>Title</i>	<i>Page Number</i>
38726	Novel Algorithms and Experimental Techniques for Quantitative Spectral Analysis of Particulates	726	44136	Fluid-Structural Interactions in Wetting and Penetration into Porous Media	740
38727	Self-Healing Adhesives and Encapsulants: Long-Term, High-Performance Weapon Components	729	44601	High-Level Decision-Support Framework for Critical-Infrastructure Protection Prioritization	386
38729	Neutron-Only Detector for JTA Tests	731	44774	Dynamic-Simulation Model of the National Security Consequences	388
38744	Adaptive Network Countermeasures	145	45279	Macroscopic Rates, Microscopic Observations, and Molecular Models of the Dissolution of Carbonate Phases	742
39017	Solution-Based Nanoengineering of Materials	534	46069	Electrical-Impedance Tomography for Opaque Multiphase Flows in Metallic Vessels	435
39212	MEMS-Based Electromechanical Acoustic-Energy Harvester	732	46070	High-Speed Micro-EDM	745
39669	Determination of Microstructural Properties with Isentropic Compression	673	46072	Electricity-Generation Production Cost Model	390
39670	Simulations of Intense Petawatt Laser Pulses with Dense Z-Pinch Plasmas	675	46684	Developing Rigid and Compliant Cardiovascular-System Models Using Rapid Prototyping	747
41193	Biomicrofuel Cell	449	46685	Nanoscale Hotspots Due to Nonequilibrium Thermal Transport	749
41194	Cognition-Driven Augmented Analyst	630	46686	Micro External Combustion Engine: The P3 Engine Prototype	752
41427	Predicting and Validating MEMS Interface Reliability	546	46687	Exploiting Polarimetric Information in Synthetic-Aperture Radar Images for Automatic Target Recognition	284
41674	Microengine for Advanced Power Generation	147	46688	Moving-Target Identification Using Ultrahigh-Range Resolution Data	285
41726	Direct Simulation of Solid-Fluid Systems	734	47516	Effectiveness of Dielectrophoretic and Electrokinetic Filters/Concentrators for Collecting Smallpox and Anthrax Surrogates from Raw Samples	754
42461	Support-Active Site Interactions in Heterogeneous Catalysts	736			
42483	An Analysis of the Automotive Industry as a Source for Weapon Components and Manufacturing Processes	738			

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<i>Project Number</i>	<i>Title</i>	<i>Page Number</i>	<i>Project Number</i>	<i>Title</i>	<i>Page Number</i>
47517	Mathematical and Algorithmic Issues in Multiphysics Couplings	755	49167	Radiolytic Reduction of Carbonaceous Gases During Coal Gasification for Hydrogen Production	391
47687	MEMS Adaptive Optics Devices	757	49168	Spectral Tagging	642
47688	Securing the U.S. Mail Distribution System Against the Threat of Biological and Chemical Agents	759	49170	Assessment of the Potential Impact of Disruptions in Manufacturing Supply Chains	766
47795	Lipid Membranes on Nanostructured Silicon	761	49367	Proton Beam Shield	393
48212	Combating Terrorism and Homeland Security	24	49767	Microoptical Radar: Enabling Multiple Solutions to the War on Terrorism	27
48213	Underground Hunter Robots: Reconnaissance, Clearing, and Securing of Underground Tunnel Complexes Using Robotic Vehicles	25	49769	Resin Infusion Between Double Flexible Tooling	768
48339	Combating the Chem-Bio Threat Using Sandia Assets: Need for a Technology Roadmap	763	49770	Frameworks for Nuclear Process Transparency and Control	395
48340	Numerical Methods for the Study of Hydrocarbon Combustion	764	49771	155-mm Munitions Reutilization Study	288
48341	Chemically Stressed Glass Structural Elements	632	49772	Studies on the Disbonding Initiation of Interfacial Cracks	770
48746	Digital Signal Processing for Acoustic-Seismic Target Identification	634	49773	Principles for Network-Security Mechanisms Utilizing Network Address Translation	30
48751	Terahertz Propagation in Telecommunication Optical Fibers	635	49864	Aviation Security	644
48764	Rapid Screening for Biological Infection	637	49914	Effect of Machining Parameters on Tool Life	771
48765	Investigation of Bluetooth Capabilities and Vulnerabilities	639	49915	Critical Technology Development for Hard Target Defeat High-G Tolerant Fuze and High Explosives	291
			50000	Protection of Sensitive Computers	646
			50001	Unmanned and Unattended Response Capability for Homeland Defense	293

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<i>Project Number</i>	<i>Title</i>	<i>Page Number</i>	<i>Project Number</i>	<i>Title</i>	<i>Page Number</i>
50065	War on Terrorism	452	51541	Optical Tagging Technologies	654
50066	Application of Nonlethal Weapons to Counterterrorism	295	51706	Feasibility Study of an Integrated-Systems Solution to the Problem of Radiological Dispersal Devices	32
50121	Particle "Front End" for Compact WMD Threat-Detection Systems: Integrated Microsystem Concepts for Intelligent Particle Collection, Separation, Preconcentration, and Processing	149	51708	A Maneuvering, Hypersonic Pathfinder/Test-Bed	298
50395	Assessment and Identification of Appropriate μ Power Technologies for μ Sensors and Other Applications	647	52173	Micromechanical Spectrum-Analyzer System	75
50396	Compliant Membranes for MEMS Microphones	773	52174	Inelastic Deformation Mechanism in Shocked Sapphire Single Crystals	781
50717	Multiscale Experimental/Numerical Study	774	52175	Feasibility Study: Development of a Computational Sociopsychological Model for Understanding Terrorist Behavior	35
50772	Cellular Observatory: Simultaneous Time- and Frequency-Resolved Microscopy	776	52176	Feasibility of Microsensors for the War on Terror	37
50858	Near-Real-Time Site Characterization for Assured HDBT Defeat	777	52216	Thermobaric Weapons Signatures	656
50973	Multispectral Data-Exploitation Advancements	649	52395	Feasibility of Using Pulsed Intense Ion Beams to Improve Wear Behavior of Metals and Plastics	299
51534	A Fully Integrated Sensor-Based Critical Facility and Border Defense System	397	52397	Feasibility Study for Improved Nonlethal Weapon Based on Disruption of Postural Reflexes	38
51536	Concept Definition for an Integrated Biodefense System	296	52796	Portable Endospore Detection System for Real-Time Anthrax Screening	782
51537	Ironless Permanent Magnet Actuator	780	52797	Design and Control of the Magnetic Properties of Nanoparticles	784
51538	Response Analysis Tactical Simulation	652	52825	Aerospace Vehicle Trajectory Optimization System by Primer Vector Methods	785
51540	Introspection, Integration, and Intercession (I^3) Toward Self-Healing Critical Infrastructures	398	52826	Algorithm Development for Smart Antennas	786

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<i>Project Number</i>	<i>Title</i>	<i>Page Number</i>	<i>Project Number</i>	<i>Title</i>	<i>Page Number</i>
52974	Class B Fire-Suppression Capabilities of a Modified Sandia CBW Decon Foam	658	53464	Atomic-Scale Scanning-Tunneling Microscopy Measurements of Nucleation and Growth of Ge/Si Alloy Structures	792
52976	Failure Analysis and Surety Design of Composite Patching Systems	787	53465	Micro-/Nanoscale Thermomechanical Manufacturing	793
52977	Flow Control and Mixing in Microfluidic Devices	788	53681	Design of Biospecific Surfaces to Control Specific Cellular Responses	794
53339	Wire-Initiation Dynamics and Monochromatic Imaging	789	53682	High Field Effects of GaN HEMTs	795
53340	Rapid Syndrome Validation Project (RSVP) Hypothesis Testing and Development	103	54210	Cognitive Models Applied to Human Effectiveness in National Security Environments	796
53342	Investigations into the Transient Analysis of System Reliability/Availability Via Cumulant Functions	790	54211	Nanomagnetic Films	797
53372	Topological Layout for the Optimal Design of Electrostatically Actuated MEMS	791	54213	A Multiscale Approach to Modeling Carbon Nanotubes	798
53373	Detection, Classification, and Multitarget Tracking in a Sensor-Rich Environment	40			

Appendix B: Awards/Recognition List

<i>Awards/Recognition</i>	<i>Project Number</i>	<i>Project Title</i>
E. O. Lawrence Award	11130	Molecular Integrated Microsystems (MIMS)
Outstanding paper for 2002 Nuclear and Space Radiation Effects Conference	26523	Radiation Aging of Stockpile and Space-Based Microelectronics
Asian-American Engineer of the Year Award: Dr. Shawn-Yu Lin	26556	Photonic Crystals for Enhancing Thermophotovoltaic Energy Conversion

Appendix C: Project Performance Measures

		Performance Statistics (Number of)											Project Qualitative Assessment		
Project Title	Project #	Refereed Publications	All Other Reports and Publications	Patent Disclosures	Patent Applications	Patents	Copyrights	Students	Post-docs	Permanent Staff Hired*	Awards	New Non-LDRD-Funded Projects†	% Milestones Completed	Goals Status**	Hypotheses Status***
A Novel Microcombustor for Sensor and Thermal-Energy Management Applications in Microsystems	10718	2			1			1		1	1		90%	2	6
Radiation-Induced Prompt Photocurrents in Microelectronics: Physics	10719												90%	2	8
Volumetric Displacement Control (VDC) of Manufacturing Tools	10721		3	1	2			1		1			100%	1	6
Process-Based Quality Tools to Verify Cleaning and Surface Preparation	10722		3					5	1	2			90%	2	6
Fabrication of Three-Dimensional Microstructures Using Soft Lithography	10723		1										70%	2	7
High-Speed 2-D Hadamard Transform Spectral Imager for IR Applications	10724	2		1	1								75%	3	6
A Micro-GC–Based Controller for Energy-Intensive Processes	10725	3		2									100%	2	6
Micro-High-G Acceleration Recorder	10727												95%	2	6
Algorithmic Advances in Computational Structural Biology	10728	1					1	2					67%	2	8
Ultraminiaturization of RF Circuitry	10729												70%	3	6
SOI–Based High-Aspect-Ratio Si Bulk Micromachining for MEMS Applications	10733												95%	2	7
Next-Generation Output-Based Process Control: An Integration of Modeling, Sensors, and Intelligent Data Analysis	10734		1	1			1	3					100%	1	6
Physical Basis for Interfacial Traction-Separation Models	10735		5										90%	2	6
Dynamic Range Imaging for Terrain Mapping, Position Determination, and Obstacle Avoidance in Autonomous Navigation	10736			1	1								70%	3	8
Diagnostics for Joining Solidification/Microstructural Simulations	10740	5	8					1					100%	1	6
Effects of Microstructural Variables on the Shock-Wave Response of PZT 95/5	10741	1											85%	2	7
Mechanisms of Dislocation Grain-Boundary Interaction	10742	9							1				50%	2	6
Defining the Frontiers of Vertical, External-Cavity, Surface-Emitting Lasers	10744	2											20%	4	7
Predicting Function of Biological Macromolecules	10746	15	4						1	1			80%	2	6

Appendix C: Project Performance Measures

		Performance Statistics (Number of)											Project Qualitative Assessment		
Project Title	Project #	Refereed Publications	All Other Reports and Publications	Patent Disclosures	Patent Applications	Patents	Copyrights	Students	Post-docs	Permanent Staff Hired*	Awards	New Non-LDRD-Funded Projects†	% Milestones Completed	Goals Status**	Hypotheses Status***
Nanostructured Silicon Surfaces for Cost-Effective Photovoltaic Efficiency Improvements	10748	2				1							75%	2	8
Growth and Characterization of Quantum Dots and Quantum-Dot Devices	10749	11						1	2				80%	2	7
Automatic Design of Practical Fixtures	10751	2		1				2					100%	2	6
Distributed, Reconfigurable, Homogeneous Microrobotic Systems	10752				3	2							100%	1	7
Robust Planning for Autonomous Navigation of Mobile Robots in Unstructured, Dynamic Environments	10753												60%	3	8
Functional Materials for Electrochemomechanical Actuation of Microvalves and Micropumps	10754				1	1		1					50%	3	7
New Architectures for Micro-Total-Analytical Systems	10756	1		2		2		2		1			100%	1	6
Large-Scale Nonlinear Optimization Arising from PDE Models	10757	3	2					4		1			100%	1	6
Making the Connection Between Microstructure and Mechanics	10761	11	2					1					90%	1	6
Self-Assembled Tamper-Detection Seals	10762			1	1		1						100%	1	6
Control Strategies for Homogeneous Charge-Compression Ignition (HCCI) Engines	10763		1		1				2				100%	1	6
Energetic-Material Burn and Detonation at the Mesoscale	10765	1		1						2			80%	1	7
Heterogeneous Integration of Optoelectronic Arrays and Microelectronics	10766	4											80%	4	7
IMEEMS Packaging and Interconnection Technology	10770			10	5	3		2					95%	2	6
Silicon/Carbon Nanocomposites for Rechargeable Battery Applications	10771		3	2				1	1				95%	2	6
Intense Directed-Energy Theory Initiative	10772												100%	1	6
Biosensors Based on the Electrical Impedance of Tethered Lipid Bilayers on Planar Electrodes	10774	1						3	1				75%	2	7
Miniature Sensors for BW Agents Using Fatty-Acid Profiles	10775		7	1	1			3		1			70%	2	
Enhanced-Sensitivity Acoustic-Wave Biosensor Arrays	10776		1					3	1				85%	2	7
Parallel Methods for Coupling Circuit- and Device-Scale Simulations	10777						1	1					75%	1	7
A JAVA-Based Tool for Multifidelity Modeling of Coupled Systems	10778	5	2	1				1					75%	3	7

Appendix C: Project Performance Measures

Project Title	Project #	Performance Statistics (Number of)											Project Qualitative Assessment		
		Refereed Publications	All Other Reports and Publications	Patent Disclosures	Patent Applications	Patents	Copyrights	Students	Post-docs	Permanent Staff Hired*	Awards	New Non-LDRD-Funded Projects†	% Milestones Completed	Goals Status**	Hypotheses Status***
Switchable Hydrophobic-Hydrophilic Surfaces	10779	2		2				1	1				90%	1	6
Nanostructured Materials Integrated in Microfabricated Optical Devices	10780	3			1			3	3				80%	2	6
Microfabrication of Electromagnetic Devices	10783			1									75%	3	7
GaAs MOEMS Technology	10784	2		1	2	1		2	1				80%	2	6
Integrated Microsensors for Autonomous Microrobots	10785	1		1									85%	3	7
Silicon-Integrated Planar Microbatteries	10786	1		1									90%	3	7
Small-Scale Multiaxial Deformation Experiments on Solder for High-Fidelity Model Development	10788	6	1					1	1	1			95%	1	8
All-Ceramic Battery	10789	3			2	2		3	1	5			80%	2	7
Computer Numerically Controlled Micromachines	10793	2		2	1								95%	2	6
Surface-Micromachined Mechanical Timer	10795			1		1		2					95%	2	6
High-Efficiency Optical MEMS by the Integration of Photonic Lattices with Surface MEMS	10796	1	1	2	1								100%	1	6
Molecular Integrated Microsystems (MIMS)	11130	21		14	8	4		3	5	3	1		100%	1	6
Pseudostationary Separation Materials for Highly Parallel Microseparations (PECASE)	16167	6											100%	1	6
Novel Coatings for Microelectromechanical (MEM) Devices (PECASE)	17230	7						3	1				90%	2	6
Use of Apatite and Substituted Apatites for <i>In Situ</i> Barriers for Radionuclide Containment and Waste Stabilization and Arsenic Removal from Potable Water	19991	2		2	2								100%	1	6
Regional Dynamic Simulation Modeling and Analysis of Integrated Nuclear Futures	21559	1											100%	1	7
Theoretical Study of Sb as a Surfactant in Epitaxy of III-V Materials	22854	2											0%	11	
Mesoscale Wide-Bandwidth Linear Magnetic Actuators	26508												75%	3	7
Levitated Three-Axis Microaccelerometer	26509												80%	3	7
Microfabrication Processes Combining Focused Ion-Beam Machining and Thin-Film Vapor-Deposition Techniques	26510	2	1	3				1					100%	1	6
Resolving Fundamental Limits of Adhesive Bonding in Microfabrication	26511	3			1			1					100%	1	7

