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*Laboratory Directed
Research and Development
Annual Report*

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"...exceptional service in the national interest."

Science and technology are at the heart of 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 revolutionizes 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.

**FY 1997
Funding Levels
(MIL \$)**

Laboratory Directed Research and Development Program Overview

C. E. Meyers

"Almost every laboratory has found that the most important innovation often comes from the scientists' independent ideas or actions."

*The Packard Panel, May 1983,
Federal Laboratory Review Panel:
report of the
White House Science Council
Office of Science and Technology Policy*

Sandia's value as a national resource is our world-class science, technology, and engineering. These capabilities must remain on the cutting edge because the safety, security, and reliability of U.S. nuclear weapons depend directly on them. Under the guidance of Sandia's Laboratory Director and with the DOE's concurrence, the Laboratory Directed Research and Development (LDRD) Program provides the flexibility to invest in long-term, high-risk, and potentially high-payoff research activities that stretch Sandia's science and technology capabilities.

LDRD supports Sandia's four primary strategic objectives: nuclear weapons; nonproliferation and materials control; energy and critical infrastructure; and emerging national security threats. To meet these objectives, LDRD promotes creative and innovative research and development by funding initiatives that are inspired by technology needs, often high risk, and that attract exceptional research talent across disciplines.

Sandia's LDRD Program provides the leadership necessary to do the right research in the right way. The insight that management brings to the knowledge generated from basic research will allow Sandia to manage its intellectual assets for the benefit of the entire nation. The LDRD Program has three strategic goals:

- to conduct leading-edge research supporting all mission assignments,

**FY 1997
Selected Statistics**

Full-time staff	270
Smallest project	\$11K
Average project	\$315K
Average project (FTE)	1.19
Largest project	\$2.9M
1ST-year projects	128
2ND-year projects	69
3RD-year projects	21

**FY 1997
Performance**

Refereed publications	371
Other publications	247
Patent disclosures	65
Patent applications	31
Patents	23
Copyrights	9

**Completed milestones
focus project performance on
negotiated metrics.**

A majority of projects have dual-use applications.

especially those with an emphasis on national security;

- to provide scientific and technical leadership through increased emphasis on external collaborations; and
- to improve communication about and support for the program.

Future work will continue to emphasize collaborations, solidifying Sandia's position in the forefront of the global research and development community. The LDRD Program will continue to develop and promote the tools necessary to assess the impact and value of ongoing and future research.

Throughout its history, exploratory research at Sandia has reflected changing societal, political, and environmental needs. A perceived nuclear threat prompted the Atomic Energy Act of 1954, fostering research and development to maximize scientific and industrial progress. During the Arab oil embargo, the Energy Research and Development Administration redirected research toward energy-related concerns. In 1977 Congressional legislation (Public Law 95-39) led to employee-suggested research, which assumed its present form as LDRD in 1991.

Authorized by federal law and implemented under DOE Order 413.2, LDRD is Sandia's sole source of discretionary research funds. LDRD is funded

by an assessment on all costed work at Sandia. Atomic energy defense activities are supported directly by 67 percent of LDRD projects, although atomic energy defense activities provide only 48 percent of LDRD annual funding. More than 90 percent of LDRD projects provide benefits in basic and applied research to national security needs. In FY 1997, LDRD funded 218 projects in eleven programmatic areas.

LDRD uses recognized metrics to track and assess research impact both qualitatively and quantitatively. Metrics include intellectual properties, programmatic performance, citations in relevant literature, and customer satisfaction. The intellectual properties metric is based on patents and copyrights. These have been trending upward. For 1997, patents totaled 23, or 35 percent of all patents issued to Sandia during the year. Copyrights totaled 9.

The programmatic performance metric is based on awards and milestones completed. The LDRD Program plays a major role in allowing Sandia to remain at the leading edge of research and technology. As a result, work performed in LDRD projects has earned many of the nationally and internationally recognized awards for excellence in research. *R&D*

Magazine's R&D 100 Awards acknowledge the most promising technologies emerging from industrial, academic, and federal laboratories. In 1997 five of Sandia's eight R&D 100 awards were associated with LDRD-supported projects. Also, FY 1997 LDRD projects completed 72 percent of their milestones.

The metric based on citations in relevant literature pioneered by the Institute for Scientific Information focuses on institutional and national performance measures. This analytic method measures impact on the scientific community by tallying the number of times published research is cited by other researchers. At least four thousand of the most influential journals worldwide are reviewed. Citations of Sandia's LDRD-related published papers were tallied in research publications from thirteen federal laboratories, the top one hundred twelve federally funded U.S. universities, and eleven internationally recognized corporations. Citations of Sandia's LDRD-related publications ranked 1.24 times the world average in engineering science, 1.30 times the world average in materials science, and 2.07 times the world average in physics. Sandia's LDRD projects ranked competitively with institutions such as Caltech and Harvard. Over the

Goals and hypothesis status reveal the dynamics of research as each project unfolds.

past five years, we have outperformed many prestigious institutions (including the Massachusetts Institute of Technology, IBM, DuPont, and other laboratories), placing Sandia LDRD in the top 10 percent of institutions conducting physical science research.

Customer satisfaction is measured through surveys and awards to determine success in meeting expectations.

Outcomes are the best measure of achievement for LDRD-funded work. As previously discussed, citation analysis measures impact, and impact presents a barometer of intellectual debt. The ultimate measure of success is customer satisfaction with the product.

In FY 1997, LDRD provided \$71.1 million to fund 218 projects (selected from 1,371 submitted).

For FY 1997, the Sandia LDRD Program was divided into four principal elements: Core Science and Technology Competencies, Systems and Technology Solutions, National Grand Challenges, and Reserve. Principal elements were further subdivided into areas as follows: **Core Science and Technology Competencies** (Materials Science and Technology, Computer Sciences, Electronics and Photonics, and Phenomenological Modeling and Engineering Simulation), **Systems and Technology Solutions** (Manufacturing Science and Technology, Life-Cycle Systems, Information Systems, Precision Sensing and Analysis, Environmental

Sciences, Risk and Reliability, and Focused Technologies), **National Grand Challenges**, and **Reserve**. Investment areas are profiled at the beginning of each section. Each area funded projects that strengthened Sandia's core science and technology base and focused on future DOE and national needs. The projects permitted Sandia staff to explore innovative scientific and technological opportunities that hold high potential for payoff in future applications. Many of these projects have led to tangible new tasks and programs.

The majority of FY 1997 projects had both defense and industrial (dual-use) applications and, at the same time, supported all DOE critical technologies. Clearly, the LDRD Program plays a key role in allowing Sandia to provide "exceptional service in the national interest" and is truly the link from today to tomorrow.