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Appendix C: Project Performance Measures

Project Title	Project #	Performance Statistics (Number of)											Project Qualitative Assessment		
		Refereed Publications	All Other Reports and Publications	Patent Disclosures	Patent Applications	Patents	Copyrights	Students	Post-docs	Permanent Staff Hired*	Awards	New Non-LDRD-Funded Projects†	% Milestones Completed	Goals Status**	Hypotheses Status***
Rapid Ultrasensitive Chemical-Fingerprint Detection of Chemical and Biochemical Warfare Agents	26533	1		1				2	1				75%	11	7
Advanced Unattended Ground-Sensor Technology	26534												75%	3	7
The Endowment of Simulator Agents with Humanlike Episodic Memory	26535	1						2				1	100%	1	7
An Advanced Learning Model for Agent Behavior	26537		2					1					100%	1	6
Threat-Assessment Study for Short-Pulse Laser Technologies in Directed-Energy and Countersensor Applications	26538											1	100%	1	6
Algorithms for Improved Performance in Cryptographic Protocols	26539		1	1									100%	1	7
Low-Cost Digital Radar for Fuzing, Tags, SAR Imaging, and Targeting	26540		3	3				3				2	95%	1	7
Triggered Isomer Research	26541							1		4			80%	2	7
A Scientific Basis for Robotic Ground-Vehicle Design	26542							3				2	90%	2	7
Adaptive and Mobile Ground Sensors	26543												95%	2	7
Algorithm Development for Prognostic Health Monitoring and Maintenance	26544	1						2				1	90%	2	8
New Mechanism for Upset of Electronics	26545										1	1	95%	2	7
Flexible Robotic Maintenance Facility	26546		1										100%	1	8
Distributed Autonomous Navigation	26547		1										50%	3	7
Obstacle Detection for Autonomous Navigation	26548							4		6			100%	1	6
Very High Temperature Gas-Cooled Reactor	26549		2										95%	2	6
Solid-State Ballistic Chemical Sensors	26550				1			1	1				75%	4	6
Novel Catalytic Systems for Energy-Efficient Feedstock Hydrocarbon Separations	26551	3	1					2	2				90%	1	7
A Model of Infrastructure Interdependency Using Communication Agents	26552		2									4	100%	1	7
Microchemical Sensors for Characterization and Monitoring of Volatile Contaminants	26553	2		3	1			2	1	1		4	100%	1	7
Investigation of Potential Applications of Self-Assembled Nanostructured Materials in Nuclear-Waste Management	26554	8		1	1			1	2	5			100%	1	6
Development of Detection Techniques and Diagnostics for Airborne Carbon Nanoparticles	26555		1									1	50%	3	7

Appendix C: Project Performance Measures

		Performance Statistics (Number of)										Project Qualitative Assessment			
Project Title	Project #	Refereed Publications	All Other Reports and Publications	Patent Disclosures	Patent Applications	Patents	Copyrights	Students	Post-docs	Permanent Staff Hired*	Awards	New Non-LDRD-Funded Projects†	% Milestones Completed	Goals Status**	Hypotheses Status***
Photonic Crystals for Enhancing Thermophotovoltaic Energy Conversion	26556	1		2	2						1		100%	1	6
Specific Anion Nanoengineered Sorbents for Water Purification	26557	5			3			1		1			100%	2	7
Development of a Microoptic Gyroscope	26559							2					80%	1	7
Synergistic Merging of Multispectral Transient Radiometry and Multispectral Imaging Technology for Enhanced Global Situational Awareness Through Accurate Geolocation	26560												90%	2	6
New Glass Technology for Enhanced Architectural Surety	26561	2	8					2		1		1	70%	3	6
Compact UV Laser Source for Chemical and Biological Sensing	26562	2						1				1	90%	1	7
Advanced Digital Detectors for Neutron Imaging	26563			2	2							1	90%	3	7
Microfabricated Acoustic Spectrum Analyzer	26564			1				2					90%	3	7
Enabling Analytical and Modeling Tools for Enhanced Disease Surveillance	26565	7	2									2	100%	1	8
Microtransmitter for Tag, Beacon, and Data-Exfiltration Applications	26566												100%	2	6
Extensibility of Knowledge-Based Human-Agent Simulation	26567	1							1	2		1	100%	1	6
Secure Authenticated Sensor Packs	26568	1											90%	1	6
Remote Monitoring of Difficult, Real-Time Targets Using Video SAR Technique	26569		1	1								1	90%	2	6
Coating Chemical Preconcentrators to Improve Chemical-Agent Collection	26572												100%	3	7
Ultralow-Power Spread-Spectrum Receivers for Microtags to Improve Security During Critical Operations	26573			1	3							1	100%	1	6
Detection and Exploitation of Spread-Spectrum Waveforms	26574		3		1								90%	1	8
Small-Power Direct-Conversion Microfluid Systems Using Logistical Fuels	26575	1						3	1				80%	3	8
High-Bandwidth Optical-Data Interconnects for Satellite Applications	26576	2						1	1			1	80%	3	7
Robust Chemometrics for Remote Spectral Sensing	26577	3	3	2	2								95%	1	6
Deployable Large-Aperture Optics System for Remote-Sensing Applications	26578	1				1		2		2	1		90%	2	6

Appendix C: Project Performance Measures

Project Title	Project #	Performance Statistics (Number of)											Project Qualitative Assessment		
		Refereed Publications	All Other Reports and Publications	Patent Disclosures	Patent Applications	Patents	Copyrights	Students	Post-docs	Permanent Staff Hired*	Awards	New Non-LDRD-Funded Projects†	% Milestones Completed	Goals Status**	Hypotheses Status***
MicroChemLab Technologies for Early Detection of Pathogen Exposure	26579	2							1				80%	1	6
Intelligent Tracking of the Telepresent Rapid-Aiming Platform	26580									3			100%	1	6
Molecular-Scale Studies of Single-Channel Membrane Pores	26581								1				80%	2	7
Efficient Massively Parallel Techniques for Protein Structure Generation	26582	2	2									1	100%	1	7
Mapping Membrane Protein Interactions in Cell-Signaling Systems	26583	1											80%	3	7
Interconnection Technology for Next Generation of Integrated Microsystems	26770												90%	1	6
Effect of Dielectric Photoelectric Effect on Surface Breakdown	26781				1			1				1	50%	3	8
A Revolution in Lighting: Building the Science and Technology Base for Ultraefficient Solid-State Lighting	27328	22	3	2	1			2	1	2		2	100%	1	7
Use of Intense Ion Beams for Surface Modification and Creation of New Materials	28763	1		1								1	100%	1	6
Low-Intensity Laser Triggering of Spark Gaps	28764												60%	3	7
Z-Pinch Power-Plant System Development	28769	2											100%	1	7
Recyclable Transmission Line Concept for Z-Pinch IFE	28770	1	4										100%	1	6
Suppression of Electron Emission from Conductors	28771		1										80%	2	8
Solid-State Switch for Advanced Pulsed Power	28772			1	1							1	90%	3	7
Laboratory-Scale Coherent Multikilovolt X-Ray Sources for Advanced Imaging Applications	28775												80%	2	
Interfacial Bioscience Grand Challenge (IBIG)	28776	5		1				2	3	4			80%	3	
High-Throughput Instruments, Methods, and Informatics for Systems Biology	32574	7	7	2	1					2		1	100%	1	
Low-Work-Function Material Development for the Microminiature Thermionic Converter	32807		1	1		2							90%	1	
Autonomous Microexplosive Subsurface Tracing System	32809												80%	2	
Security Models of Agent-Based Coalitions	32815			2			1						75%	2	
Vulnerability Assessment of National Power Grid	32816	1	1										100%	1	
Molecular Simulations of MEMS and Membrane Coatings (PECASE)	32817							2			2		80%	2	

Appendix C: Project Performance Measures

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Appendix C: Project Performance Measures

Project Title	Project #	Performance Statistics (Number of)											Project Qualitative Assessment		
		Refereed Publications	All Other Reports and Publications	Patent Disclosures	Patent Applications	Patents	Copyrights	Students	Post-docs	Permanent Staff Hired*	Awards	New Non-LDRD-Funded Projects†	% Milestones Completed	Goals Status**	Hypotheses Status***
Science-Based Sensing of Phase Transformations in Steels	38608			2	2								100%	1	
Physical and Electronic Changes Caused by Membrane Signaling as a Transduction Pathway in Affinity-Based Biosensors	38609							3					85%	2	
Graduated Embodiment for Sophisticated Agent Evolution and Optimization	38610	1	1					2					90%	2	
Stochastic Programming for Enterprise Modeling—Optimization for Nondeterministic Simulation	38611		2								1		90%	4	
Robust Message Routing for Mobile (Wireless) <i>Ad Hoc</i> Networks	38612							1					95%	1	
Scalable Fault-Tolerant Algorithms for Linear-Scaling Coupled-Cluster Electronic Structure Methods	38613												100%	1	
Micromagnetic Suspension	38614							1					90%	1	
Sensitivities for Large-Scale Simulation Codes	38615				2			1					100%	1	
Engineered Superconductivity in Electron-Hole Bilayers	38616							1	1	2			80%	2	
Silicon-Based RF MEMS Components	38617												100%	4	
2-D Arrayed Resonant Subwavelength Gratings	38618	2							1				90%	2	
Nanoelectromechanical Oscillators (NEMOs) for RF Filtering	38619	10		1				1					80%	2	7
Continuous-Wave Intersubband Terahertz Sources	38620												80%	2	7
Microsystems for Chemical Signature and Reagent Delivery	38621			1									70%	2	7
Microfluidic Cellular Sample Pretreatment	38622			2						1			75%	2	7
Automated Visual Direction of Mobile Manipulation	38623		1										100%	2	8
Miniature Fourier-Transform Ion-Mobility Spectrometer for Real-Time Detection and Identification of Explosives and Chemical Agents	38624	1	2	1	1								85%	2	7
CONOPS Development for Automated Systems	38625												90%	4	7
Rapid Mitigation and Decontamination of Toxic Industrial Chemicals	38626												100%	1	6
EM Interactions with Systems to Enhance Security	38627												100%	1	8
Adaptive Awareness for Personal and Small-Group Decision Making	38628		1					2					90%	2	7

Appendix C: Project Performance Measures

		Performance Statistics (Number of)											Project Qualitative Assessment		
Project Title	Project #	Refereed Publications	All Other Reports and Publications	Patent Disclosures	Patent Applications	Patents	Copyrights	Students	Post-docs	Permanent Staff Hired*	Awards	New Non-LDRD-Funded Projects†	% Milestones Completed	Goals Status**	Hypotheses Status***
Use of Seismic and Acoustic Responses to Assess Bomb Damage to Underground Facilities	38629		1										95%	2	7
Free-Space Electrooptic Sampling and Remote Mapping of Electromagnetic Fields from Emitting Structures Using Femtosecond Terahertz Transceivers	38655								1	1			80%	2	6
Kinematics-Based Video Compression Using a Foveated-Imaging Sensor for Remote Telepresence Applications	38658	1	1	1									60%	4	6
Information Assurance for Wireless <i>Ad Hoc</i> Networks	38659	1						1					100%	1	7
Low-Toxicity Hypergolic Propellant System Using H2O2 Oxidizer	38661												75%	2	7
Natural-Gas Production Problems: Solutions, Methodologies, and Modeling	38662	3	2					1					100%	1	7
High-Efficiency Turbine Blade Coatings	38664						1			1			73%	2	7
Time-Domain Reflectometry for Remote, Real-Time Water-Quantity/-Quality Monitoring of Ephemeral Streams	38665							5					90%	2	7
Research and Development of Mathematical Algorithms to Define and Quantify Critical Infrastructure Interdependencies	38667												100%	1	7
Functionalized Nanoelectrode Arrays for <i>In Situ</i> Identification and Quantification of Regulated Chemicals in Water	38668	2	2					1	1				90%	2	8
Hybrid Infrastructure Cryptography	38669			1				1					100%	1	7
Validated Modeling of Distributed-Energy Resources at Distribution Voltages	38672												90%	2	7
Water Desalination	38673	2		2				1	1				33%	1	7
Revolutionary Systems for Catalytic Combustion and Diesel Catalytic Particulate Traps	38674		4	1				1	1				100%	1	7
Potential Application of Microsensor Technology in Radioactive-Waste Management—with Emphasis on Headspace Gas Detection	38677							1		7			100%	1	6
Surety Enhancement for Wireless Automated-Control Networks	38678												95%	2	8
Advanced Nuclear-Engineering Analysis Technology	38679							1					90%	1	7
Identification of Chemical Plumes: Range-Resolved IR Lidar Enabled by New Photonic Technologies	38681	3		1	2								90%	3	7
Multiscale Thermal Modeling	38682							1					90%	1	8

Appendix C: Project Performance Measures

Project Title	Project #	Performance Statistics (Number of)											Project Qualitative Assessment		
		Refereed Publications	All Other Reports and Publications	Patent Disclosures	Patent Applications	Patents	Copyrights	Students	Post-docs	Permanent Staff Hired*	Awards	New Non-LDRD-Funded Projects†	% Milestones Completed	Goals Status**	Hypotheses Status***
A Robust, Coupled Approach for Atomistic-Continuum Simulation	38684												70%	3	7
Microscale Rarefied-Gas Dynamics and Surface Interactions for EUVL and MEMS Applications	38685												80%	2	7
High-Fidelity Frictional Models for MEMS	38686		2										100%	2	7
Soot Formation, Transport, and Radiation in Unsteady Diffusion Flames	38687								1				85%	2	7
The Basics of Aqueous Nanofluidics: "Interphase" Structure and Surface Forces	38688	6	6	1									80%	2	7
Design, Synthesis, and Characterization of Soft-Matter Nanolayer Superlattices	38689												100%	1	7
Photocontrol of Nanointeractions in Microsystems	38690												67%	2	8
Electrochemically Deposited Alloys with Tailored Nanostructures for LIGA Micromachines	38691								1	1			75%	3	7
Nanostructured Materials for Directed Transport of Excitation Energy	38692								2				90%	2	7
Modeling Local Chemistry in the Presence of Collective Phenomena	38693												85%	1	7
Passive-Legged, Multisegmented Robotic Vehicle	38695												90%	2	6
Low-Cost Photonic Lattice Structures for Remote Sensing	38696		1	2	1				1				90%	3	7
Security Monitoring and Management with Information Technology (SUMMIT)	38698		1										100%	1	8
Novel Methods for Ultracompact, Ultralow-Power Communications	38699												90%	2	7
Collaborative Approach in System Design and Protection	38700							1					100%	1	7
Novel Tagging Technologies for the Tracking and Authentication of Documents, Property, and Other Items	38701												80%	3	7
A Revolutionary Long-Lived Power Supply: The Icosahedral Boride Semiconductor (IBS) Beta Cell	38702	1											70%	3	7
Remote-Sensing Data Exploitation for Geologic Characterization of Difficult Targets	38703												85%	1	7
The Effects of Varying Humidity on Copper-Sulfide Film Formation	38705	4						1		1			100%	1	7
Detecting and Tracking the Active Insider Using 3-D Detection Technology	38706							1		2			100%	1	6

Appendix C: Project Performance Measures

Project Title	Project #	Performance Statistics (Number of)											Project Qualitative Assessment		
		Refereed Publications	All Other Reports and Publications	Patent Disclosures	Patent Applications	Patents	Copyrights	Students	Post-docs	Permanent Staff Hired*	Awards	New Non-LDRD-Funded Projects†	% Milestones Completed	Goals Status**	Hypotheses Status***
Microfabricated Dielectrophoretic Sample-Preparation System	38707		1	2	2			1					90%	3	7
Automation of Microelectronic Physical Analysis	38708							1					75%	4	
Nonlinear Optical Limiters Using Photonic-Bandgap Structures for Sensor Protection	38712									1			90%	2	7
Secure MPLS Control Plane for Internet Connectivity	38713	1	1					2		1			100%	1	7
Integrated-Sensor Network Chip	38714	1						3					100%	1	7
Self-Organization of Software	38716									1			95%	1	6
Nanoscale Energetic Materials by Inverse Micellar Synthesis	38717			1									80%	2	7
Modeling of Rock Penetration	38718												80%	2	7
Nanoconverter	38719												80%	2	8
Novel Proton-Exchange Membrane Materials for the Advancement of Direct Methanol Fuel-Cell Technology	38720	4		1									92%	1	6
Communicating with the <i>In Vivo</i> Sensor	38721		3										100%	1	6
Agile, Microsystems-Enabled Receiver	38722							3		1			90%	2	7
Linking Geosciences to Emerging Bioengineering Technologies	38723	1											100%	1	7
Energy Storage: Leaving Chemistry in the Dust	38724												90%	2	
Novel Algorithms and Experimental Techniques for Quantitative Spectral Analysis of Particulates	38726												85%	2	7
Self-Healing Adhesives and Encapsulants: Long-Term, High-Performance Weapon Components	38727												100%	1	
Neutron-Only Detector for JTA Tests	38729												90%	1	6
Adaptive Network Countermeasures	38744							3		2			80%	3	7
Solution-Based Nanoengineering of Materials	39017								1				100%	1	7
MEMS-Based Electromechanical Acoustic-Energy Harvester	39212		1					1					80%	1	7
Determination of Microstructural Properties with Isentropic Compression	39669												80	2	7
Simulations of Intense Petawatt Laser Pulses with Dense Z-Pinch Plasmas	39670	1	1					1					85	2	7
Biomicrofuel Cell	41193		6	1				4	3				90	2	7

Appendix C: Project Performance Measures

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Project Title	Project #	Performance Statistics (Number of)											Project Qualitative Assessment		
		Refereed Publications	All Other Reports and Publications	Patent Disclosures	Patent Applications	Patents	Copyrights	Students	Post-docs	Permanent Staff Hired*	Awards	New Non-LDRD-Funded Projects†	% Milestones Completed	Goals Status**	Hypotheses Status***
Micro-/Nanoscale Thermomechanical Manufacturing ****	53465														9
Design of Biospecific Surfaces to Control Specific Cellular Responses ****	53681														9
High Field Effects of GaN HEMTs ****	53682														9
Cognitive Models Applied to Human Effectiveness in National Security Environments ****	54210														9
Nanomagnetic Films ****	54211														9
A Multiscale Approach to Modeling Carbon Nanotubes ****	54213														9
		352	209	133	76	27	10	213	68	82	12	44			

† Identification of new non-LDRD-funded projects is now completed in the fiscal year following the annual report.

* Permanent Staff Hired. Laboratories operate under manpower cap. There are no increases in permanent staff.

** Goals Status

- 1 - Goals Met
- 2 - Goals Substantially Met
- 3 - Goals Partially Met
- 4 - Goals Substantially Modified
- 5 - Goals Not Met
- 11 - Project Terminated

*** Hypothesis Status

- 6 - Hypotheses Proved
- 7 - Hypotheses Remains Unchanged
- 8 - Hypotheses Modified
- 9 - Hypotheses Redefined
- 10 - Hypotheses Disproved
- 11 - Project Terminated

****These projects represent university fellowships and are not included in the totals.

Appendix D: DOE Critical Technologies

Pg #	Title	Project #	Science of Complex Systems	Modeling & Simulation of Complex Systems	High-Performance Computing	Nuclear Weapons Predictive Capability (Classified)	Safety Assessments & Engineering	Use Control & Security	Nonproliferation & Verification	Dynamic Testing in Severe Environments	High-Energy-Density Materials	Laser Technology	Pulsed Power and Accelerators	Microelectronics and Photonics	Nuclear Materials	Engineered Materials	Flexible Manufacturing	Environmentally Conscious Manufacturing	Intelligent Machines and Robotics	Waste Management	Other
302	A Novel Microcombustor for Sensor and Thermal-Energy Management Applications in Microsystems	10718							•					•				•			
153	Radiation-Induced Prompt Photocurrents in Microelectronics: Physics	10719			•									•							
42	Volumetric Displacement Control (VDC) of Manufacturing Tools	10721															•		•		
45	Process-Based Quality Tools to Verify Cleaning and Surface Preparation	10722												•		•	•	•			
48	Fabrication of Three-Dimensional Microstructures Using Soft Lithography	10723												•		•	•				
549	High-Speed 2-D Hadamard Transform Spectral Imager for IR Applications	10724							•												
305	A Micro-GC-Based Controller for Energy-Intensive Processes	10725	•				•	•	•	•						•	•	•	•	•	
210	Micro-High-G Acceleration Recorder	10727								•				•							
106	Algorithmic Advances in Computational Structural Biology	10728		•	•																
679	Ultraminiaturization of RF Circuitry	10729							•					•							
155	SOI-Based High-Aspect-Ratio Si Bulk Micromachining for MEMS Applications	10733												•					•		
455	Next-Generation Output-Based Process Control: An Integration of Modeling, Sensors, and Intelligent Data Analysis	10734	•						•							•	•				
457	Physical Basis for Interfacial Traction-Separation Models	10735														•					
212	Dynamic Range Imaging for Terrain Mapping, Position Determination, and Obstacle Avoidance in Autonomous Navigation	10736		•				•				•		•					•		
460	Diagnostics for Joining Solidification/ Microstructural Simulations	10740		•												•					
464	Effects of Microstructural Variables on the Shock-Wave Response of PZT 95/5	10741		•							•					•					
467	Mechanisms of Dislocation Grain-Boundary Interaction	10742	•	•												•					

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Pg #	Title	Project #	Science of Complex Systems	Modeling & Simulation of Complex Systems	High-Performance Computing	Nuclear Weapons Predictive Capability (Classified)	Safety Assessments & Engineering	Use Control & Security	Nonproliferation & Verification	Dynamic Testing in Severe Environments	High-Energy-Density Materials	Laser Technology	Pulsed Power and Accelerators	Microelectronics and Photonics	Nuclear Materials	Engineered Materials	Flexible Manufacturing	Environmentally Conscious Manufacturing	Intelligent Machines and Robotics	Waste Management	Other
158	Defining the Frontiers of Vertical, External-Cavity, Surface-Emitting Lasers	10744										•		•							
78	Predicting Function of Biological Macromolecules	10746	•	•	•																
308	Nanostructured Silicon Surfaces for Cost-Effective Photovoltaic Efficiency Improvements	10748												•		•		•			
160	Growth and Characterization of Quantum Dots and Quantum-Dot Devices	10749	•		•							•		•		•					•
51	Automatic Design of Practical Fixtures	10751	•	•	•	•										•	•		•		
214	Distributed, Reconfigurable, Homogeneous Microrobotic Systems	10752		•															•		
216	Robust Planning for Autonomous Navigation of Mobile Robots in Unstructured, Dynamic Environments	10753	•							•									•		
469	Functional Materials for Electrochemomechanical Actuation of Microvalves and Micropumps	10754	•											•		•					
537	New Architectures for Micro-Total-Analytical Systems	10756	•						•					•							
108	Large-Scale Nonlinear Optimization Arising from PDE Models	10757			•																
472	Making the Connection Between Microstructure and Mechanics	10761	•	•												•					
551	Self-Assembled Tamper-Detection Seals	10762						•	•												
311	Control Strategies for Homogeneous Charge-Compression Ignition (HCCI) Engines	10763		•	•																
401	Energetic-Material Burn and Detonation at the Mesoscale	10765	•	•			•			•	•					•	•				
163	Heterogeneous Integration of Optoelectronic Arrays and Microelectronics	10766			•									•					•		
53	IMEMS Packaging and Interconnection Technology	10770						•						•			•				
314	Silicon/Carbon Nanocomposites for Rechargeable Battery Applications	10771									•					•					
217	Intense Directed-Energy Theory Initiative	10772	•	•	•							•	•	•					•		

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Pg #	Title	Project #	Science of Complex Systems	Modeling & Simulation of Complex Systems	High-Performance Computing	Nuclear Weapons Predictive Capability (Classified)	Safety Assessments & Engineering	Use Control & Security	Nonproliferation & Verification	Dynamic Testing in Severe Environments	High-Energy-Density Materials	Laser Technology	Pulsed Power and Accelerators	Microelectronics and Photonics	Nuclear Materials	Engineered Materials	Flexible Manufacturing	Environmentally Conscious Manufacturing	Intelligent Machines and Robotics	Waste Management	Other
82	Biosensors Based on the Electrical Impedance of Tethered Lipid Bilayers on Planar Electrodes	10774							•					•					•	•	
165	Miniature Sensors for BW Agents Using Fatty-Acid Profiles	10775							•					•							
168	Enhanced-Sensitivity Acoustic-Wave Biosensor Arrays	10776		•					•					•							
111	Parallel Methods for Coupling Circuit- and Device-Scale Simulations	10777			•																
114	A JAVA-Based Tool for Multifidelity Modeling of Coupled Systems	10778		•																	
475	Switchable Hydrophobic-Hydrophilic Surfaces	10779	•											•		•					
84	Nanostructured Materials Integrated in Microfabricated Optical Devices	10780	•						•					•		•					
170	Microfabrication of Electromagnetic Devices	10783						•						•		•					
172	GaAs MOEMS Technology	10784												•							
174	Integrated Microsensors for Autonomous Microrobots	10785	•						•					•					•		
177	Silicon-Integrated Planar Microbatteries	10786						•	•			•		•					•		
404	Small-Scale Multiaxial Deformation Experiments on Solder for High-Fidelity Model Development	10788		•										•		•					
478	All-Ceramic Battery	10789												•		•			•		
56	Computer Numerically Controlled Micromachines	10793										•		•					•		
680	Surface-Micromachined Mechanical Timer	10795						•						•							
180	High-Efficiency Optical MEMS by the Integration of Photonic Lattices with Surface MEMS	10796										•		•					•		
438	Molecular Integrated Microsystems (MIMS)	11130												•		•					
682	Pseudostationary Separation Materials for Highly Parallel Microseparations (PECASE)	16167														•					•
685	Novel Coatings for Microelectromechanical (MEM) Devices (PECASE)	17230	•	•	•		•	•	•	•				•	•	•	•	•	•	•	•

Appendix D: DOE Critical Technologies

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Pg #	Title	Project #	Science of Complex Systems	Modeling & Simulation of Complex Systems	High-Performance Computing	Nuclear Weapons Predictive Capability (Classified)	Safety Assessments & Engineering	Use Control & Security	Nonproliferation & Verification	Dynamic Testing in Severe Environments	High-Energy-Density Materials	Laser Technology	Pulsed Power and Accelerators	Microelectronics and Photonics	Nuclear Materials	Engineered Materials	Flexible Manufacturing	Environmentally Conscious Manufacturing	Intelligent Machines and Robotics	Waste Management	Other
237	Low-Cost Digital Radar for Fuzing, Tags, SAR Imaging, and Targeting	26540							•					•							•
239	Triggered Isomer Research	26541	•								•										
241	A Scientific Basis for Robotic Ground-Vehicle Design	26542							•										•		•
243	Adaptive and Mobile Ground Sensors	26543						•	•										•		
245	Algorithm Development for Prognostic Health Monitoring and Maintenance	26544		•															•		
248	New Mechanism for Upset of Electronics	26545	•	•									•	•							
250	Flexible Robotic Maintenance Facility	26546		•													•		•		
253	Distributed Autonomous Navigation	26547	•							•									•	•	
255	Obstacle Detection for Autonomous Navigation	26548						•	•										•		
321	Very High Temperature Gas-Cooled Reactor	26549					•		•						•					•	
324	Solid-State Ballistic Chemical Sensors	26550	•											•				•			
327	Novel Catalytic Systems for Energy-Efficient Feedstock Hydrocarbon Separations	26551																•			•
330	A Model of Infrastructure Interdependency Using Communication Agents	26552	•	•																	
540	Microchemical Sensors for Characterization and Monitoring of Volatile Contaminants	26553							•					•						•	
333	Investigation of Potential Applications of Self-Assembled Nanostructured Materials in Nuclear-Waste Management	26554														•				•	
336	Development of Detection Techniques and Diagnostics for Airborne Carbon Nanoparticles	26555																•			•
339	Photonic Crystals for Enhancing Thermophotovoltaic Energy Conversion	26556												•		•					
341	Specific Anion Nanoengineered Sorbents for Water Purification	26557	•	•	•		•									•		•		•	
554	Development of a Microoptic Gyroscope	26559							•			•		•							

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Pg #	Title	Project #	Science of Complex Systems	Modeling & Simulation of Complex Systems	High-Performance Computing	Nuclear Weapons Predictive Capability (Classified)	Safety Assessments & Engineering	Use Control & Security	Nonproliferation & Verification	Dynamic Testing in Severe Environments	High-Energy-Density Materials	Laser Technology	Pulsed Power and Accelerators	Microelectronics and Photonics	Nuclear Materials	Engineered Materials	Flexible Manufacturing	Environmentally Conscious Manufacturing	Intelligent Machines and Robotics	Waste Management	Other
556	Synergistic Merging of Multispectral Transient Radiometry and Multispectral Imaging Technology for Enhanced Global Situational Awareness Through Accurate Geolocation	26560		•	•				•												•
558	New Glass Technology for Enhanced Architectural Surety	26561						•		•						•					
561	Compact UV Laser Source for Chemical and Biological Sensing	26562							•			•		•							
564	Advanced Digital Detectors for Neutron Imaging	26563						•	•				•	•	•						
566	Microfabricated Acoustic Spectrum Analyzer	26564						•	•					•					•		
569	Enabling Analytical and Modeling Tools for Enhanced Disease Surveillance	26565		•																	
573	Microtransmitter for Tag, Beacon, and Data-Exfiltration Applications	26566							•												
574	Extensibility of Knowledge-Based Human-Agent Simulation	26567	•	•			•	•	•										•		
576	Secure Authenticated Sensor Packs	26568						•	•					•					•		
579	Remote Monitoring of Difficult, Real-Time Targets Using Video SAR Technique	26569							•												
581	Coating Chemical Preconcentrators to Improve Chemical-Agent Collection	26572							•							•					
542	Ultralow-Power Spread-Spectrum Receivers for Microtags to Improve Security During Critical Operations	26573							•					•					•		
583	Detection and Exploitation of Spread-Spectrum Waveforms	26574		•	•				•												
585	Small-Power Direct-Conversion Microfluid Systems Using Logistical Fuels	26575							•												•
587	High-Bandwidth Optical-Data Interconnects for Satellite Applications	26576			•				•			•		•							
589	Robust Chemometrics for Remote Spectral Sensing	26577							•										•		
593	Deployable Large-Aperture Optics System for Remote-Sensing Applications	26578		•					•					•		•					

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Pg #	Title	Project #	Science of Complex Systems	Modeling & Simulation of Complex Systems	High-Performance Computing	Nuclear Weapons Predictive Capability (Classified)	Safety Assessments & Engineering	Use Control & Security	Nonproliferation & Verification	Dynamic Testing in Severe Environments	High-Energy-Density Materials	Laser Technology	Pulsed Power and Accelerators	Microelectronics and Photonics	Nuclear Materials	Engineered Materials	Flexible Manufacturing	Environmentally Conscious Manufacturing	Intelligent Machines and Robotics	Waste Management	Other
596	MicroChemLab Technologies for Early Detection of Pathogen Exposure	26579							•			•				•					
599	Intelligent Tracking of the Telepresent Rapid-Aiming Platform	26580																			•
87	Molecular-Scale Studies of Single-Channel Membrane Pores	26581	•	•																	
89	Efficient Massively Parallel Techniques for Protein Structure Generation	26582	•		•																•
92	Mapping Membrane Protein Interactions in Cell-Signaling Systems	26583		•																	•
544	Interconnection Technology for Next Generation of Integrated Microsystems	26770							•					•					•		
420	Effect of Dielectric Photoelectric Effect on Surface Breakdown	26781	•	•		•	•						•								
442	A Revolution in Lighting: Building the Science and Technology Base for Ultraefficient Solid-State Lighting	27328												•							
661	Use of Intense Ion Beams for Surface Modification and Creation of New Materials	28763											•			•		•			
663	Low-Intensity Laser Triggering of Spark Gaps	28764											•								
664	Z-Pinch Power-Plant System Development	28769	•	•							•		•		•	•	•		•		
666	Recyclable Transmission Line Concept for Z-Pinch IFE	28770		•									•								
669	Suppression of Electron Emission from Conductors	28771								•	•		•			•					
671	Solid-State Switch for Advanced Pulsed Power	28772										•	•	•							
257	Laboratory-Scale Coherent Multikilovolt X-Ray Sources for Advanced Imaging Applications	28775										•									
447	Interfacial Bioscience Grand Challenge (IBIG)	28776							•												•
95	High-Throughput Instruments, Methods, and Informatics for Systems Biology	32574	•											•							
343	Low-Work-Function Material Development for the Microminiature Thermionic Converter	32807	•	•							•			•		•					