Sandia's LDRD process begins when executive management establishes a framework for strategy and investments, followed by a call for proposals. Electronic submittal of proposal briefs has increased the number of ideas submitted and minimized the time invested in preparation. Each proposal is assessed for technical merit, growth potential, impact on future laboratory activities, and the degree to which it supports Sandia's strategic goals. Projects proposed for extension beyond one year must submit a request for continuation of funding, showing progress achieved to date

toward the objectives and describing the tasks to be performed in the next year.

Proposals are subjected to two independent evaluations. An independent technical review evaluates the technical content of the proposed work, the technical approach proposed, and the technical potential of the project. Proposals are technically scored, ranked, and subjected to a programmatic evaluation by one of several review boards. In this evaluation, a proposal is reviewed with regard to its growth potential, its impact on future laboratory activities, and how the work supports Sandia's strategic intent. Selected projects are submitted to DOE headquarters for concurrence.

An important factor in determining proposal approval is the degree of collaboration involved. Sandia's LDRD Program has created partnerships with industry, government, and academe. This collaborative network enables us to keep pace with rapid technological change, alleviate duplication of effort, and increase the flow of knowledge. Collaborations doubled from FY 1996 to FY 1997, from 29 percent to 63 percent of all projects.

A continuing need for Sandia's LDRD Program is clear. The program is respected for the excellence of its innovative research and teamwork that continue to support the nation's science and technology needs. Sandia's LDRD will continue to conceive and nurture ideas for technologies that anticipate the DOE's emerging mission.

C

reating new materials and processes that enhance national security and benefit industry is the objective of the Materials Science and Technology investment area. Projects originate materials and develop products that behave predictably during the fabrication, production, and aging processes. Predictable behavior helps

designers choose materials and processes according to the kinds of stress that products must endure. Products range from mechanical, electronic, optic, chemical, and magnetic to "smart" devices that operate on atomic and subatomic levels.

There are three categories of Materials Science and Technology projects: (1) research to develop scientifically based materials and processing models that use massively parallel computers to predict material and product behavior; (2) direct fabrication projects that build three-dimensional structures atom by atom, molecule by molecule, or particle by particle; and (3) nanotechnology projects that apply engineering at the atomic scale to develop intelligent materials and microdevices.

Scientists are currently working to enable weapons components to be made directly from a computer model. This process will allow a metal, polymer, or composite part to be created by spraying the material in layers as detailed in the model. This new materials technology may revolutionize weapons production and has a wide range of industrial applications.

Nanotechnology expertise is being applied to use surface impurities — to an advantage — in semiconductor thin films. Massively parallel computers, used to model atomic-scale interactions, and atom-tracking microscopes are enabling scientists to develop a toolkit that converts surface impurities to useful features, which, in turn, will improve semiconductor devices of the future.

MATERIALS SCIENCE & TECHNOLOGY

Top: A strip of pure copper is cold-spray-deposited directly onto the unprepared surface of a ceramic chip carrier. Because the copper remains at essentially room temperature during deposition, oxidation of the copper does not occur even though it is being laid down in an open-air environment.

Below: A new cold-spray deposition process can rapidly lay down thick, low-oxide metal layers at or very near room temperature without the melting or vaporization normally required in traditional thermal-spray or vapor-deposition processes.

Physico-Chemical Stability of Solid Surfaces

T. A. Michalske, G. L. Kellogg, D. R. Jennison, P. J. Feibelman

The application of physico-chemical phenomena to either increase machinability of hard materials, improve the wear resistance of cutting surfaces, or enhance sintering of particle compacts can have a large economic impact on technologies ranging from materials-forming processes to oil-well drilling. Unfortunately, the broad application of these physico-chemical principles is limited by our ability to predict the optimum conditions for a wide variety of materials surfaces. Predictive models must be built upon an understanding of the elementary events involved in surface damage and mobility. Sandia is developing a new approach to examine the fundamental mechanisms controlling physico-chemical surface stability that combines (1) atomic-scale control of surface contact forces and displacements under well-controlled adsorbate conditions using the interfacial force microscope (IFM), (2) atomic-level imaging of surface and near-surface structure and defects using field ion microscopy (FIM) and transmission electron microscopy (TEM), and (3) first-principles modeling of the effect of surface stress on adsorbate bonding interactions and the subsequent generation of surface damage. This unique combination of approaches will provide new insights into observed physico-chemical phenomena and provide the basis for developing true predictive models that are

needed for wide application of these important new approaches to modifying the surface sensitive properties of materials.

Having completed the necessary physical and electronic modifications to the IFM that permit operation in ultra-high vacuum (UHV), we designed and conducted a series of experiments to explore the role of liquid-metal adsorbers on the mechanical properties of clean metal surfaces and interfaces. In these experiments, we were able, for the first time, to clean the IFM probe tip and the substrate surface and to directly measure the mechanical interactions as these metal surfaces were brought together in UHV conditions. In conventional force microscopy, the proximity of the tip is determined by physically contacting the substrate prior to any actual force measurements. Since clean metal surfaces interact so strongly, we had to invent a new method by which we could obtain data on the first approach to the substrate. By applying a bias voltage to the tip, we were able to guide it into position for the first measurement using the field-emitted electron intensity. With this new experimental technique developed, we conducted experiments that contrast the mechanical interaction for a clean Au surface against one covered with monolayers of Hg. Since Hg is a classic embrittling agent for gold, we used these experiments to study the details of the embrittling process. Our results showed, contrary to expectations, that monolayer coverage of Hg actually strengthened the mechanical bond between the clean metals by greater than a factor of six. In addition, these measurements showed for the first time that

the liquid metal actually softens the Au substrate surface, allowing an adhesive instability as the outermost atomic layer of metal atoms "jump" across to form the adhesive bond. During the remainder of the year we completed instrumentation that allows us to measure the atomic-scale contact area as a function of interaction force so that we can directly deduce the chemical influence on the surface mechanical response.

These atomic-level mechanical measurements were complemented by macroscopic wear studies conducted by our university collaborator. Using a unique microscroting apparatus, he demonstrated the effect of liquid embrittling metals on the surface wear of Al. His results show a dramatic softening of the Al surface by Ga (a known embrittling agent for Al). This softening is consistent with our atomic-scale IFM measurements for the Hg/Au system.

Publications

Refereed

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Sol-Gel Preservation of Mankind's Cultural Heritage in Objects Constructed of Stone

C. J. Brinker, R. T. Cygan, K. L. Nagy, C. S. Ashley, A. Sellinger

This was the final year of a three-year effort focused on the development of customized treatments for the preservation of carbonate minerals (limestone and marble) against weathering. The goal of this project is to design a protection system that passivates these stones against subsequent chemical and physical degradation and consolidates the material to impart strength and to arrest further granular deterioration.