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Pg #	Title	Project #	Science of Complex Systems	Modeling & Simulation of Complex Systems	High-Performance Computing	Nuclear Weapons Predictive Capability (Classified)	Safety Assessments & Engineering	Use Control & Security	Nonproliferation & Verification	Dynamic Testing in Severe Environments	High-Energy-Density Materials	Laser Technology	Pulsed Power and Accelerators	Microelectronics and Photonics	Nuclear Materials	Engineered Materials	Flexible Manufacturing	Environmentally Conscious Manufacturing	Intelligent Machines and Robotics	Waste Management	Other
258	Microfuzze	34698	•							•						•			•		
514	Exploration of New Multivariate Spectral Calibration Algorithms	34699		•					•		•						•	•	•	•	
696	Development of Experimental Verification Techniques for Nonlinear Deformation and Fracture	35376		•										•		•					
699	Microcontact Printing of Nanoparticle Arrays	36901	•											•			•				
703	Mathematical Analysis of Deception	36902	•	•	•		•	•	•										•		•
704	A System-Dynamics Approach to Modeling Water Demand	36904	•	•																	
69	Microfabrication with Femtosecond-Laser Processing	38605							•			•		•			•				
71	Mesoscale Controlled Motion for a Microfluidic Drop Ejector	38606												•		•	•				
73	Science-Based Sensing of Phase Transformations in Steels	38608											•			•	•	•			
101	Physical and Electronic Changes Caused by Membrane Signaling as a Transduction Pathway in Affinity-Based Biosensors	38609							•			•		•							
130	Graduated Embodiment for Sophisticated Agent Evolution and Optimization	38610																	•		
133	Stochastic Programming for Enterprise Modeling—Optimization for Nondeterministic Simulation	38611		•																	
136	Robust Message Routing for Mobile (Wireless) <i>Ad Hoc</i> Networks	38612		•	•																
138	Scalable Fault-Tolerant Algorithms for Linear-Scaling Coupled-Cluster Electronic Structure Methods	38613		•	•				•		•										
140	Micromagnetic Suspension	38614		•	•																
142	Sensitivities for Large-Scale Simulation Codes	38615		•	•																
193	Engineered Superconductivity in Electron-Hole Bilayers	38616	•											•		•					

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Pg #	Title	Project #	Science of Complex Systems	Modeling & Simulation of Complex Systems	High-Performance Computing	Nuclear Weapons Predictive Capability (Classified)	Safety Assessments & Engineering	Use Control & Security	Nonproliferation & Verification	Dynamic Testing in Severe Environments	High-Energy-Density Materials	Laser Technology	Pulsed Power and Accelerators	Microelectronics and Photonics	Nuclear Materials	Engineered Materials	Flexible Manufacturing	Environmentally Conscious Manufacturing	Intelligent Machines and Robotics	Waste Management	Other
195	Silicon-Based RF MEMS Components	38617						•	•					•					•		
197	2-D Arrayed Resonant Subwavelength Gratings	38618							•			•		•							
200	Nanoelectromechanical Oscillators (NEMOs) for RF Filtering	38619						•	•					•							
203	Continuous-Wave Intersubband Terahertz Sources	38620							•			•		•							
205	Microsystems for Chemical Signature and Reagent Delivery	38621							•					•		•		•			
207	Microfluidic Cellular Sample Pretreatment	38622	•	•										•							
261	Automated Visual Direction of Mobile Manipulation	38623						•	•								•		•	•	
263	Miniature Fourier-Transform Ion-Mobility Spectrometer for Real-Time Detection and Identification of Explosives and Chemical Agents	38624							•									•		•	•
266	CONOPS Development for Automated Systems	38625	•	•	•			•											•		•
268	Rapid Mitigation and Decontamination of Toxic Industrial Chemicals	38626							•												•
270	EM Interactions with Systems to Enhance Security	38627											•								
272	Adaptive Awareness for Personal and Small-Group Decision Making	38628	•	•	•		•	•				•		•					•		•
274	Use of Seismic and Acoustic Responses to Assess Bomb Damage to Underground Facilities	38629	•	•					•												
277	Free-Space Electrooptic Sampling and Remote Mapping of Electromagnetic Fields from Emitting Structures Using Femtosecond Terahertz Transceivers	38655							•			•		•							
279	Kinematics-Based Video Compression Using a Foveated-Imaging Sensor for Remote Telepresence Applications	38658						•	•					•					•		
281	Information Assurance for Wireless <i>Ad Hoc</i> Networks	38659			•			•	•										•		•
283	Low-Toxicity Hypergolic Propellant System Using H2O2 Oxidizer	38661									•					•					

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Pg #	Title	Project #	Science of Complex Systems	Modeling & Simulation of Complex Systems	High-Performance Computing	Nuclear Weapons Predictive Capability (Classified)	Safety Assessments & Engineering	Use Control & Security	Nonproliferation & Verification	Dynamic Testing in Severe Environments	High-Energy-Density Materials	Laser Technology	Pulsed Power and Accelerators	Microelectronics and Photonics	Nuclear Materials	Engineered Materials	Flexible Manufacturing	Environmentally Conscious Manufacturing	Intelligent Machines and Robotics	Waste Management	Other
354	Natural-Gas Production Problems: Solutions, Methodologies, and Modeling	38662	•	•																	
356	High-Efficiency Turbine Blade Coatings	38664	•												•						
358	Time-Domain Reflectometry for Remote, Real-Time Water-Quantity/-Quality Monitoring of Ephemeral Streams	38665																			•
361	Research and Development of Mathematical Algorithms to Define and Quantify Critical Infrastructure Interdependencies	38667	•	•																	
364	Functionalized Nanoelectrode Arrays for <i>In Situ</i> Identification and Quantification of Regulated Chemicals in Water	38668					•		•									•		•	•
367	Hybrid Infrastructure Cryptography	38669		•				•											•		•
369	Validated Modeling of Distributed-Energy Resources at Distribution Voltages	38672		•																	
370	Water Desalination	38673														•		•		•	
373	Revolutionary Systems for Catalytic Combustion and Diesel Catalytic Particulate Traps	38674														•	•	•			
376	Potential Application of Microsensor Technology in Radioactive-Waste Management—with Emphasis on Headspace Gas Detection	38677					•		•					•						•	
378	Surety Enhancement for Wireless Automated-Control Networks	38678		•	•																•
380	Advanced Nuclear-Engineering Analysis Technology	38679		•	•		•		•												
383	Identification of Chemical Plumes: Range-Resolved IR Lidar Enabled by New Photonic Technologies	38681	•					•	•	•		•		•		•		•	•	•	•
422	Multiscale Thermal Modeling	38682	•	•	•									•							
424	A Robust, Coupled Approach for Atomistic-Continuum Simulation	38684		•	•		•									•					
427	Microscale Rarefied-Gas Dynamics and Surface Interactions for EUVL and MEMS Applications	38685	•	•								•		•							
430	High-Fidelity Frictional Models for MEMS	38686	•	•				•						•							

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Pg #	Title	Project #	Science of Complex Systems	Modeling & Simulation of Complex Systems	High-Performance Computing	Nuclear Weapons Predictive Capability (Classified)	Safety Assessments & Engineering	Use Control & Security	Nonproliferation & Verification	Dynamic Testing in Severe Environments	High-Energy-Density Materials	Laser Technology	Pulsed Power and Accelerators	Microelectronics and Photonics	Nuclear Materials	Engineered Materials	Flexible Manufacturing	Environmentally Conscious Manufacturing	Intelligent Machines and Robotics	Waste Management	Other
620	Microfabricated Dielectrophoretic Sample-Preparation System	38707		•					•							•	•				
623	Automation of Microelectronic Physical Analysis	38708							•					•							
624	Nonlinear Optical Limiters Using Photonic-Bandgap Structures for Sensor Protection	38712										•		•		•					
626	Secure MPLS Control Plane for Internet Connectivity	38713		•	•				•												
628	Integrated-Sensor Network Chip	38714	•						•										•		
706	Self-Organization of Software	38716	•	•	•																
707	Nanoscale Energetic Materials by Inverse Micellar Synthesis	38717	•								•										
709	Modeling of Rock Penetration	38718	•	•	•	•				•											
712	Nanoconverter	38719												•							
713	Novel Proton-Exchange Membrane Materials for the Advancement of Direct Methanol Fuel-Cell Technology	38720	•								•					•				•	
715	Communicating with the <i>In Vivo</i> Sensor	38721												•		•			•		
718	Agile, Microsystems-Enabled Receiver	38722							•					•							
721	Linking Geosciences to Emerging Bioengineering Technologies	38723	•	•	•		•		•							•				•	
724	Energy Storage: Leaving Chemistry in the Dust	38724									•				•						
726	Novel Algorithms and Experimental Techniques for Quantitative Spectral Analysis of Particulates	38726		•							•							•			
729	Self-Healing Adhesives and Encapsulants: Long-Term, High-Performance Weapon Components	38727												•		•					
731	Neutron-Only Detector for JTA Tests	38729				•															
145	Adaptive Network Countermeasures	38744																			•
534	Solution-Based Nanoengineering of Materials	39017	•	•										•		•	•				

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Pg #	Title	Project #	Science of Complex Systems	Modeling & Simulation of Complex Systems	High-Performance Computing	Nuclear Weapons Predictive Capability (Classified)	Safety Assessments & Engineering	Use Control & Security	Nonproliferation & Verification	Dynamic Testing in Severe Environments	High-Energy-Density Materials	Laser Technology	Pulsed Power and Accelerators	Microelectronics and Photonics	Nuclear Materials	Engineered Materials	Flexible Manufacturing	Environmentally Conscious Manufacturing	Intelligent Machines and Robotics	Waste Management	Other
732	MEMS-Based Electromechanical Acoustic-Energy Harvester	39212	•	•						•				•							
673	Determination of Microstructural Properties with Isentropic Compression	39669											•								
675	Simulations of Intense Petawatt Laser Pulses with Dense Z-Pinch Plasmas	39670	•	•							•		•								
449	Biomicrofuel Cell	41193	•						•					•		•	•	•	•		
630	Cognition-Driven Augmented Analyst	41194	•	•					•										•		
546	Predicting and Validating MEMS Interface Reliability	41427	•	•	•		•	•		•				•		•	•	•	•		
147	Microengine for Advanced Power Generation	41674		•					•					•			•		•		
734	Direct Simulation of Solid-Fluid Systems	41726	•	•	•																
736	Support-Active Site Interactions in Heterogeneous Catalysts	42461	•													•		•			
738	An Analysis of the Automotive Industry as a Source for Weapon Components and Manufacturing Processes	42483	•	•	•					•				•			•		•		
740	Fluid-Structural Interactions in Wetting and Penetration into Porous Media	44136	•	•										•			•				
386	High-Level Decision-Support Framework for Critical-Infrastructure Protection Prioritization	44601	•	•																	
388	Dynamic-Simulation Model of the National Security Consequences	44774		•																	
742	Macroscopic Rates, Microscopic Observations, and Molecular Models of the Dissolution of Carbonate Phases	45279	•	•																•	
435	Electrical-Impedance Tomography for Opaque Multiphase Flows in Metallic Vessels	46069	•	•																	•
745	High-Speed Micro-EDM	46070															•	•			
390	Electricity-Generation Production Cost Model	46072		•																	
747	Developing Rigid and Compliant Cardiovascular-System Models Using Rapid Prototyping	46684															•				

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Pg #	Title	Project #	Science of Complex Systems	Modeling & Simulation of Complex Systems	High-Performance Computing	Nuclear Weapons Predictive Capability (Classified)	Safety Assessments & Engineering	Use Control & Security	Nonproliferation & Verification	Dynamic Testing in Severe Environments	High-Energy-Density Materials	Laser Technology	Pulsed Power and Accelerators	Microelectronics and Photonics	Nuclear Materials	Engineered Materials	Flexible Manufacturing	Environmentally Conscious Manufacturing	Intelligent Machines and Robotics	Waste Management	Other
749	Nanoscale Hotspots Due to Nonequilibrium Thermal Transport	46685		•										•		•					
752	Micro External Combustion Engine: The P3 Engine Prototype	46686												•							
284	Exploiting Polarimetric Information in Synthetic-Aperture Radar Images for Automatic Target Recognition	46687	•		•																
285	Moving-Target Identification Using Ultrahigh-Range Resolution Data	46688	•		•																
754	Effectiveness of Dielectrophoretic and Electrokinetic Filters/Concentrators for Collecting Smallpox and Anthrax Surrogates from Raw Samples	47516	•											•						•	•
755	Mathematical and Algorithmic Issues in Multiphysics Couplings	47517		•	•																
757	MEMS Adaptive Optics Devices	47687							•	•		•		•				•	•	•	
759	Securing the U.S. Mail Distribution System Against the Threat of Biological and Chemical Agents	47688								•			•								
761	Lipid Membranes on Nanostructured Silicon	47795	•													•					
24	Combating Terrorism and Homeland Security	48212	•	•																	
25	Underground Hunter Robots: Reconnaissance, Clearing, and Securing of Underground Tunnel Complexes Using Robotic Vehicles	48213		•					•	•									•		
763	Combating the Chem-Bio Threat Using Sandia Assets: Need for a Technology Roadmap	48339		•																	
764	Numerical Methods for the Study of Hydrocarbon Combustion	48340		•	•																
632	Chemically Stressed Glass Structural Elements	48341														•					•
634	Digital Signal Processing for Acoustic-Seismic Target Identification	48746		•															•		
635	Terahertz Propagation in Telecommunication Optical Fibers	48751							•												
637	Rapid Screening for Biological Infection	48764										•		•							

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Pg #	Title	Project #	Science of Complex Systems	Modeling & Simulation of Complex Systems	High-Performance Computing	Nuclear Weapons Predictive Capability (Classified)	Safety Assessments & Engineering	Use Control & Security	Nonproliferation & Verification	Dynamic Testing in Severe Environments	High-Energy-Density Materials	Laser Technology	Pulsed Power and Accelerators	Microelectronics and Photonics	Nuclear Materials	Engineered Materials	Flexible Manufacturing	Environmentally Conscious Manufacturing	Intelligent Machines and Robotics	Waste Management	Other
149	Particle "Front End" for Compact WMD Threat-Detection Systems: Integrated Microsystem Concepts for Intelligent Particle Collection, Separation, Preconcentration, and Processing	50121							•												
647	Assessment and Identification of Appropriate μ Power Technologies for μ Sensors and Other Applications	50395												•							
773	Compliant Membranes for MEMS Microphones	50396	•				•	•	•	•				•					•		
774	Multiscale Experimental/Numerical Study	50717														•					
776	Cellular Observatory: Simultaneous Time- and Frequency-Resolved Microscopy	50772	•									•									
777	Near-Real-Time Site Characterization for Assured HDBT Defeat	50858				•															
649	Multispectral Data-Exploitation Advancements	50973		•	•				•												
397	A Fully Integrated Sensor-Based Critical Facility and Border Defense System	51534		•										•							
296	Concept Definition for an Integrated Biodefense System	51536		•																	
780	Ironless Permanent Magnet Actuator	51537																			•
652	Response Analysis Tactical Simulation	51538		•					•												
398	Introspection, Integration, and Intercession (I3): Toward Self-Healing Critical Infrastructures	51540	•	•			•														
654	Optical Tagging Technologies	51541							•												
32	Feasibility Study of an Integrated-Systems Solution to the Problem of Radiological Dispersal Devices	51706		•					•						•					•	
298	A Maneuvering, Hypersonic Pathfinder/Test-Bed	51708			•									•		•			•		
75	Micromechanical Spectrum-Analyzer System	52173	•											•							
781	Inelastic Deformation Mechanism in Shocked Sapphire Single Crystals	52174	•	•									•								

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Appendix E: Major National Programs

Pg #	Title	Project #	Waste Management	Energy Efficiency	Renewable Energy	ES&H	Environmental Restoration	Fossil Energy	Radioactive-Waste Management	Economic Impact	Energy Research	Intelligence & National Security	Nuclear Energy	Science Education & Technical Information	Defense Programs	Department of Defense (DoD)	Other Federal Agencies*	Other (Industry, Consortia...)**	Other Federal Agencies* Other (Industry, Consortia...)**
302	A Novel Microcombustor for Sensor and Thermal-Energy Management Applications in Microsystems	10718		•							•				•	•			
153	Radiation-Induced Prompt Photocurrents in Microelectronics: Physics	10719													•	•	•		*Defense Threat Reduction Agency
42	Volumetric Displacement Control (VDC) of Manufacturing Tools	10721													•	•	•		**Industrial machining and metrology
45	Process-Based Quality Tools to Verify Cleaning and Surface Preparation	10722								•					•		•		**Industry
48	Fabrication of Three-Dimensional Microstructures Using Soft Lithography	10723								•		•			•	•	•	•	*DARPA, **Industry
549	High-Speed 2-D Hadamard Transform Spectral Imager for IR Applications	10724										•							
305	A Micro-GC-Based Controller for Energy-Intensive Processes	10725	•	•	•	•	•	•		•					•	•			
210	Micro-High-G Acceleration Recorder	10727													•	•			
106	Algorithmic Advances in Computational Structural Biology	10728															•		*OBER (DOE)
678	Ultraminiaturization of RF Circuitry	10729										•			•	•			
155	SOI-Based High-Aspect-Ratio Si Bulk Micromachining for MEMS Applications	10733										•			•				
455	Next-Generation Output-Based Process Control: An Integration of Modeling, Sensors, and Intelligent Data Analysis	10734								•					•	•			
457	Physical Basis for Interfacial Traction-Separation Models	10735													•				
212	Dynamic Range Imaging for Terrain Mapping, Position Determination, and Obstacle Avoidance in Autonomous Navigation	10736							•	•		•			•	•	•	•	*DoD, Commerce, **Industry
460	Diagnostics for Joining Solidification/ Microstructural Simulations	10740												•			•		**Materials Processing
464	Effects of Microstructural Variables on the Shock-Wave Response of PZT 95/5	10741													•				
467	Mechanisms of Dislocation Grain-Boundary Interaction	10742									•				•				
158	Defining the Frontiers of Vertical, External-Cavity, Surface-Emitting Lasers	10744													•	•			
78	Predicting Function of Biological Macromolecules	10746									•								

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Pg #	Title	Project #	Waste Management	Energy Efficiency	Renewable Energy	ES&H	Environmental Restoration	Fossil Energy	Radioactive-Waste Management	Economic Impact	Energy Research	Intelligence & National Security	Nuclear Energy	Science Education & Technical Information	Defense Programs	Department of Defense (DoD)	Other Federal Agencies*	Other (Industry, Consortia...)**	Other Federal Agencies* Other (Industry, Consortia...)**
308	Nanostructured Silicon Surfaces for Cost-Effective Photovoltaic Efficiency Improvements	10748			•					•	•								
160	Growth and Characterization of Quantum Dots and Quantum-Dot Devices	10749												•	•	•			
51	Automatic Design of Practical Fixtures	10751													•	•			
214	Distributed, Reconfigurable, Homogeneous Microrobotic Systems	10752										•			•	•			
216	Robust Planning for Autonomous Navigation of Mobile Robots in Unstructured, Dynamic Environments	10753					•					•			•	•	•		*CIA, FBI
469	Functional Materials for Electrochemomechanical Actuation of Microvalves and Micropumps	10754																•	**Industry
537	New Architectures for Micro-Total-Analytical Systems	10756								•					•	•		•	**Microsystems
108	Large-Scale Nonlinear Optimization Arising from PDE Models	10757													•				
472	Making the Connection Between Microstructure and Mechanics	10761									•				•				
551	Self-Assembled Tamper-Detection Seals	10762							•			•			•				
311	Control Strategies for Homogeneous Charge-Compression Ignition (HCCI) Engines	10763		•							•								
401	Energetic-Material Burn and Detonation at the Mesoscale	10765													•	•			
163	Heterogeneous Integration of Optoelectronic Arrays and Microelectronics	10766										•		•	•				
53	IMEMS Packaging and Interconnection Technology	10770								•					•			•	**Industry
314	Silicon/Carbon Nanocomposites for Rechargeable Battery Applications	10771		•							•					•	•	•	*CIA, NASA, NSA, ..., **Industry
217	Intense Directed-Energy Theory Initiative	10772			•		•				•	•	•	•	•	•			
82	Biosensors Based on the Electrical Impedance of Tethered Lipid Bilayers on Planar Electrodes	10774	•				•					•				•			
165	Miniature Sensors for BW Agents Using Fatty-Acid Profiles	10775	•									•			•	•		•	**Industry
168	Enhanced-Sensitivity Acoustic-Wave Biosensor Arrays	10776										•		•	•	•			

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Pg #	Title	Project #	Waste Management	Energy Efficiency	Renewable Energy	ES&H	Environmental Restoration	Fossil Energy	Radioactive-Waste Management	Economic Impact	Energy Research	Intelligence & National Security	Nuclear Energy	Science Education & Technical Information	Defense Programs	Department of Defense (DoD)	Other Federal Agencies*	Other (Industry, Consortia...)**	Other Federal Agencies* Other (Industry, Consortia...)**
111	Parallel Methods for Coupling Circuit- and Device-Scale Simulations	10777													•				
114	A JAVA-Based Tool for Multifidelity Modeling of Coupled Systems	10778													•				
475	Switchable Hydrophobic-Hydrophilic Surfaces	10779									•								
84	Nanostructured Materials Integrated in Microfabricated Optical Devices	10780										•			•	•			
170	Microfabrication of Electromagnetic Devices	10783								•	•	•		•	•	•			
172	GaAs MOEMS Technology	10784										•				•			
174	Integrated Microsensors for Autonomous Microrobots	10785				•	•					•				•			
177	Silicon-Integrated Planar Microbatteries	10786		•						•	•	•			•				
404	Small-Scale Multiaxial Deformation Experiments on Solder for High-Fidelity Model Development	10788								•					•				
478	All-Ceramic Battery	10789						•			•			•			•	**American Battery Consortium	
56	Computer Numerically Controlled Micromachines	10793														•	•	**Industry	
680	Surface-Micromachined Mechanical Timer	10795										•			•	•			
180	High-Efficiency Optical MEMS by the Integration of Photonic Lattices with Surface MEMS	10796								•					•	•			
438	Molecular Integrated Microsystems (MIMS)	11130									•	•			•				
682	Pseudostationary Separation Materials for Highly Parallel Microseparations (PECASE)	16167								•	•					•	•	•	*NIH, EPA, **Industry
685	Novel Coatings for Microelectromechanical (MEM) Devices (PECASE)	17230	•	•	•	•	•	•	•	•	•	•	•	•	•	•		•	**Industry
317	Use of Apatite and Substituted Apatites for <i>In Situ</i> Barriers for Radionuclide Containment and Waste Stabilization and Arsenic Removal from Potable Water	19991	•				•												
319	Regional Dynamic Simulation Modeling and Analysis of Integrated Nuclear Futures	21559	•	•				•		•	•		•						
689	Theoretical Study of Sb as a Surfactant in Epitaxy of III-V Materials	22854													•				

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Pg #	Title	Project #	Waste Management	Energy Efficiency	Renewable Energy	ES&H	Environmental Restoration	Fossil Energy	Radioactive-Waste Management	Economic Impact	Energy Research	Intelligence & National Security	Nuclear Energy	Science Education & Technical Information	Defense Programs	Department of Defense (DoD)	Other Federal Agencies*	Other (Industry, Consortia...)**	Other Federal Agencies* Other (Industry, Consortia...)**
59	Mesoscale Wide-Bandwidth Linear Magnetic Actuators	26508								•		•			•	•			
62	Levitated Three-Axis Microaccelerometer	26509										•			•	•	•	•	*NASA, JPL, DoD, **Commercial
64	Microfabrication Processes Combining Focused Ion-Beam Machining and Thin-Film Vapor-Deposition Techniques	26510										•			•				
66	Resolving Fundamental Limits of Adhesive Bonding in Microfabrication	26511								•		•			•	•		•	**Industry
118	Parallel Atomistic Computing for Failure Analysis of Micromachines	26512									•			•	•	•		•	**Industry
120	Implementation of Fault Tolerance in Scientific Simulation Application Software	26513											•		•	•			
122	Smart-Sensor Technology for Joint Test Assembly Flights	26514													•				
124	Multilevel Methods for Nonlinear Structural Mechanics	26515													•				
126	Algorithmic Support for Commodity-Based Parallel Computing Systems	26516									•				•				
128	Parallel Repartitioning for Optimal Solver Performance	26517									•				•				
182	III-Antimonide/Nitride-Based Semiconductors for Optoelectronic Materials and Device Studies	26518								•		•			•	•			
184	The Integration of Advanced Photonics and MEMS	26519								•		•			•	•			
407	Uncertainty Propagation in Models of Thermo-fluid Systems	26520									•				•				
409	Filtered Rayleigh-Scattering Diagnostic for Multiparameter Thermal/Fluids Measurements	26521									•				•				
412	A Physically Based Approach to Modeling Ductile Fracture	26522									•				•	•			
415	Radiation Aging of Stockpile and Space-Based Microelectronics	26523													•				
417	Large-Deformation Solid-Fluid Interaction Via a Level-Set Approach	26524								•					•	•		•	**Industry
480	Magnetic-Field Effects on Vacuum-Arc Plasmas	26525													•				
481	Microstructural and Continuum Evolution Modeling of Sintering	26526																•	**Industry (ceramic and powder metals processing)

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Pg #	Title	Project #	Waste Management	Energy Efficiency	Renewable Energy	ES&H	Environmental Restoration	Fossil Energy	Radioactive-Waste Management	Economic Impact	Energy Research	Intelligence & National Security	Nuclear Energy	Science Education & Technical Information	Defense Programs	Department of Defense (DoD)	Other Federal Agencies*	Other (Industry, Consortia...)**	Other Federal Agencies* Other (Industry, Consortia...)**
485	Assuring Ultraclean Environments in Microsystem Packages: Irreversible and Reversible Getters	26527													•				
487	Biocompatible Self-Assembly of Nanomaterials for Bio-MEMS and Insect Reconnaissance	26528	•				•				•	•				•	•	•	*DARPA, **Hewlett Packard
490	Nanoclusters for Supercapacitors	26529													•	•			
492	First-Principles Determination of Dislocation Properties	26530									•								
219	Air Sterilization and Decontamination	26531	•			•									•				
221	Data Fusion and Visualization of MASINT Results for Underground Facility Characterization	26532														•			
223	Rapid Ultrasensitive Chemical-Fingerprint Detection of Chemical and Biochemical Warfare Agents	26533	•			•	•			•	•	•				•	•		*NN-20
226	Advanced Unattended Ground-Sensor Technology	26534										•			•	•			
229	The Endowment of Simulator Agents with Humanlike Episodic Memory	26535										•	•		•	•			
232	An Advanced Learning Model for Agent Behavior	26537										•		•		•			
553	Threat-Assessment Study for Short-Pulse Laser Technologies in Directed-Energy and Countersensor Applications	26538										•			•	•			
234	Algorithms for Improved Performance in Cryptographic Protocols	26539										•			•	•			
237	Low-Cost Digital Radar for Fuzing, Tags, SAR Imaging, and Targeting	26540										•			•	•	•	•	*DOE NN&DP, DARPA, DTRA, **Industry
239	Triggered Isomer Research	26541									•				•	•			
241	A Scientific Basis for Robotic Ground-Vehicle Design	26542										•				•			
243	Adaptive and Mobile Ground Sensors	26543										•			•	•			
245	Algorithm Development for Prognostic Health Monitoring and Maintenance	26544											•			•		•	**Machine Tool Industry, Aerospace Industry
248	New Mechanism for Upset of Electronics	26545										•			•	•			
250	Flexible Robotic Maintenance Facility	26546														•		•	**Industry
253	Distributed Autonomous Navigation	26547					•					•			•	•	•		*CIA,FBI

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Pg #	Title	Project #	Waste Management	Energy Efficiency	Renewable Energy	ES&H	Environmental Restoration	Fossil Energy	Radioactive-Waste Management	Economic Impact	Energy Research	Intelligence & National Security	Nuclear Energy	Science Education & Technical Information	Defense Programs	Department of Defense (DoD)	Other Federal Agencies*	Other (Industry, Consortia...)**	Other Federal Agencies* Other (Industry, Consortia...)**
255	Obstacle Detection for Autonomous Navigation	26548					•		•			•		•	•	•			
321	Very High Temperature Gas-Cooled Reactor	26549	•	•					•	•			•						
324	Solid-State Ballistic Chemical Sensors	26550		•												•		•	**Industry
327	Novel Catalytic Systems for Energy-Efficient Feedstock Hydrocarbon Separations	26551						•			•						•	•	*DOE/OIT, **Chem/Petro Industry
330	A Model of Infrastructure Interdependency Using Communication Agents	26552								•		•				•			
540	Microchemical Sensors for Characterization and Monitoring of Volatile Contaminants	26553	•			•	•	•	•								•		*EPA
333	Investigation of Potential Applications of Self-Assembled Nanostructured Materials in Nuclear-Waste Management	26554	•				•		•				•						
336	Development of Detection Techniques and Diagnostics for Airborne Carbon Nanoparticles	26555		•	•			•			•						•	•	*NASA, EPA, **Industry (auto)
339	Photonic Crystals for Enhancing Thermophotovoltaic Energy Conversion	26556		•	•					•	•		•						
341	Specific Anion Nanoengineered Sorbents for Water Purification	26557	•			•	•			•			•				•	•	*EPA, USDA, **Water Treatment Industry
554	Development of a Microoptic Gyroscope	26559										•			•			•	**Automotive Industry
556	Synergistic Merging of Multispectral Transient Radiometry and Multispectral Imaging Technology for Enhanced Global Situational Awareness Through Accurate Geolocation	26560										•			•	•			
558	New Glass Technology for Enhanced Architectural Surety	26561										•			•	•	•	•	*GAO, **Industry
561	Compact UV Laser Source for Chemical and Biological Sensing	26562						•			•				•	•			
564	Advanced Digital Detectors for Neutron Imaging	26563							•		•	•	•		•	•			
566	Microfabricated Acoustic Spectrum Analyzer	26564										•			•	•			
569	Enabling Analytical and Modeling Tools for Enhanced Disease Surveillance	26565													•	•	•		*Centers for Disease Control and Prevention
573	Microtransmitter for Tag, Beacon, and Data-Exfiltration Applications	26566										•				•			

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Pg #	Title	Project #	Waste Management	Energy Efficiency	Renewable Energy	ES&H	Environmental Restoration	Fossil Energy	Radioactive-Waste Management	Economic Impact	Energy Research	Intelligence & National Security	Nuclear Energy	Science Education & Technical Information	Defense Programs	Department of Defense (DoD)	Other Federal Agencies*	Other (Industry, Consortia...)**	Other Federal Agencies* Other (Industry, Consortia...)**
574	Extensibility of Knowledge-Based Human-Agent Simulation	26567										•	•		•	•			
576	Secure Authenticated Sensor Packs	26568										•			•				
579	Remote Monitoring of Difficult, Real-Time Targets Using Video SAR Technique	26569										•				•			
581	Coating Chemical Preconcentrators to Improve Chemical-Agent Collection	26572										•			•	•	•		*Federal Aviation Administration
542	Ultralow-Power Spread-Spectrum Receivers for Microtags to Improve Security During Critical Operations	26573										•			•	•	•	•	*NASA, Navy, Army, NIJ, **Communications Industry
583	Detection and Exploitation of Spread-Spectrum Waveforms	26574										•				•			
585	Small-Power Direct-Conversion Microfluid Systems Using Logistical Fuels	26575									•	•			•	•			
587	High-Bandwidth Optical-Data Interconnects for Satellite Applications	26576										•				•			
589	Robust Chemometrics for Remote Spectral Sensing	26577										•				•			
593	Deployable Large-Aperture Optics System for Remote-Sensing Applications	26578										•			•	•	•		*NASA, AFRL, NRO, DARPA
596	MicroChemLab Technologies for Early Detection of Pathogen Exposure	26579				•									•				
599	Intelligent Tracking of the Telepresent Rapid-Aiming Platform	26580														•	•		*DOE
87	Molecular-Scale Studies of Single-Channel Membrane Pores	26581									•			•					
89	Efficient Massively Parallel Techniques for Protein Structure Generation	26582																•	**Biotechnology
92	Mapping Membrane Protein Interactions in Cell-Signaling Systems	26583															•	•	*NIH, **University Collaborators
544	Interconnection Technology for Next Generation of Integrated Microsystems	26770										•			•	•			
420	Effect of Dielectric Photoelectric Effect on Surface Breakdown	26781											•		•	•	•	•	*FAA, Office of Pipeline Safety, **Microsystems Industry
442	A Revolution in Lighting: Building the Science and Technology Base for Ultraefficient Solid-State Lighting	27328		•						•	•	•							