This year's work focused on several areas: (1) deposition of synthetic passivants, passivant/consolidant systems, novel functionalized silsesquioxanes, and commercial consolidating coatings onto calcite materials, (2) characterization of calcium leaching behavior under conditions that simulate acid rain, (3) molecular modeling to determine relative ranking of passivant molecules based on binding energies, optimum binding configuration, packing densities, and interactions with water, (4) evaluation of surface changes in uncoated and coated single-crystal calcite using scanning probe microscopy and environmental scanning electron microscopy (SEM), and (5) preliminary strength tests of treated limestone cores using three-point bend tests.

This work fills a critical need for a science-based solution to the wholesale loss of limestone and marble historic buildings and objets d'art to environmental damage. As such, it received recognition during 1997 from the scientific and conservation community in reports by Science News (cover story), Art in America, the Associated Press, and the BBC. This work has relevance to other potential applications where stabilization of mineral surfaces against chemical degradation is required, e.g., chemical migration in hazardous-waste storage areas, groundwater protection, and sealants for concrete structures.

Ideal stone preservation schemes must address both chemical and physical

modes of deterioration. Effective treatments must (1) passivate mineral surfaces against further attack, (2) prevent water adsorption, and (3) consolidate the surface. Conservators demand that the treatment be easy to apply to objects ranging from small objets d'art to entire buildings, remain ultraviolet (UV)-stable, and leave the appearance of the stone unaltered. Alkoxysilane-based commercial treatments, in use since the 1960s to protect sandstone (silicate rock), are only minimally protective of limestone and marble (carbonate rock). We based our protection strategy for carbonate-based minerals on customized bifunctional passivating agents that act as calcium-coupling molecules and provide attachment sites for *in situ* polymerization of a subsequent consolidating layer.

We employed molecular modeling methods to determine relative ranking of binding energies for candidate passivant molecules. We used empirical forcefields, based on observed structural and spectroscopic data, to define the interatomic energies for the passivant molecules, calcite surfaces, and the intermolecular interactions during sorption and binding of the molecule to a surface. We completed energy minimization calculations to obtain the optimum binding configuration and associated binding energy. We examined calcite cleavage and common calcite crystal faces, along with the interaction of passivant molecule on mono-atom-layer steps between the selected surfaces. The computer simulations provide an effective screening tool for determining the most ideal passivant molecule for calcite surfaces, and for guiding the synthesis of passivant materials.

Molecular dynamics (MD) and packing simulations provide further analysis of passivant densities and water interactions. We compared recent calculations of relative binding energies of passivants with calcium ion (gas-phase results) with the binding to the calcite surface. These results suggest there is a strong tendency toward dissolution for strongly sorbed anionic passivants.

Dissolution experiments using passivated calcite confirmed this trend.

We selected three candidate passivant molecules based on their likely bonding configurations with calcite: (1) silylaminocarboxylates (SAAC) with three carboxylate ligands, (2) silylphosphonates (SAP) with two strong P-O bonds, and (3) aminoethylaminopropylsilanes (AEAPS) with two N-based ligands. All three classes have a silanol tail that combines with the alkoxysilane consolidant (e.g., polymerized tetraethoxysilane [TEOS]) to provide mechanical and UV stability. We also evaluated novel epoxy functionalized passivant systems containing cationic photoinitiators, which polymerize the epoxy moieties using natural sunlight. We used treatment with commercial stone treatment products as a weathering benchmark.

Computer simulations suggest a binding order (strongest to weakest) of SAAC>SAP>TEOS>AEAPS. Calcite dissolution rate experiments show that the actual order of effectiveness is reversed from that predicted; i.e., AEAPS-treated samples showed low dissolution rate while SAAC-treated samples had high rates. The contradictory trend in dissolution rates suggests a threshold binding energy above which the passivant actually enhances the dissolution. Although the binding energy of AEAPS is less than that of SAAC and SAP, AEAPS binds strongly enough to reduce the dissolution of calcium when exposed to simulated acid rain conditions. All passivants exhibited even slower dissolution rates when linked to a consolidant layer. The AEAPS passivant in combination with a TEOS consolidant slowed the dissolution rate to 1/10 that of uncoated calcite. Even unoptimized, this combination coating was more effective than one common commercial consolidant (Conservare OH).

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3502.030

Catalytic Membrane Sensors

T. J. Boyle, R. C. Hughes, T. J. Gardner, A. G. Sault, C. J. Brinker

The goal of this project is to develop a catalytic membrane-based sensor (CMS) with enhanced sensitivity and specificity through modification of a Sandia-developed Pd/Ni-based hydrogen sensor. We will accomplish this through overlays of size-selective gas-separation membrane and an ion-exchangeable titanate catalyst. Our goal is to process these CMS elements into an array that utilizes different catalysts and membranes. This will enable us to significantly improve both the selectivity and the specificity via pattern-recognition (PR) methodologies.

We successfully accomplished a majority of the main objectives: (1) integration of the individual components of the CMS cell, which required (a) determination of the optimal processing temperature for the bottom sol-gel membrane, (b) generation of a surface acoustic-wave (SAW) device, (c) characterization of the activity and selectivity of these various Rh/HTO (rhodium/hydrous titania oxide) catalysts to determine whether the catalysts prepared via the double alkoxide route behave differently from Rh/HTO materials prepared via the standard TIPT/NaOH/MeOH process, and (d) optimization of the coatings of active catalysts in conjunction with membrane coatings, (2) optimization of the fabrication of the CMS cell, (3) successful demonstration of the prototype CMS cell, and (4) the combination of two CMS cells.

We optimized the most important aspect of this project—processing the bottom membrane. Some unusual properties that we discovered after introducing this membrane were (1) enhanced oxygen detection (allows for explosive-gas detection), and (2) poison resistance (simple, fast coating). We also showed the NaTi(OR)_5 double alkoxide layer to be modified by ion exchange to form a RhTi(OR)_5 complex. Based on analysis it appears this simple double alkoxide behaves in an analogous manner as the standard HTO precursor; we are investigating it as the starting solution for SAW devices. We successfully added the ion-exchanged catalyst layer on top of the $\text{A2}^{**}/\text{Ti}$ modified layer and found it to be compatible with the sensor.

Currently we are adding the top sandwich layer to generate the first CMS. We will test this for separation of different-sized molecules. We are investigating new bottom sol-gel layers to determine their effects on the sensor. We are generating new catalyst layers that utilize RhTi alkoxides to reduce the

amount of processing by eliminating the ion-exchange step. We will compare these to existing catalysts and also investigate integration of the various CMS cells.

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Photonic Bandgap Structures as a Gateway to Nano-Photonics

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The goal of this project is to explore the fundamental physics of a new class of photonic materials, photonic bandgap (PBG) structures, and to exploit their unique properties for the design and implementation of photonic devices on a nanometer-length scale for the control and confinement of light. The low-loss, highly reflective, and quantum interference nature of a PBG material makes it one of the most promising candidates for realizing an extremely high-Q resonant cavity, >100,000, for optoelectronic applications, and for the exploration of novel photonic physics, such as photonic localization, tunneling, and modification of spontaneous emission rate. Moreover, the PBG concept affords us with a new opportunity to design and tailor photonic properties in very much the same way we manipulate, or bandgap engineer, electronic properties through modern epitaxy.

We successfully demonstrated one of the world's first PBG lasers at $\lambda=920\text{--}930\text{ nm}$. The design uses higher-order bandgap, which allows us to use a much bigger post diameter $d=250\text{ nm}$. We observed lasing in the light-current curve. Thus, our data are more convincing than those from a leading research university. Our next effort is to optimize photonic lattice structure design, shorten cavity length, and invoke antireflection coating to bring down lasing threshold to the $\sim\text{mW}$ range.

We successfully fabricated both PBG-resonant cavity and 90-degree waveguide bend structure at 1.3- μm spectral regime. We achieved a state-of-the-art aspect ratio, 1:15, for the posts (diameter $d=220\text{ nm}$ and height $h=3200\text{ nm}$). We used a new coupling scheme that allows single-mode waveguiding for a deep-etch, 3- μm structure. This approach simplified our process steps because only one reactive ion-beam etch

(RIE) is required rather than two. The deep-etched waveguide structure is essential since it ensures that light is well collimated as it comes out of the waveguide, and thus less leaky when it passes through the photonic lattice. Also, in our design, we used two bends so we can measure reflection in a transmission setup. Experimental testing is under progress using the Idler signal, which is tunable from 900 nm–1800 nm, from a Coherent Optical Parametric Amplifier laser system in our laboratory.

We designed a new 2-D honeycomb lattice that poses higher-order bandgap and has a complete bandgap. Since it is a 2-D dielectric lattice instead of a 2-D hole lattice, fabrication is relatively easier. It has a gap size of $\sim 10\%$, which corresponds to a very wide bandwidth of 90 nm and should act as a good reflecting mirror. To take initiative to be ahead of the rest of the world in PBG research, we started working on 3-D photonic lattice. We chose the so-called 3-D layer-by-layer structure as it fits to Sandia's strength in nanofabrication and planarization. On the theoretical side, we established a collaboration with the inventor of the structure.

In the millimeter-wave regime, we also designed, built, and tested a 45-degree-bend beam splitter. We showed that the PBG beam splitter is highly efficient, $> 95\%$, and its splitting angle is much larger than the conventional angles of 5–10 degrees.

We can claim success with one of the most challenging problems of the past 10 years in the field of PBG research.

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Wide-Bandgap Compound Semiconductors to Enable Novel Semiconductor Devices

M. H. Crawford, A. F. Wright, E. D. Jones, S. R. Lee, J. Han, E. J. Heller, W. W. Chow

Sandia proposes an interdisciplinary investigation into the growth and physical properties of wide-bandgap compound semiconductors for the purpose of enabling both optoelectronic and microelectronic device development. The AlGaInN material system is widely considered to be essential to the development of a wide array of ultraviolet (UV) and blue optical devices as well as high-temperature microelectronics. A critical limiting factor in the demonstration of advanced III-N-based devices is the lack of an in-depth understanding of the physics and chemistry that govern the unique properties of these materials. The proposed work focuses on the investigation of the physical properties of the AlGaInN material system. Analytical investigations include calculations to determine bandstructure and development of a model for optical gain and lasing that will include an exact treatment of Coulomb effects. We will perform steady-state and time-resolved luminescence to evaluate the nature of defect states in these materials as well as to study the excitonic properties that we expect to be enhanced for wide-bandgap semiconductors. We will perform magnetoluminescence experiments to determine energy dispersion and effective masses and will directly compare these results with bandstructure calculations. A final aspect of our proposal is an evaluation of how various processing techniques that are relevant for device fabrication, such as post-growth annealing, reactive ion etching, and implantation, affect the optical and electronic properties of the III-N materials.

One milestone was to further expand our models of gain, absorption, and refractive index, and compare the results to experiments. Our approach, based on the Semiconductor Bloch equations with carrier correlations treated at the level of quantum kinetic theory in the Markovian limit, gives a consistent treatment of plasma and excitonic effects, both of which are important under lasing conditions. Also, as experimental optical

data suggested the importance of local fluctuations in the InGaN/AlGaIn heterostructure, we included inhomogeneous broadening due to spatial variations in the quantum-well (QW) thickness or composition in the theory by a statistical average of the homogeneously broadened spectra.

We satisfied one of our most critical milestones, to supply III-N materials for these experiments. We significantly modified our metalorganic vapor phase epitaxy (MOVPE) III-N growth reactor to expand our growth capabilities and grew a number of high-quality GaN and AlGaIn bulk films as well as InGaIn single QW structures. One of our experimental milestones involved performing pressure-dependent magneto-photoluminescence (PL) measurements on III-N materials to determine exciton binding energies and elucidate the nature of emission resonances. We performed low-temperature PL experiments on GaN bulk films, employing magnetic fields up to 30 tesla. The exciton energy shift in magnetic field can be related to the conduction-band/valence-band reduced mass μ by $E = 1/2R^*g^2$ where $R^* = me^4/2\hbar^2$ is the effective rydberg energy (exciton binding energy), m is the reduced mass, e is the dielectric constant, and $g = \hbar\omega_c/2R^*$ is the ratio of the cyclotron energy and the effective rydberg. For GaN, $R^* = 25$ meV and for 30 tesla, the cyclotron energy is thought to be near 5 meV. It was clear from these experiments, however, that higher magnetic fields than were accessible previously would be necessary to make a simultaneous determination of the exciton binding energy R^* and the reduced mass μ . We therefore scheduled time on the 60-tesla pulsed magnet.

Another experimental milestone involved performing time-resolved PL experiments on the III-N materials to evaluate radiative recombination mechanisms in these materials. Our experiments first required constructing a UV-visible time-resolved spectroscopy

setup including a picosecond Ti:Sapphire laser pumping a nonlinear conversion module, which enabled the spectral regions of 260–325 nm and 375–490 nm to be achieved from frequency tripling and doubling, respectively. We performed the experiments both at room temperature and at 10° K, with laser excitation at 280 nm and powers of 0.1–3 mW. One striking result is the significantly long decay of InGaIn alloys ($t = 600$ psec) versus the GaN bulk regions ($t = 60$ psec). These data support the hypothesis that local variations in the InGaIn QW result in localized excitons with substantially increased decay rates relative to free excitons (such as in the GaN bulk regions).