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Pg #	Title	Project #	Waste Management	Energy Efficiency	Renewable Energy	ES&H	Environmental Restoration	Fossil Energy	Radioactive-Waste Management	Economic Impact	Energy Research	Intelligence & National Security	Nuclear Energy	Science Education & Technical Information	Defense Programs	Department of Defense (DoD)	Other Federal Agencies*	Other (Industry, Consortia...)**	Other Federal Agencies* Other (Industry, Consortia...)**
661	Use of Intense Ion Beams for Surface Modification and Creation of New Materials	28763									•		•		•	•			
663	Low-Intensity Laser Triggering of Spark Gaps	28764									•				•	•			
6664	Z-Pinch Power-Plant System Development	28769	•	•							•		•	•	•				
666	Recyclable Transmission Line Concept for Z-Pinch IFE	28770									•		•		•				
669	Suppression of Electron Emission from Conductors	28771									•				•	•			
671	Solid-State Switch for Advanced Pulsed Power	28772									•		•		•	•			
257	Laboratory-Scale Coherent Multikilovolt X-Ray Sources for Advanced Imaging Applications	28775													•	•			
447	Interfacial Bioscience Grand Challenge (IBIG)	28776								•	•						•	•	*NIH, **Biotech Industry
95	High-Throughput Instruments, Methods, and Informatics for Systems Biology	32574			•		•					•		•					
343	Low-Work-Function Material Development for the Microminiature Thermionic Converter	32807		•							•		•			•			
346	Autonomous Microexplosive Subsurface Tracing System	32809					•	•			•							•	**Petroleum Industry
349	Security Models of Agent-Based Coalitions	32815										•				•			
351	Vulnerability Assessment of National Power Grid	32816									•	•				•	•	•	*FERC, NERC, NRC, FBI, **Electric Power Utilities
691	Molecular Simulations of MEMS and Membrane Coatings (PECASE)	32817		•							•				•				
196	Aging Mechanisms in Dormant MEMS Structures	32913									•				•				
99	Biomimetic Chloroplasts: An Integrated Microdevice Power Source	32914	•		•		•		•		•			•					
494	Study of Polymer Spin-Coating for Photolithographic Semiconductors in Near-Zero-Gravity Environment	32915												•				•	**Semiconductor
188	MEMS in μ Fluid Channels	32923								•		•							
191	Dispersive Photonics for Next-Generation Sensors and Microsystems	33602										•				•			

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496	Understanding Metal Vaporization from Transient High-Fluence Laser Irradiation	34465								•					•				
498	Mechanics and Tribology of MEMS Materials	34466		•								•			•	•	•	•	*NIH, **Industry
502	Dynamics of Metal/Ceramic Interfaces	34467									•								
504	<i>In Situ</i> Characterization of Soft Solution Processes for Nanoscale Growth	34468												•					
506	Determination of Critical Length Scales for Corrosion Processes Using Microelectroanalytical Techniques	34469		•						•		•			•	•			**Industry
508	LIGA Microsystems Aging: Evaluation and Mitigation	34478													•	•			
511	Science-Based Processing of Field-Structured Composites	34485	•									•			•				
693	Self-Assembly of Polymers in Confined Geometries	34692									•				•				
695	Building Conscious Machines Based on the Architecture of Visual Cortex in the Primate Brain	34693										•			•	•			
258	Microfuze	34698													•	•			
514	Exploration of New Multivariate Spectral Calibration Algorithms	34699	•		•		•	•			•	•			•				
696	Development of Experimental Verification Techniques for Nonlinear Deformation and Fracture	35376													•				
699	Microcontact Printing of Nanoparticle Arrays	36901		•						•				•					
703	Mathematical Analysis of Deception	36902										•	•	•	•	•	•	•	*Other Federal Agencies, **Industry, Consortia, etc.
704	A System-Dynamics Approach to Modeling Water Demand	36904			•							•		•			•		*U.S. Geological Survey, U.S. Bureau of Reclamation
69	Microfabrication with Femtosecond-Laser Processing	38605														•		•	**Industrial machining
71	Mesoscale Controlled Motion for a Microfluidic Drop Ejector	38606														•			**Industry
73	Science-Based Sensing of Phase Transformations in Steels	38608		•												•		•	**Automotive Industry
101	Physical and Electronic Changes Caused by Membrane Signaling as a Transduction Pathway in Affinity-Based Biosensors	38609										•		•	•	•			

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Pg #	Title	Project #	Waste Management	Energy Efficiency	Renewable Energy	ES&H	Environmental Restoration	Fossil Energy	Radioactive-Waste Management	Economic Impact	Energy Research	Intelligence & National Security	Nuclear Energy	Science Education & Technical Information	Defense Programs	Department of Defense (DoD)	Other Federal Agencies*	Other (Industry, Consortia...)**	Other Federal Agencies* Other (Industry, Consortia...)**
130	Graduated Embodiment for Sophisticated Agent Evolution and Optimization	38610								•		•			•				
133	Stochastic Programming for Enterprise Modeling—Optimization for Nondeterministic Simulation	38611													•				
136	Robust Message Routing for Mobile (Wireless) <i>Ad Hoc</i> Networks	38612													•				
138	Scalable Fault-Tolerant Algorithms for Linear-Scaling Coupled-Cluster Electronic Structure Methods	38613		•			•	•			•								
140	Micromagnetic Suspension	38614									•				•				
142	Sensitivities for Large-Scale Simulation Codes	38615									•				•				
193	Engineered Superconductivity in Electron-Hole Bilayers	38616									•	•							
195	Silicon-Based RF MEMS Components	38617								•		•			•	•	•	•	*NSA, **Wireless Communications Industry
197	2-D Arrayed Resonant Subwavelength Gratings	38618										•				•			
200	Nanoelectromechanical Oscillators (NEMOs) for RF Filtering	38619										•			•	•			
203	Continuous-Wave Intersubband Terahertz Sources	38620										•				•			
205	Microsystems for Chemical Signature and Reagent Delivery	38621					•			•		•			•				
207	Microfluidic Cellular Sample Pretreatment	38622					•					•			•	•	•	•	*NIH, **BioMEMS Industry
261	Automated Visual Direction of Mobile Manipulation	38623	•				•		•			•	•		•	•			
263	Miniature Fourier-Transform Ion-Mobility Spectrometer for Real-Time Detection and Identification of Explosives and Chemical Agents	38624	•			•	•									•			
266	CONOPS Development for Automated Systems	38625										•	•		•	•			
268	Rapid Mitigation and Decontamination of Toxic Industrial Chemicals	38626										•				•	•		*Department of Justice
270	EM Interactions with Systems to Enhance Security	38627														•			
272	Adaptive Awareness for Personal and Small-Group Decision Making	38628										•		•	•	•			

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274	Use of Seismic and Acoustic Responses to Assess Bomb Damage to Underground Facilities	38629										•			•	•		
277	Free-Space Electrooptic Sampling and Remote Mapping of Electromagnetic Fields from Emitting Structures Using Femtosecond Terahertz Transceivers	38655										•			•	•		
279	Kinematics-Based Video Compression Using a Foveated-Imaging Sensor for Remote Telepresence Applications	38658										•				•		
281	Information Assurance for Wireless <i>Ad Hoc</i> Networks	38659							•						•	•		
283	Low-Toxicity Hypergolic Propellant System Using H ₂ O ₂ Oxidizer	38661										•			•	•		
354	Natural-Gas Production Problems: Solutions, Methodologies, and Modeling	38662						•			•							
356	High-Efficiency Turbine Blade Coatings	38664									•		•					
358	Time-Domain Reflectometry for Remote, Real-Time Water-Quantity/-Quality Monitoring of Ephemeral Streams	38665					•							•			•	*U.S. Geological Survey, U.S. Bureau of Reclamation, Army Corps of Engineers
361	Research and Development of Mathematical Algorithms to Define and Quantify Critical Infrastructure Interdependencies	38667			•			•		•			•					
364	Functionalized Nanoelectrode Arrays for <i>In Situ</i> Identification and Quantification of Regulated Chemicals in Water	38668	•			•	•		•	•		•				•	•	**Water Analysis
367	Hybrid Infrastructure Cryptography	38669										•			•			
369	Validated Modeling of Distributed-Energy Resources at Distribution Voltages	38672		•	•			•			•			•	•	•		
370	Water Desalination	38673	•	•	•		•									•	•	• *DoS, EPA, **Industry, State/Local Gov'ts
373	Revolutionary Systems for Catalytic Combustion and Diesel Catalytic Particulate Traps	38674	•					•										
376	Potential Application of Microsensor Technology in Radioactive-Waste Management—with Emphasis on Headspace Gas Detection	38677	•			•	•		•									
378	Surety Enhancement for Wireless Automated-Control Networks	38678						•		•	•						•	**Industry

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380	Advanced Nuclear-Engineering Analysis Technology	38679		•							•		•						
383	Identification of Chemical Plumes: Range-Resolved IR Lidar Enabled by New Photonic Technologies	38681	•				•	•		•	•	•			•	•	•	•	*NASA, **GTI, API
422	Multiscale Thermal Modeling	38682													•	•		•	**Industry
424	A Robust, Coupled Approach for Atomistic-Continuum Simulation	38684									•				•	•			
427	Microscale Rarefied-Gas Dynamics and Surface Interactions for EUVL and MEMS Applications	38685									•				•	•		•	**Industry, EUVL, MEMS
430	High-Fidelity Frictional Models for MEMS	38686											•	•	•				
433	Soot Formation, Transport, and Radiation in Unsteady Diffusion Flames	38687									•				•	•	•		*NIST, NASA
518	The Basics of Aqueous Nanofluidics: "Interphase" Structure and Surface Forces	38688									•				•				
521	Design, Synthesis, and Characterization of Soft-Matter Nanolayer Superlattices	38689													•			•	**Optics
523	Photocontrol of Nanointeractions in Microsystems	38690													•				
526	Electrochemically Deposited Alloys with Tailored Nanostructures for LIGA Micromachines	38691									•				•				
528	Nanostructured Materials for Directed Transport of Excitation Energy	38692					•			•	•			•		•			
530	Modeling Local Chemistry in the Presence of Collective Phenomena	38693													•	•			
601	Passive-Legged, Multisegmented Robotic Vehicle	38695										•			•	•			
603	Low-Cost Photonic Lattice Structures for Remote Sensing	38696										•			•	•			
605	Security Monitoring and Management with Information Technology (SUMMIT)	38698										•			•	•			
607	Novel Methods for Ultracompact, Ultralow-Power Communications	38699										•			•	•	•		*National Reconnaissance Office
609	Collaborative Approach in System Design and Protection	38700										•			•	•			
610	Novel Tagging Technologies for the Tracking and Authentication of Documents, Property, and Other Items	38701										•				•			

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612	A Revolutionary Long-Lived Power Supply: The Icosahedral Boride Semiconductor (IBS) Beta Cell	38702	•						•				•		•	•			
615	Remote-Sensing Data Exploitation for Geologic Characterization of Difficult Targets	38703										•			•	•			
532	The Effects of Varying Humidity on Copper-Sulfide Film Formation	38705													•	•			
618	Detecting and Tracking the Active Insider Using 3-D Detection Technology	38706										•				•	•		*DOE
620	Microfabricated Dielectrophoretic Sample-Preparation System	38707					•					•			•	•			
623	Automation of Microelectronic Physical Analysis	38708										•							
624	Nonlinear Optical Limiters Using Photonic-Bandgap Structures for Sensor Protection	38712										•			•	•			
626	Secure MPLS Control Plane for Internet Connectivity	38713										•			•	•			
628	Integrated-Sensor Network Chip	38714										•			•				
706	Self-Organization of Software	38716									•	•			•	•			
707	Nanoscale Energetic Materials by Inverse Micellar Synthesis	38717													•	•			
709	Modeling of Rock Penetration	38718													•	•			
712	Nanoconverter	38719													•				
713	Novel Proton-Exchange Membrane Materials for the Advancement of Direct Methanol Fuel-Cell Technology	38720		•	•					•	•			•	•	•		•	**Transportation
715	Communicating with the <i>In Vivo</i> Sensor	38721								•					•	•			
718	Agile, Microsystems-Enabled Receiver	38722														•			
721	Linking Geosciences to Emerging Bioengineering Technologies	38723	•			•	•	•				•		•	•	•			
724	Energy Storage: Leaving Chemistry in the Dust	38724									•		•		•	•		•	**Industry
726	Novel Algorithms and Experimental Techniques for Quantitative Spectral Analysis of Particulates	38726													•				

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729	Self-Healing Adhesives and Encapsulants: Long-Term, High-Performance Weapon Components	38727													•			•	**Aerospace
731	Neutron-Only Detector for JTA Tests	38729													•				
145	Adaptive Network Countermeasures	38744														•			
534	Solution-Based Nanoengineering of Materials	39017			•						•								
732	MEMS–Based Electromechanical Acoustic-Energy Harvester	39212		•							•					•			
673	Determination of Microstructural Properties with Isentropic Compression	39669												•	•				
675	Simulations of Intense Petawatt Laser Pulses with Dense Z-Pinch Plasmas	39670									•		•		•	•			
449	Biomicrofuel Cell	41193		•	•			•		•	•	•			•	•		•	**Power & Auto Industries
630	Cognition-Driven Augmented Analyst	41194										•			•	•			
546	Predicting and Validating MEMS Interface Reliability	41427	•	•	•	•	•	•	•	•	•	•	•	•	•			•	**Industry
147	Microengine for Advanced Power Generation	41674									•	•				•			
734	Direct Simulation of Solid-Fluid Systems	41726		•				•		•	•			•	•			•	**1581 CRADA
736	Support–Active Site Interactions in Heterogeneous Catalysts	42461						•										•	**Industry (chemical manufacturing)
738	An Analysis of the Automotive Industry as a Source for Weapon Components and Manufacturing Processes	42483		•				•			•	•			•	•			
740	Fluid-Structural Interactions in Wetting and Penetration into Porous Media	44136												•				•	**CRMPC CRADA, Others
386	High-Level Decision-Support Framework for Critical-Infrastructure Protection Prioritization	44601			•					•	•	•	•		•	•	•		*FEMA, FBI, Office of Homeland Security
388	Dynamic-Simulation Model of the National Security Consequences	44774		•	•			•		•			•						
742	Macroscopic Rates, Microscopic Observations, and Molecular Models of the Dissolution of Carbonate Phases	45279	•				•				•			•					
435	Electrical-Impedance Tomography for Opaque Multiphase Flows in Metallic Vessels	46069						•		•	•							•	**Chemical and Fossil Energy Industries
745	High-Speed Micro-EDM	46070													•	•			