We examined plasma etch-induced damage in the III-N materials, and specifically how plasma etching under different conditions affects both the optical and electrical properties of the materials. We evaluated both inductively coupled plasma (ICP) and electron cyclotron resonance (ECR) plasma-induced damage of GaN. While the exact nature of surface oxides and surface states in GaN are not well understood, the data show that the PL efficiency can be strongly affected by exposure to an Ar plasma and is highly sensitive to the plasma conditions.

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Synthesis and Modeling of Field-Structured Anisotropic Composites

J. E. Martin, C. P. Tigges, R. A. Anderson

Sandia developed the computer modeling, synthesis, and processing capability to create novel anisotropic polymer/ceramic and polymer/metal composite materials by applying external electric or magnetic fields to systems consisting of a polymerizable continuous phase into which particles having an electric permittivity or magnetic permeability mismatch are suspended. A uniaxial field creates 1-D particle chains, a well-known effect, but we found that biaxial fields (e.g., rotating fields) create 2-D particle sheets in the plane of the field. We captured these structures by polymerizing the continuous phase during a field anneal. A key aspect of this program is the modeling of these structures, which allows accurate prediction of the resultant material properties and intelligent control of the evolution of structure in these materials.

We conducted computer simulations of the evolution of structure in a two-component fluid consisting of a liquid phase and a dispersed colloidal phase subjected to either uniaxial or biaxial fields. Our primary objective was to understand the mechanism and kinetics of coarsening and the emergence of crystallinity. Using an efficient, linear- N simulation method, we studied systems of $N=10,000$ particles over the concentration range of 10–50 vol%. We used a variety of methods to characterize the structures that emerge, including the anisotropy of the conductivity, capacitance and dipolar interaction energy, 2-D pair correlation, principal moments of the gyration tensor, velocity correlation functions, microcrystallinity and coordination number, and the optical attenuation length. We concluded that athermal coarsening is effectively driven by the

presence of defect structures and that as the concentration increases, the structures progressively lose the well-known "chain" anisotropy evinced at low concentration. The equilibrium phase in a uniaxial field is the *bct* lattice, but in the biaxial field case, we found that the equilibrium phase is the *fcc* lattice, though the *hcp* lattice is very close in energy.

We incorporated Brownian motion into the modeling to investigate the effect of simulated anneals, where the temperature is slowly quenched to zero, on the resultant material structures and anisotropy. We found that a linear temperature anneal, from above the melting temperature to absolute zero in 75 ms, gives structures that are dramatically different, containing a high degree of crystallinity, few defects, and large dielectric and optical anisotropies. This work shows that control of the quench path is an important factor in producing highly field-structured composites.

We developed a simulation of field-structured composites in shear and found a surprising effect. With a uniaxial field along the z -axis and shear flow along the x -axis, hexagonal plates spontaneously form in the x - z plane, i.e., orthogonal to the axis of fluid vorticity. These simulations also compute the fluid stress, and we find that the shear stress in a biaxial field is more than twice that expected for a uniaxial field. These findings indicate routes to improved fluid response.

Finally, a failure mechanism in neutron generators is dielectric breakdown through the filled encapsulant. To investigate whether field structuring can ameliorate this problem, we investigated the breakdown of field-structured composites of BaTiO_3 particles in a thermosetting resin. We were surprised to find that orthogonal to the field-cure axis, the dielectric breakdown strength is 50% greater than the unstructured sample—a significant increase. To understand the physics behind this, we developed a simple model of breakdown that maps the composite material onto a

resistor/superconductor network. This model does indeed show a 50% increase in the breakdown voltage, and shows that field structuring of encapsulants might address a leading problem in neutron-generator performance.

We investigated the phenomena of field-induced transparency in a sample of submicron-size magnetite particles. We suspended these particles in glycerin and placed them inside a solenoid. We illuminated the sample with a laser beam directed along the solenoid axis and applied a voltage to the sample, generating a magnetic field parallel to the beam. At low particle concentrations the transmitted light intensity grew by four decades in a short time. Viewed in an alternative way, the time dependence of the transmitted intensity allows us to probe fundamental aspects of the coarsening kinetics in field-structured composite

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Model Determination and Validation for Reactive Wetting Processes

F. G. Yost, E. J. O'Toole, P. A. Sackinger

Sandia showed that dissolutive wetting initially yields a metastable equilibrium. This report describes a compact model for the kinetics of approach to this metastable state. The technique for constructing these kinetics stems from the early work of Onsager and begins with a relationship for the entropy production. From this, we can write directly a coupled set of nonlinear, ordinary differential equations. We solved the equations numerically for the wetted area and compared them with experimental data. The model captures many of the subtle complexities of dissolutive wetting such as multiple metastable states.

We described thermodynamic equilibrium conditions for a spreading droplet that is simultaneously dissolving a solid substrate. We established the kinetic equations for wetting in the manner of Onsager. We solved these equations numerically and compared them with experimental data. We found that good agreement can be obtained by using this technique to describe wetting kinetics in the Sn-Bi on Bi system. We also found that time-varying quantities, such as atom fraction Bi dissolved in the liquid, converge to the values expected from the metastable equilibrium analysis.

Early in the dissolutive wetting process, the system follows a sequence of short-lived metastable states in which the Laplace equation for the liquid-vapor interface is the only requirement even close to being met. Under slow wetting conditions, the liquid surface is likely to be spherical, but the curvature of this interface will depend on the extent of dissolution. This work showed that long after wetting and spreading stop, the liquid-solid interface has still not reached equilibrium, judging from its nonspherical shape, even though substrate dissolution is sensibly complete. The Laplace requirement for this interface is not met, so the system is

metastable and will remain so for a long period of time. This period of time makes measurement of the equilibrium contact angle of this interface untenable and inefficient. We demonstrated that it may be possible to estimate the true equilibrium contact angle when dissolution is complete and the Laplace condition for the liquid-vapor interface is met. For the Bi-Sn system at 240°C, this angle is approximately 15°, and the solid-liquid surface tension is approximately 183 ergs/cm². We showed that the predicted equilibrium contact angle is relatively constant, as was the contact angle, over a wide range of alloy compositions. Although the drop diameter increased with increasing Sn content, it did so because the dissolution process made more fluid available. The equilibrium wetting configuration should be and was experimentally shown to be scale invariant.

The solid-vapor interface appeared to be flat in all of the experiments. We showed that gravitational forces are too small to cause any distortion of this interface near the wetting line. We found no significant wetting effect due to substrate grain size, and there did not appear to be any significant preferential dissolution at emerging grain boundaries. The wetting of single-crystal substrates appeared to be very similar to wetting of small-grained substrates. This behavior is certainly not to be expected in general, since evidence to the contrary has been reported in the literature for decades.

The classical approach to capillary problems ignores microstructure and defects. It contains the implicit assumption that all phases of the system are homogeneous and structureless, which, of course, bears no resemblance to reality except for systems that are totally liquid. Analysis of this wetting problem should consider, for example, grain boundaries in the substrate and reaction product phases in addition to phase interfaces. Such a structure is metastable and will evolve to equilibrium only after a very long period of time, if ever.

To investigate the atomic behavior of liquids at interfaces during wetting, we

simulated wetting in the Ag-Cu system using molecular dynamics (MD) with atomic potentials and observed both atomic dynamics and structural correlations at the liquid-solid interface. We found that spreading is prompted by interactions between the liquid and the substrate surface that cause the liquid layer in contact with the substrate to take on some of the symmetry of the substrate surface and result in the formation of a liquid monolayer that extends beyond the major part of the liquid droplet.

We also showed that, in certain systems, a region of high spatial correlation exists in the liquid near the solid-liquid interface. This correlated region is produced by mutual kinetic and potential interactions of the liquid and solid atoms. We found dislocations and other defects in this region that may influence wetting kinetics by allowing a mechanism for slip of liquid over the substrate near the wetting line. We derived a relationship for wetting rate and effective viscosity based on the existence of glissile dislocations. Careful study of the interfacial defects observed here may reveal important information on the nature of slip in wetting systems.

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Refereed

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Scanning Probe-Based Processes for Nanometer-Scale Device Fabrication

T. M. Mayer, S. A. Casalnuovo, J. A. Simmons

Development of nanometer-scale technologies requires a novel physics base that includes fabrication processes, characterization techniques, and materials properties allowing reliable performance of devices at this very small-length scale. This project's goal is to expand Sandia's expertise in scanning probe-based fabrication and characterization of nanostructures. Our objective is to achieve an order-of-magnitude decrease in feature size compared to conventional fabrication technology. This order-of-magnitude jump in our ability to make small structures opens new areas of fundamental physics research on the properties of mesoscopic structures, and enables new types of electronic and sensing devices with enhanced functionality, speed, and reliability. We are exploring approaches to nanostructure fabrication and characterization using scanning probe-based (scanning-tunneling microscopy [STM], atomic force microscopy [AFM]) methods. We also are developing numerical simulations of localized electric field and emission current to explore mechanisms and characterize limits to processing techniques. We emphasized novel fabrication processes and characterization of physical, chemical, and electronic effects in nanostructures. We will integrate critical nanoscale components with conventional test structures to allow full electrical accessibility. We investigated molecular layer resists based on simple adsorbed atoms and molecules that can be patterned by electron-induced desorption or reaction. We also are developing direct-write fabrication processes for nanoscale fabrication using electric fields and the low-energy electron flux from an STM to directly induce deposition processes leading to nanostructure formation. We will evaluate novel high-sensitivity chemical-sensor prototypes based on alteration of electrical properties of nanowires by adsorption or absorption of gases.

We concentrated on construction of a new STM nanofabrication facility and continued process development and refinement of simulations of scanning probe-based fabrication processes. We designed and constructed a new STM facility with several features specifically adapted to nanofabrication processes. The instrument incorporates an increased scan range and optical access to the tip region via a low-power microscope to facilitate alignment and connection of STM-fabricated features with existing structures and electrical bonding pads. Thermal management design features and kinematic sample mounting also allow variable temperature processing and reproducible sample placement. Construction of the instrument is complete; however, we are currently correcting several unanticipated design flaws. We continued our characterization of selective chemical vapor deposition (CVD) processes for nanostructure fabrication and investigated anodic oxidation by an AFM tip as an alternate nanoscale lithography. We adapted our nanofabrication simulation code to explore effects of electric fields, mechanical forces, and emission current-induced heating on surface modification processes in scanning probes. We showed that for a W tip interacting with a Au surface, surface diffusion of Au adatoms in a lateral electric-field gradient is responsible for formation of nanometer-scale bumps on the Au surface, suggesting another practical method for controlled fabrication of nanoscale structures.

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Ultra-Hard Multilayer Coatings

T. A. Friedmann, P. Provencio, P. B. Mirkarimi, D. L. Medlin, D. M. Follstaedt, J. A. Knapp, M. T. Dugger, K. F. McCarty, N. A. Missert

Sandia is exploring the production of ceramic multilayer structures that are potentially harder than any natural or artificial material. Diamond and cubic boron nitride (cBN) are the two hardest substances known to man. Numerous proven technologies rely on the superior mechanical properties of these materials. The question arises: Is it possible to manufacture a material that is harder than diamond? In theory, the answer is yes. Experiments indicate that properly grown multilayer coatings of two materials are harder than either of the materials making up the individual layers. The increase in hardness is due mainly to the resistance of dislocation flow across the interfaces between phases of different elasticity. This experimental fact leads to the possibility that a new class of ultra-hard materials—harder than diamond—can be made by growing the appropriate multilayer film.

We propose to establish the state-of-the-art in ultra-hard multilayers by synergistically merging Sandia capabilities. This work is a combination of growth, analysis, and theoretical modeling capabilities at Sandia that could possibly lead to a revolutionary jump in both materials understanding and performance—a material harder than diamond.

(1) We developed a new multilayer a-tC (amorphous tetrahedral carbon) material that is thick, stress-free, adherent, low friction, and with hardness and stiffness near that of diamond. The new a-tC material is deposited by pulsed-laser deposition (PLD) at room temperature, and fully stress-relieved by a short thermal anneal at 600°C. Repeated deposition and annealing steps build up a thick multilayer. We measured 88 GPa hardness, 1100 GPa Young's modulus, and 0.1 friction coefficient (under high load). Significantly, these results are all well within the range reported for crystalline diamond. However, this material has significant advantages over thin-film diamond: a-tC is smooth, processed at lower temperatures, and can be grown on a much broader range of

substrates. This breakthrough will enable a host of applications that we are actively pursuing in microelectromechanical systems (MEMs), sensors, LIGA (an acronym from German words for lithography, electroforming, and molding), etc.

(2) We drastically improved our cBN films grown by ion-assisted PLD (IAPLD). We combined x-ray reflectivity, Fourier transform infrared (FTIR), and transmission electron microscopy (TEM) characterization to optimize the IAPLD process to obtain films that have the bulk density of cBN (and presumably high hardness), a columnar grain structure with greatly reduced hBN inclusions and smooth surfaces. Thus, we are now ready to deposit by PLD multilayers of (arguably) the two hardest substances known to man—stress-relieved a-tC and cBN, due to breakthroughs directly resulting from this project.

(3) Another highlight of our efforts includes development of an electron cyclotron resonance (ECR) ion-assisted sputtering process for B4C that is compatible with our improved cBN deposition process developed in FY96. We are using this process to synthesize cBN/B4C multilayers.

(4) We vastly improved our finite-element modeling (FEM) techniques to extract yield, elastic stresses, and hardness from nanoindentation curves.

(5) We made progress in modeling dislocation sources and the role they play in pileups as a step toward modeling dislocations in multilayers.