Appendix E: Major National Programs

Pg #	Title	Project #	Waste Management	Energy Efficiency	Renewable Energy	ES&H	Environmental Restoration	Fossil Energy	Radioactive-Waste Management	Economic Impact	Energy Research	Intelligence & National Security	Nuclear Energy	Science Education & Technical Information	Defense Programs	Department of Defense (DoD)	Other Federal Agencies*	Other (Industry, Consortia...)**	Other Federal Agencies* Other (Industry, Consortia...)**
390	Electricity-Generation Production Cost Model	46072		•	•			•											
747	Developing Rigid and Compliant Cardiovascular-System Models Using Rapid Prototyping	46684											•						
749	Nanoscale Hotspots Due to Nonequilibrium Thermal Transport	46685										•			•	•		•	**Microelectronics Industry
752	Micro External Combustion Engine: The P3 Engine Prototype	46686		•	•														
284	Exploiting Polarimetric Information in Synthetic-Aperture Radar Images for Automatic Target Recognition	46687										•				•			
285	Moving-Target Identification Using Ultrahigh-Range Resolution Data	46688										•				•			
754	Effectiveness of Dielectrophoretic and Electrokinetic Filters/Concentrators for Collecting Smallpox and Anthrax Surrogates from Raw Samples	47516	•			•			•			•			•	•	•	•	*NIH, **Biotechnology, bioterrorism
755	Mathematical and Algorithmic Issues in Multiphysics Couplings	47517	•					•	•						•			•	**Industry
757	MEMS Adaptive Optics Devices	47687	•	•		•	•	•	•	•		•				•			
759	Securing the U.S. Mail Distribution System Against the Threat of Biological and Chemical Agents	47688				•						•					•		*U.S. Postal Service
761	Lipid Membranes on Nanostructured Silicon	47795			•							•				•			
24	Combating Terrorism and Homeland Security	48212										•				•			
25	Underground Hunter Robots: Reconnaissance, Clearing, and Securing of Underground Tunnel Complexes Using Robotic Vehicles	48213					•					•			•	•	•		*DOJ
763	Combating the Chem-Bio Threat Using Sandia Assets: Need for a Technology Roadmap	48339														•	•		*GSA
764	Numerical Methods for the Study of Hydrocarbon Combustion	48340		•				•			•				•	•			
632	Chemically Stressed Glass Structural Elements	48341										•			•	•			
634	Digital Signal Processing for Acoustic-Seismic Target Identification	48746										•			•	•			
635	Terahertz Propagation in Telecommunication Optical Fibers	48751										•							

Appendix E: Major National Programs

Pg #	Title	Project #	Waste Management	Energy Efficiency	Renewable Energy	ES&H	Environmental Restoration	Fossil Energy	Radioactive-Waste Management	Economic Impact	Energy Research	Intelligence & National Security	Nuclear Energy	Science Education & Technical Information	Defense Programs	Department of Defense (DoD)	Other Federal Agencies*	Other (Industry, Consortia...)**	Other Federal Agencies* Other (Industry, Consortia...)**
637	Rapid Screening for Biological Infection	48764										•							
639	Investigation of Bluetooth Capabilities and Vulnerabilities	48765												•					
391	Radiolytic Reduction of Carbonaceous Gases During Coal Gasification for Hydrogen Production	49167		•							•		•						
642	Spectral Tagging	49168															•		*Army Basic Research
766	Assessment of the Potential Impact of Disruptions in Manufacturing Supply Chains	49170								•					•				
393	Proton Beam Shield	49367								•						•			
27	Microoptical Radar: Enabling Multiple Solutions to the War on Terrorism	49767										•				•			
768	Resin Infusion Between Double Flexible Tooling	49769								•					•	•			
395	Frameworks for Nuclear Process Transparency and Control	49770									•		•						
288	155-mm Munitions Reutilization Study	49771													•	•			
770	Studies on the Disbonding Initiation of Interfacial Cracks	49772										•			•	•		•	**Electronics & Phonotics
30	Principles for Network-Security Mechanisms Utilizing Network Address Translation	49773										•				•			
644	Aviation Security	49864								•		•					•	•	*TSA, FAA, **Aviation Industry
771	Effect of Machining Parameters on Tool Life	49914								•					•				
291	Critical Technology Development for Hard Target Defeat High-G Tolerant Fuze and High Explosives	49915										•			•	•			
646	Protection of Sensitive Computers	50000										•							
293	Unmanned and Unattended Response Capability for Homeland Defense	50001	•				•		•			•			•	•			
452	War on Terrorism	50065										•				•			
295	Application of Nonlethal Weapons to Counterterrorism	50066													•				

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Pg #	Title	Project #	Waste Management	Energy Efficiency	Renewable Energy	ES&H	Environmental Restoration	Fossil Energy	Radioactive-Waste Management	Economic Impact	Energy Research	Intelligence & National Security	Nuclear Energy	Science Education & Technical Information	Defense Programs	Department of Defense (DoD)	Other Federal Agencies*	Other (Industry, Consortia...)**	Other Federal Agencies* Other (Industry, Consortia...)**
149	Particle "Front End" for Compact WMD Threat-Detection Systems: Integrated Microsystem Concepts for Intelligent Particle Collection, Separation, Preconcentration, and Processing	50121										•			•				
647	Assessment and Identification of Appropriate μ Power Technologies for μ Sensors and Other Applications	50395										•							
773	Compliant Membranes for MEMS Microphones	50396				•	•			•		•				•			
774	Multiscale Experimental/Numerical Study	50717		•										•	•	•			
776	Cellular Observatory: Simultaneous Time- and Frequency-Resolved Microscopy	50772									•								
777	Near-Real-Time Site Characterization for Assured HDBT Defeat	50858										•			•	•			
649	Multispectral Data-Exploitation Advancements	50973					•					•	•			•		•	**Industry
397	A Fully Integrated Sensor-Based Critical Facility and Border Defense System	51534								•		•							
296	Concept Definition for an Integrated Biodefense System	51536										•				•	•		*DOE Chem Bio Nonproliferation
780	Ironless Permanent Magnet Actuator	51537												•					
652	Response Analysis Tactical Simulation	51538										•				•		•	**Police/Homeland Security
398	Introspection, Integration, and Intercession (I3): Toward Self-Healing Critical Infrastructures	51540										•						•	**MIT
654	Optical Tagging Technologies	51541										•				•			
32	Feasibility Study of an Integrated-Systems Solution to the Problem of Radiological Dispersal Devices	51706	•			•			•			•	•			•	•		*FEMA
298	A Maneuvering, Hypersonic Pathfinder/ Test-Bed	51708										•			•	•			
75	Micromechanical Spectrum-Analyzer System	52173										•				•			
781	Inelastic Deformation Mechanism in Shocked Sapphire Single Crystals	52174												•	•	•			
35	Feasibility Study: Development of a Computational Sociopsychological Model for Understanding Terrorist Behavior	52175										•							

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Pg #	Title	Project #	Waste Management	Energy Efficiency	Renewable Energy	ES&H	Environmental Restoration	Fossil Energy	Radioactive-Waste Management	Economic Impact	Energy Research	Intelligence & National Security	Nuclear Energy	Science Education & Technical Information	Defense Programs	Department of Defense (DoD)	Other Federal Agencies*	Other (Industry, Consortia...)**	Other Federal Agencies* Other (Industry, Consortia...)**
37	Feasibility of Microsensors for the War on Terror	52176										•			•	•		•	**Industry
656	Thermobaric Weapons Signatures	52216										•			•	•			
299	Feasibility of Using Pulsed Intense Ion Beams to Improve Wear Behavior of Metals and Plastics	52395													•		•	•	*Department of Defense, **Materials Industry
38	Feasibility Study for Improved Nonlethal Weapon Based on Disruption of Postural Reflexes	52397											•		•	•			
782	Portable Endospore Detection System for Real-Time Anthrax Screening	52796												•	•				
784	Design and Control of the Magnetic Properties of Nanoparticles	52797								•		•		•					
785	Aerospace Vehicle Trajectory Optimization System by Primer Vector Methods	52825										•			•	•	•	•	*NASA, **DoD Defense Contractors
786	Algorithm Development for Smart Antennas	52826													•				
658	Class B Fire-Suppression Capabilities of a Modified Sandia CBW Decon Foam	52974														•	•	•	*Homeland Security, **Counterterrorism Industry
787	Failure Analysis and Surety Design of Composite Patching Systems	52976				•												•	**Industry (aeronautics)
788	Flow Control and Mixing in Microfluidic Devices	52977									•			•				•	**University Collaboration
789	Wire-Initiation Dynamics and Monochromatic Imaging	53339									•				•				
103	Rapid Syndrome Validation Project (RSVP) Hypothesis Testing and Development	53340														•	•	•	*Office of Homeland Security, **Medical
790	Investigations into the Transient Analysis of System Reliability/Availability Via Cumulant Functions	53342											•		•	•			
791	Topological Layout for the Optimal Design of Electrostatically Actuated MEMS	53372								•				•	•	•			
40	Detection, Classification, and Multitarget Tracking in a Sensor-Rich Environment	53373										•				•			
792	Atomic-Scale Scanning-Tunneling Microscopy Measurements of Nucleation and Growth of Ge/Si Alloy Structures	53464									•				•		•		*DARPA
793	Micro-/Nanoscale Thermomechanical Manufacturing	53465	•											•		•		•	**Industry, Consortia

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Pg #	Title	Project #	Waste Management	Energy Efficiency	Renewable Energy	ES&H	Environmental Restoration	Fossil Energy	Radioactive-Waste Management	Economic Impact	Energy Research	Intelligence & National Security	Nuclear Energy	Science Education & Technical Information	Defense Programs	Department of Defense (DoD)	Other Federal Agencies*	Other (Industry, Consortia...)**	Other Federal Agencies* Other (Industry, Consortia...)**
794	Design of Biospecific Surfaces to Control Specific Cellular Responses	53681										•		•	•	•			
795	High Field Effects of GaN HEMTs	53682										•			•	•			
796	Cognitive Models Applied to Human Effectiveness in National Security Environments	54210														•			
797	Nanomagnetic Films	54211		•				•			•	•			•	•			
798	A Multiscale Approach to Modeling Carbon Nanotubes	54213									•				•	•			

Appendix F: Dual-Benefit Areas and Single-Use Categories

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Pg #	Title	Project #	Aeronautics	Applied Molecular Biology	Ceramics	Composites	Computer Simulation and Modeling	Data Storage and Peripherals	Electronics and Photonics	Energy	Flexible Computer-Integrated Manufacturing	High-Definition Imaging and Displays	High-Performance Computing and Networking	High-Performance Metals and Alloys	Intelligent Processing Equipment	Material Synthesis and Processing	Medical Technology	Micro- and Nanofabrication	Micro- and Optoelectronics	Photonic Materials	Pollution Minimization, Remediation, and Waste Mgmt.	Sensors and Signal Processing	Software	Surface Transportation Technologies	Systems Management Technologies	Defense-Related (mostly or purely)	Dual-Use (defense and non-defense-related)	Non-Defense-Related (mostly or purely)
182	III-Antimonide/Nitride-Based Semiconductors for Optoelectronic Materials and Device Studies	26518							•				•						•	•							•	
184	The Integration of Advanced Photonics and MEMS	26519	•						•											•							•	
407	Uncertainty Propagation in Models of Thermo-fluid Systems	26520					•			•			•										•				•	
409	Filtered Rayleigh-Scattering Diagnostic for Multiparameter Thermal/Fluids Measurements	26521	•							•												•					•	
412	A Physically Based Approach to Modeling Ductile Fracture	26522	•				•																•				•	
415	Radiation Aging of Stockpile and Space-Based Microelectronics	26523					•		•										•				•				•	
417	Large-Deformation Solid-Fluid Interaction Via a Level-Set Approach	26524		•			•							•													•	
480	Magnetic-Field Effects on Vacuum-Arc Plasmas	26525					•						•													•		
481	Microstructural and Continuum Evolution Modeling of Sintering	26526			•		•				•					•											•	
485	Assuring Ultraclean Environments in Microsystem Packages: Irreversible and Reversible Getters	26527				•	•		•							•		•								•		
487	Biocompatible Self-Assembly of Nanomaterials for Bio-MEMS and Insect Reconnaissance	26528		•	•	•										•	•	•			•	•					•	
490	Nanoclusters for Supercapacitors	26529				•			•							•		•									•	
492	First-Principles Determination of Dislocation Properties	26530					•									•		•										•
219	Air Sterilization and Decontamination	26531		•													•							•			•	

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Pg #	Title	Project #	Aeronautics	Applied Molecular Biology	Ceramics	Composites	Computer Simulation and Modeling	Data Storage and Peripherals	Electronics and Photonics	Energy	Flexible Computer-Integrated Manufacturing	High-Definition Imaging and Displays	High-Performance Computing and Networking	High-Performance Metals and Alloys	Intelligent Processing Equipment	Material Synthesis and Processing	Medical Technology	Micro- and Nanofabrication	Micro- and Optoelectronics	Photonic Materials	Pollution Minimization, Remediation, and Waste Mgmt.	Sensors and Signal Processing	Software	Surface Transportation Technologies	Systems Management Technologies	Defense-Related (mostly or purely)	Dual-Use (defense and non-defense-related)	Non-Defense-Related (mostly or purely)
221	Data Fusion and Visualization of MASINT Results for Underground Facility Characterization	26532													•							•				•		
223	Rapid Ultrasensitive Chemical-Fingerprint Detection of Chemical and Biochemical Warfare Agents	26533		•					•							•		•			•	•					•	
226	Advanced Unattended Ground-Sensor Technology	26534													•		•					•					•	
229	The Endowment of Simulator Agents with Humanlike Episodic Memory	26535	•				•								•		•					•	•		•		•	
232	An Advanced Learning Model for Agent Behavior	26537					•						•		•								•				•	
553	Threat-Assessment Study for Short-Pulse Laser Technologies in Directed-Energy and Countersensor Applications	26538							•										•	•		•				•		
234	Algorithms for Improved Performance in Cryptographic Protocols	26539																				•	•				•	
237	Low-Cost Digital Radar for Fuzing, Tags, SAR Imaging, and Targeting	26540	•						•													•					•	
239	Triggered Isomer Research	26541								•																	•	
241	A Scientific Basis for Robotic Ground-Vehicle Design	26542					•																	•		•		
243	Adaptive and Mobile Ground Sensors	26543																				•	•			•		
245	Algorithm Development for Prognostic Health Monitoring and Maintenance	26544	•												•							•					•	
248	New Mechanism for Upset of Electronics	26545					•		•										•			•			•	•		

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Pg #	Title	Project #	Aeronautics	Applied Molecular Biology	Ceramics	Composites	Computer Simulation and Modeling	Data Storage and Peripherals	Electronics and Photonics	Energy	Flexible Computer-Integrated Manufacturing	High-Definition Imaging and Displays	High-Performance Computing and Networking	High-Performance Metals and Alloys	Intelligent Processing Equipment	Material Synthesis and Processing	Medical Technology	Micro- and Nanofabrication	Micro- and Optoelectronics	Photonic Materials	Pollution Minimization, Remediation, and Waste Mgmt.	Sensors and Signal Processing	Software	Surface Transportation Technologies	Systems Management Technologies	Defense-Related (mostly or purely)	Dual-Use (defense and non-defense-related)	Non-Defense-Related (mostly or purely)
250	Flexible Robotic Maintenance Facility	26546	•				•																•				•	
253	Distributed Autonomous Navigation	26547					•															•		•		•		
255	Obstacle Detection for Autonomous Navigation	26548													•							•		•			•	
321	Very High Temperature Gas-Cooled Reactor	26549																			•							•
324	Solid-State Ballistic Chemical Sensors	26550								•					•			•	•			•						•
327	Novel Catalytic Systems for Energy-Efficient Feedstock Hydrocarbon Separations	26551								•						•		•			•							•
330	A Model of Infrastructure Interdependency Using Communication Agents	26552					•																				•	
540	Microchemical Sensors for Characterization and Monitoring of Volatile Contaminants	26553																			•	•					•	
333	Investigation of Potential Applications of Self-Assembled Nanostructured Materials in Nuclear-Waste Management	26554			•											•		•			•	•						•
336	Development of Detection Techniques and Diagnostics for Airborne Carbon Nanoparticles	26555								•											•	•		•				•
339	Photonic Crystals for Enhancing Thermophotovoltaic Energy Conversion	26556						•	•									•	•	•								•
341	Specific Anion Nanoengineered Sorbents for Water Purification	26557					•									•					•							•
554	Development of a Microoptic Gyroscope	26559	•					•										•	•	•		•					•	