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Molecular-Scale Lubricants for Micromachine Applications

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T. A. Michalske

The goal of this project is to develop the physics and chemistry base for designing and understanding molecular-scale lubricants for the reduction of friction- and adhesion-induced failure in silicon microelectromechanical systems (MEMS). Sandia acquired this new knowledge by tailoring the molecular properties of lubricants, applying local probes that can directly monitor the response of lubricants in contact conditions, and evaluating the performance of model lubricants in MEMS devices.

Model lubricants under investigation are the silane coupling agents that form monolayer films on native oxide silicon surfaces, which is the substrate in MEMS. These molecules bind via strong surface bonds and produce a layer of hydrocarbon or fluorocarbon chains normal to the substrate. "Tailoring" the lubricants entails modifying the chain length, the chain chemical reactivity (H or F), and the density of chain structures. Thus understanding the surface chemistry of silane-silicon oxide coupling is critical. With proximal probes such as atomic force microscopy (AFM), interfacial force microscopy (IFM), and scanning near-field optical microscopy (SNOM), we examined the frictional and adhesive properties of the silane films with very high spatial resolution (< 100 nm) and sensitivity. We treated MEMS structures with silanes under identical conditions and examined them for friction and adhesion under operating conditions. Proper assessment of the lubricants requires quantitative analysis of MEMS performance at high speeds and long operating times. Our proximal probe measurements and MEMS performance analyses form a very important link for molecular dynamics (MD) simulations that, in turn, should be able to predict MEMS performance under all conditions.

Our accomplishments for FY97

include the following:

(1) We showed the formation of uniform silane films to be directly linked to the presence of water in the chemical reactions.

(2) AFM data revealed that the initial friction force resisting motion on silane-covered silicon oxide is ten times smaller than that on the bare surface. Furthermore, silane-covered surfaces exhibit a reduction in friction force with repetitive tip contact.

(3) IFM data indicate that lubricant chain lengths of less than six carbons significantly increase the adhesive forces under contact conditions; i.e., the surface free energy increases significantly for short alkane chain lengths.

(4) With our SNOM, we demonstrated that shear forces experienced by the tip depend on chain length of the lubricants (consistent with the IFM data). We began work on correlating film fluorescence with tip/chain mechanical interactions.

(5) We developed an automated image acquisition and analysis system that provides very accurate position versus time data from MEMS operating at high speeds. It is now analyzing the operation of specially designed friction devices.

(6) We discovered residue on MEMS devices, demonstrated its removal, and identified its root causes.

(7) We finished the basic code development for massively parallel (MP) molecular dynamics (MD) simulations of the silane lubricants.

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Surface-Micromachined Flexural Plate Wave Device Integrated on Silicon

B. A. Tuttle, J. A. Ruffner, D. D. Chu, D. B. Dimos, J. H. Smith, G. C. Frye, K. W. Schubert

Small, reliable chemical sensors are needed for a wide range of applications, such as weapons state-of-health monitoring, nonproliferation activities, and manufacturing emission monitoring. Advantages of flexural plate wave (FPW) architecture include improved sensitivity, reduction in operating frequency to be compatible with standard digital microelectronics and sensitivity, and sensing in liquid media. Fabrication of these miniaturized, high-reliability devices requires successful execution and integration of three technologies: acoustic sensor design, Si surface micromachining, and high-quality piezoelectric thin-film deposition.

We successfully fabricated piezoelectric lead zirconate titanate (PZT) thin films on surface-micromachined FPW structures. Sandia's team made the first surface acoustic-wave (SAW) measurements at 100 MHz on a PZT thin-film-based device. Future work will include determination of piezoelectric coupling coefficients for SAW devices and acoustic characterization of PZT thin-film/poly Si and silicon nitride (SiN) membrane structures in the FPW mode.

We performed characterization of stress versus thermal history of PZT-based thin films using a laser reflectance technique. From these measurements, we selected PZT 40/60 films of 1.2-micrometer thickness annealed at 600°C as the baseline for FPW device fabrication because of the low mechanical stress in these films. We developed processing procedures for integration of PZT thin films with FPW devices by deposition of PZT films on both macro (1 cm x 2 mm) cantilever beams and bulk micromachined cantilever beams. Proper electrode design and PZT deposition techniques were essential for the fabrication of mechanically robust devices. We measured piezoelectric coefficients on the order of 50 pC/volt, approximately 100 times that of single-crystal GaAs and 15 times greater than lithium niobate. The Sandia

Microelectronics Development Laboratory completed two out of the eight planned lots of surface-micromachined Si wafers with FPW devices. We fabricated both silicon nitride and polysilicon membrane-based devices. We demonstrated that appropriately processed PZT films can be processed on the 1-micrometer-thick membrane structures without mechanical failure. Further, our team designed and fabricated masks for SAW devices based on PZT and aluminum nitride (AlN) thin films. From these masks, we measured the first acoustic response of PZT thin films at 68 MHz and 107 MHz. We developed a polling procedure to optimize the piezoelectric response from these films deposited on lanthanum aluminate substrates. We fabricated AlN films for both prototype SAW devices and in the form of macrocantilever beams. While the macrocantilever beams indicate that our highly (001) oriented AlN films have reasonable piezoelectric response, we determined that subtle process modifications alter domain configurations and that these modifications are critical to optimizing FPW device piezoelectric response.

Publications

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3502.130

Molecular Imprinting in Aerogels for Remote Sensing of Chemical Weapons and Pesticides

D. Y. Sasaki, J. S. Schoeniger, P. I. Pohl, A. J. Ricco, M. A. Butler, C. J. Brinker

Sandia generated synthetic receptors for phosphates and phosphonates in SiO₂ xerogels via a surface molecular imprinting method. We developed the guanidine monomer, 3-trimethoxysilylpropyl-1-guanidinium chloride (1), to prepare receptor sites capable of binding with substrates through a combination of ionic and hydrogen bond interactions. Structure characterization of the xerogels via ²⁹Si (material accountability system (MAS)), nuclear magnetic resonance (NMR), and N₂ BET (Brunauer Emmett-Teller) analyses finds a highly cross-linked material with high surface area and large pore volume that is largely unaffected by functionalization with (1). High-performance liquid chromatography (HPLC) studies and binding isotherms performed in water determined that molecular imprinting affords a significant improvement in phosphate and phosphonate affinity with about a twofold increase in binding constant over a randomly functionalized xerogel and about an order of magnitude higher affinity compared to analogous small molecule receptors found in the literature.