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Pg #	Title	Project #	Aeronautics	Applied Molecular Biology	Ceramics	Composites	Computer Simulation and Modeling	Data Storage and Peripherals	Electronics and Photonics	Energy	Flexible Computer-Integrated Manufacturing	High-Definition Imaging and Displays	High-Performance Computing and Networking	High-Performance Metals and Alloys	Intelligent Processing Equipment	Material Synthesis and Processing	Medical Technology	Micro- and Nanofabrication	Micro- and Optoelectronics	Photonic Materials	Pollution Minimization, Remediation, and Waste Mgmt.	Sensors and Signal Processing	Software	Surface Transportation Technologies	Systems Management Technologies	Defense-Related (mostly or purely)	Dual-Use (defense and non-defense-related)	Non-Defense-Related (mostly or purely)
556	Synergistic Merging of Multispectral Transient Radiometry and Multispectral Imaging Technology for Enhanced Global Situational Awareness Through Accurate Geolocation	26560					•								•							•	•			•		
558	New Glass Technology for Enhanced Architectural Surety	26561			•											•											•	
561	Compact UV Laser Source for Chemical and Biological Sensing	26562							•	•												•					•	
564	Advanced Digital Detectors for Neutron Imaging	26563		•					•	•							•					•					•	
566	Microfabricated Acoustic Spectrum Analyzer	26564													•			•				•					•	
569	Enabling Analytical and Modeling Tools for Enhanced Disease Surveillance	26565					•																				•	
573	Microtransmitter for Tag, Beacon, and Data-Exfiltration Applications	26566																	•								•	
574	Extensibility of Knowledge-Based Human-Agent Simulation	26567	•				•								•		•						•	•	•		•	
576	Secure Authenticated Sensor Packs	26568							•									•				•					•	
579	Remote Monitoring of Difficult, Real-Time Targets Using Video SAR Technique	26569																				•					•	
581	Coating Chemical Preconcentrators to Improve Chemical-Agent Collection	26572														•		•				•					•	
542	Ultralow-Power Spread-Spectrum Receivers for Microtags to Improve Security During Critical Operations	26573	•						•						•		•	•	•			•					•	
583	Detection and Exploitation of Spread-Spectrum Waveforms	26574					•						•									•				•		

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661	Use of Intense Ion Beams for Surface Modification and Creation of New Materials	28763				•								•		•	•										•	
663	Low-Intensity Laser Triggering of Spark Gaps	28764							•	•																	•	
664	Z-Pinch Power-Plant System Development	28769								•	•			•	•						•	•			•		•	
666	Recyclable Transmission Line Concept for Z-Pinch IFE	28770								•																	•	
669	Suppression of Electron Emission from Conductors	28771							•	•				•		•											•	
671	Solid-State Switch for Advanced Pulsed Power	28772							•	•									•								•	
257	Laboratory-Scale Coherent Multikilovolt X-Ray Sources for Advanced Imaging Applications	28775								•						•						•					•	
447	Interfacial Bioscience Grand Challenge (IBIG)	28776		•													•					•						•
95	High-Throughput Instruments, Methods, and Informatics for Systems Biology	32574		•					•						•		•		•								•	
343	Low-Work-Function Material Development for the Microminiature Thermionic Converter	32807			•				•			•				•		•	•			•					•	
346	Autonomous Microexplosive Subsurface Tracing System	32809							•	•								•	•			•						•
349	Security Models of Agent-Based Coalitions	32815																				•			•		•	
351	Vulnerability Assessment of National Power Grid	32816					•			•			•												•		•	
691	Molecular Simulations of MEMS and Membrane Coatings (PECASE)	32817								•								•			•						•	
186	Aging Mechanisms in Dormant MEMS Structures	32913														•		•				•					•	

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99	Biomimetic Chloroplasts: An Integrated Microdevice Power Source	32914		•			•		•	•						•		•										•
494	Study of Polymer Spin-Coating for Photolithographic Semiconductors in Near-Zero-Gravity Environment	32915														•			•								•	
188	MEMS in μ Fluid Channels	32923		•													•	•	•			•					•	
191	Dispersive Photonics for Next-Generation Sensors and Microsystems	33602							•									•		•							•	
496	Understanding Metal Vaporization from Transient High-Fluence Laser Irradiation	34465	•				•		•					•	•	•	•		•				•				•	
498	Mechanics and Tribology of MEMS Materials	34466				•			•					•		•	•	•				•					•	
502	Dynamics of Metal/Ceramic Interfaces	34467			•									•				•									•	
504	<i>In Situ</i> Characterization of Soft Solution Processes for Nanoscale Growth	34468				•			•									•		•		•						•
506	Determination of Critical Length Scales for Corrosion Processes Using Microelectroanalytical Techniques	34469							•					•				•	•			•					•	
508	LIGA Microsystems Aging: Evaluation and Mitigation	34478																•									•	
511	Science-Based Processing of Field-Structured Composites	34485				•										•					•	•					•	
693	Self-Assembly of Polymers in Confined Geometries	34692					•						•			•											•	
695	Building Conscious Machines Based on the Architecture of Visual Cortex in the Primate Brain	34693									•		•		•		•										•	
258	Microfuzze	34698			•	•	•		•	•					•			•	•	•		•				•		

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514	Exploration of New Multivariate Spectral Calibration Algorithms	34699		•	•		•		•	•	•				•	•	•				•	•	•				•	
696	Development of Experimental Verification Techniques for Nonlinear Deformation and Fracture	35376					•		•									•									•	
699	Microcontact Printing of Nanoparticle Arrays	36901							•									•		•								•
703	Mathematical Analysis of Deception	36902					•	•					•		•								•		•		•	
704	A System-Dynamics Approach to Modeling Water Demand	36904					•																		•		•	
69	Microfabrication with Femtosecond-Laser Processing	38605							•		•			•		•		•	•	•							•	
71	Mesoscale Controlled Motion for a Microfluidic Drop Ejector	38606													•			•									•	
73	Science-Based Sensing of Phase Transformations in Steels	38608													•							•		•			•	
101	Physical and Electronic Changes Caused by Membrane Signaling as a Transduction Pathway in Affinity-Based Biosensors	38609		•					•								•	•	•	•		•					•	
130	Graduated Embodiment for Sophisticated Agent Evolution and Optimization	38610													•												•	
133	Stochastic Programming for Enterprise Modeling—Optimization for Nondeterministic Simulation	38611					•																				•	
136	Robust Message Routing for Mobile (Wireless) <i>Ad Hoc</i> Networks	38612	•				•		•				•		•								•				•	
138	Scalable Fault-Tolerant Algorithms for Linear-Scaling Coupled-Cluster Electronic Structure Methods	38613		•			•			•			•										•				•	

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40	Micromagnetic Suspension	38614					•											•									•	
142	Sensitivities for Large-Scale Simulation Codes	38615					•						•														•	
193	Engineered Superconductivity in Electron-Hole Bilayers	38616							•				•						•	•							•	
195	Silicon-Based RF MEMS Components	38617							•								•		•			•					•	
197	2-D Arrayed Resonant Subwavelength Gratings	38618							•									•	•	•							•	
200	Nanoelectromechanical Oscillators (NEMOs) for RF Filtering	38619							•									•				•					•	
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205	Microsystems for Chemical Signature and Reagent Delivery	38621		•		•			•						•	•	•	•			•	•					•	
207	Microfluidic Cellular Sample Pretreatment	38622		•					•								•	•	•			•					•	
261	Automated Visual Direction of Mobile Manipulation	38623									•				•						•	•					•	
263	Miniature Fourier-Transform Ion-Mobility Spectrometer for Real-Time Detection and Identification of Explosives and Chemical Agents	38624																			•	•					•	
266	CONOPS Development for Automated Systems	38625					•						•		•							•	•		•		•	
268	Rapid Mitigation and Decontamination of Toxic Industrial Chemicals	38626																			•			•			•	
270	EM Interactions with Systems to Enhance Security	38627							•																	•		
272	Adaptive Awareness for Personal and Small-Group Decision Making	38628					•		•			•	•		•		•	•	•			•	•		•		•	

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274	Use of Seismic and Acoustic Responses to Assess Bomb Damage to Underground Facilities	38629					•											•					•			•		
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279	Kinematics-Based Video Compression Using a Foveated-Imaging Sensor for Remote Telepresence Applications	38658	•						•			•										•					•	
281	Information Assurance for Wireless <i>Ad Hoc</i> Networks	38659					•						•									•	•				•	
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354	Natural-Gas Production Problems: Solutions, Methodologies, and Modeling	38662								•																		•
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358	Time-Domain Reflectometry for Remote, Real-Time Water-Quantity/-Quality Monitoring of Ephemeral Streams	38665																				•						•
361	Research and Development of Mathematical Algorithms to Define and Quantify Critical Infrastructure Interdependencies	38667					•																		•			•
364	Functionalized Nanoelectrode Arrays for <i>In Situ</i> Identification and Quantification of Regulated Chemicals in Water	38668		•					•						•	•	•	•			•	•					•	
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370	Water Desalination	38673														•	•	•									•		
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376	Potential Application of Microsensor Technology in Radioactive-Waste Management—with Emphasis on Headspace Gas Detection	38677							•												•	•						•	
378	Surety Enhancement for Wireless Automated-Control Networks	38678					•			•			•				•											•	
380	Advanced Nuclear-Engineering Analysis Technology	38679					•			•																		•	
383	Identification of Chemical Plumes: Range-Resolved IR Lidar Enabled by New Photonic Technologies	38681							•	•							•	•	•	•	•	•					•		
422	Multiscale Thermal Modeling	38682					•		•									•	•	•	•						•		
424	A Robust, Coupled Approach for Atomistic-Continuum Simulation	38684					•							•				•					•				•		
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620	Microfabricated Dielectrophoretic Sample-Preparation System	38707		•			•									•	•	•				•	•				•	
623	Automation of Microelectronic Physical Analysis	38708							•																	•		
624	Nonlinear Optical Limiters Using Photonic-Bandgap Structures for Sensor Protection	38712							•									•	•	•		•				•		
626	Secure MPLS Control Plane for Internet Connectivity	38713					•					•											•				•	
628	Integrated-Sensor Network Chip	38714					•																		•		•	
706	Self-Organization of Software	38716					•					•		•								•					•	
707	Nanoscale Energetic Materials by Inverse Micellar Synthesis	38717																•								•		
709	Modeling of Rock Penetration	38718					•																			•		
712	Nanoconverter	38719																•	•								•	
713	Novel Proton-Exchange Membrane Materials for the Advancement of Direct Methanol Fuel-Cell Technology	38720				•				•						•		•			•						•	
715	Communicating with the <i>In Vivo</i> Sensor	38721		•					•						•	•	•	•				•					•	
718	Agile, Microsystems-Enabled Receiver	38722	•						•									•				•					•	

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721	Linking Geosciences to Emerging Bioengineering Technologies	38723		•	•	•	•			•		•	•			•	•				•						•	
724	Energy Storage: Leaving Chemistry in the Dust	38724	•							•																•		
726	Novel Algorithms and Experimental Techniques for Quantitative Spectral Analysis of Particulates	38726		•	•		•										•	•				•	•				•	
729	Self-Healing Adhesives and Encapsulants: Long-Term, High-Performance Weapon Components	38727				•			•							•	•									•		
731	Neutron-Only Detector for JTA Tests	38729							•											•						•		
145	Adaptive Network Countermeasures	38744					•																•		•		•	
534	Solution-Based Nanoengineering of Materials	39017			•				•											•		•					•	
732	MEMS-Based Electromechanical Acoustic-Energy Harvester	39212	•				•		•													•					•	
673	Determination of Microstructural Properties with Isentropic Compression	39669												•												•		
675	Simulations of Intense Petawatt Laser Pulses with Dense Z-Pinch Plasmas	39670					•			•																	•	
449	Biomicrofuel Cell	41193		•		•				•						•	•	•									•	
630	Cognition-Driven Augmented Analyst	41194					•								•							•	•		•		•	
546	Predicting and Validating MEMS Interface Reliability	41427	•	•	•	•	•	•	•	•	•	•	•	•	•	•	•	•	•	•	•	•	•	•	•	•	•	
147	Microengine for Advanced Power Generation	41674								•								•									•	
734	Direct Simulation of Solid-Fluid Systems	41726					•			•			•										•					•

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634	Digital Signal Processing for Acoustic-Seismic Target Identification	48746													•							•					•	
635	Terahertz Propagation in Telecommunication Optical Fibers	48751							•						•						•	•					•	
637	Rapid Screening for Biological Infection	48764															•					•					•	
639	Investigation of Bluetooth Capabilities and Vulnerabilities	48765																					•					•
391	Radiolytic Reduction of Carbonaceous Gases During Coal Gasification for Hydrogen Production	49167					•			•						•					•							•
642	Spectral Tagging	49168														•						•					•	
766	Assessment of the Potential Impact of Disruptions in Manufacturing Supply Chains	49170			•				•		•				•			•	•						•		•	
393	Proton Beam Shield	49367			•										•												•	
27	Microoptical Radar: Enabling Multiple Solutions to the War on Terrorism	49767	•						•			•							•								•	
768	Resin Infusion Between Double Flexible Tooling	49769				•																					•	
395	Frameworks for Nuclear Process Transparency and Control	49770								•												•					•	
288	155-mm Munitions Reutilization Study	49771	•						•																	•		
770	Studies on the Disbonding Initiation of Interfacial Cracks	49772				•			•							•		•	•			•					•	
30	Principles for Network-Security Mechanisms Utilizing Network Address Translation	49773					•					•													•		•	
644	Aviation Security	49864					•		•			•					•					•			•		•	

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771	Effect of Machining Parameters on Tool Life	49914									•																•	
291	Critical Technology Development for Hard Target Defeat High-G Tolerant Fuze and High Explosives	49915							•									•				•				•		
646	Protection of Sensitive Computers	50000																					•				•	
293	Unmanned and Unattended Response Capability for Homeland Defense	50001					•														•			•	•		•	
452	War on Terrorism	50065					•								•											•		
295	Application of Nonlethal Weapons to Counterterrorism	50066																				•					•	
149	Particle "Front End" for Compact WMD Threat-Detection Systems: Integrated Microsystem Concepts for Intelligent Particle Collection, Separation, Preconcentration, and Processing	50121																•				•					•	
647	Assessment and Identification of Appropriate μ Power Technologies for μ Sensors and Other Applications	50395							•										•			•					•	
773	Compliant Membranes for MEMS Microphones	50396	•						•						•		•	•	•			•		•	•		•	
774	Multiscale Experimental/ Numerical Study	50717	•				•						•					•									•	
776	Cellular Observatory: Simultaneous Time- and Frequency-Resolved Microscopy	50772		•													•	•				•					•	
777	Near-Real-Time Site Characterization for Assured HDBT Defeat	50858																				•				•		
649	Multispectral Data-Exploitation Advancements	50973													•							•	•				•	

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38	Feasibility Study for Improved Nonlethal Weapon Based on Disruption of Postural Reflexes	52397															•										•	
782	Portable Endospore Detection System for Real-Time Anthrax Screening	52796		•													•	•		•							•	
784	Design and Control of the Magnetic Properties of Nanoparticles	52797		•		•											•	•	•			•					•	
785	Aerospace Vehicle Trajectory Optimization System by Primer Vector Methods	52825	•				•																			•		
786	Algorithm Development for Smart Antennas	52826																•				•				•		
658	Class B Fire-Suppression Capabilities of a Modified Sandia CBW Decon Foam	52974															•				•						•	
787	Failure Analysis and Surety Design of Composite Patching Systems	52976				•	•									•							•					•
788	Flow Control and Mixing in Microfluidic Devices	52977		•			•										•	•				•						•
789	Wire-Initiation Dynamics and Monochromatic Imaging	53339								•																	•	
103	Rapid Syndrome Validation Project (RSVP) Hypothesis Testing and Development	53340															•										•	
790	Investigations into the Transient Analysis of System Reliability/ Availability Via Cumulant Functions	53342					•																				•	
791	Topological Layout for the Optimal Design of Electrostatically Actuated MEMS	53372					•		•		•		•										•				•	
40	Detection, Classification, and Multitarget Tracking in a Sensor-Rich Environment	53373																				•				•		

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