We showed through these initial studies that molecular receptor sites for phosphonates and phosphates can be prepared in sol-gel materials using a simple surface imprinting procedure with the guanidine monomer 3-trimethoxysilyl propyl-1-guanidinium chloride. The imprinting method does not explicitly provide size and shape imprinting in the matrix, which is a general feature of molecular imprinting. However, we chose

the method to be compatible with the sol-gel matrix, provide quantitative surface functionalization while maintaining high surface area and large pore size, and allow rapid equilibration of the receptor sites to solution. Affinities measured in aqueous solutions of phosphate and phenylphosphonic acid substrates to these imprinted xerogels are one to two orders of magnitude higher than analogous small molecule receptors, including pre-organized bis- and tris-guanidine receptors. The guanidine-phosphonate pairing on the gel surface shows evidence of contributions from both ionic and hydrogen bonding interactions in aqueous solution. Additionally, interfacial phenomena from the receptor residing on the gel surface appear to heighten binding affinity. We found the matrix to play a major role in the efficiency of the receptor site. The surface anionic charge of the silica gel may reduce binding affinity at pH > 2 and completely overwhelm the receptor site at pH 8 and above. We anticipate that by tailoring the matrix surface, we can improve the specificity of the receptors, which will result in highly efficient molecular recognition materials for aqueous systems.

Publications

Refereed

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Smart Interface Bonding Alloys (SIBA): Tailoring Thin-Film Mechanical Properties

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Sandia will explore the use of the newly discovered strain-stabilized 2-D interfacial alloys as smart interface bonding alloys (SIBA). We will use these materials as templates for the heteroepitaxial growth of metallic thin films. SIBAs are formed by two metallic components that mix at an interface to relieve strain and prevent dislocations from forming in subsequent thin-film growth. The composition of the SIBA is determined locally by the amount of strain, and therefore can react "smartly" to areas of the highest strain to relieve dislocations. In this way, we can use SIBA to tailor the dislocation structure of thin films.

This project will include growth, characterization, and modeling of films grown using SIBA templates. Characterization will include atomic imaging of the dislocations structure, measurement of the mechanical properties of the film using interfacial force microscopy (IFM) and nanoindenter, and measurement of the electronic structure of the SIBA with synchrotron photoemission. We will also examine resistance of films to sulfidation and oxidation. We will use the Paragon parallel processing computer to calculate the structure of the SIBA and thin films in order to develop the ability to predict and tailor SIBA and thin-film behavior.

This work will lead to the development of a new class of thin-film materials with properties tailored by varying the composition of the SIBA, serving as a buffer layer to relieve the strain between the substrate

and the thin film. Such films will have improved mechanical and corrosion resistance, allowing application as protective barriers for weapons applications. They will also exhibit enhanced electrical conductivity and reduced electromigration, making them particularly suitable for application as interconnects and other electronic needs.

In the first two years of the program, we successfully laid the groundwork, both experimental and theoretical, to test the effectiveness of SIBA materials in enhancing the mechanical properties of thin films. IFM is now at the stage where we can directly investigate the atomistic process of stiffness and plastic deformation. We developed and refined this with our studies of Au single-crystal surfaces. Simulations of these processes are now completely under way on the Paragon computer, and we are at the stage in which we can incorporate more complex structures, such as that of SIBA materials. We showed that SIBA materials do, in fact, inhibit dislocation formation as we originally predicted. With this groundwork, we are ready in the last year of our program to definitively test SIBA materials.

Our accomplishments in FY97 include the following:

- Measured IFM indentation curves for Au(111) and investigated role of surface steps.
- Developed and debugged indentation modeling code on Paragon computer.
- Developed an algorithm for automated identification of dislocations in complex structures.
- Modeled indentation on Au(111) and Au(100).
- Measured dislocation structure of Ag film grown on SIBA material.
- Measured stability of SIBA interface.

Publications

Refereed

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Understanding and Control of Energy Transfer Mechanisms in Optical Ceramics

J. C. Barbour, D. M. Follstaedt, J. A. Knapp, M. B. Sinclair, D. R. Jennison, B. G. Potter, Jr.

Sandia developed a new material strategy for rare-earth (RE) hosts. In this approach, we modified the optical performance of the dopant through atomic-level engineering of its local structural environment in a nanocomposite, optical ceramic host material. To this end, we experimentally manipulated and theoretically modeled the local environment of RE ions in multiphase, multicomponent composites produced in thin-film form. These efforts will lead to a greater understanding of RE/host interactions for improved luminescence efficiency and lifetimes in this important new class of photonic materials and will provide a means to control dopant optical behavior previously unattainable using conventional single-phase ceramics. The versatility of this strategy will allow next-generation optical components with even more stringent operational requirements to be attained, e.g., blue light sources for high-density optical data storage and compact, integrable optical amplifier elements. We employed both direct optical evaluation of the dopant behavior and theoretical structural modeling and simulation to evaluate these novel host materials. We successfully modeled the local atomic structure in the vicinity of RE dopants using a powerful Sandia-developed

QUEST computational approach based on local density functional theory. In alumina, we will extend this technique to model the difference in tetrahedral versus octahedral site symmetry on the density of electronic and vibrational states, and for the first time it will allow the investigation of a variety of dopant site types characteristic of multiphase hosts (e.g., interfaces and clusters).

We examined RE optical behavior in various single- and two-phase hosts. High-index, alumina thin films are of current interest as active and passive waveguide materials for high-area-density integrated photonic devices. We produced alumina thin films using an electron-cyclotron-resonance (ECR) plasma and pulsed laser deposition (PLD). These techniques provide a process for simultaneous RE doping during film synthesis. We used the results of temperature-dependent, laser-excited photoluminescence (PL) measurements to monitor the impact of host-phase structure on the RE optical behavior in both ion-implanted bulk material and *in situ* doped thin films. We evaluated these findings in the context of preliminary molecular dynamics/crystal field (MD/CF) analyses of Er-doped alpha and gamma alumina. We used the effects of low-energy ions from a biased ECR plasma during growth of alumina and La_2O_3 to modify the density and crystalline quality of these oxide films. We varied the type of phase formed for alumina with the ion-assisted growth from amorphous to crystalline gamma alumina. We examined the PL properties of different Er-doped Al- and La-oxide phases and, through comparison of the

PL spectra, discussed the local environment of Er in these oxide materials. We also made two-phase materials with alumina as the matrix and RE-doped zirconia-tellurite glass (ZTG) using PLD and examined the PL properties in the same manner as that for the pure RE-doped alumina films. These PLD samples proved the original hypothesis that a greater luminescence efficiency could be achieved as a result of modifying the local environment of the RE ion. That is, the RE ion contained in the ZTG was more efficient than that in the alumina alone, and this enhanced efficiency was maintained when we embedded clusters of the doped ZTG in the alumina matrix.

Publications

Refereed

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Integrated Thin-Film Structures for IR Imaging

J. A. Ruffner, P. G. Clem, R. D. Nasby, R. W. Schwartz, W. L. Warren, B. A. Tuttle, C. J. Brinker

Sandia successfully integrated a thermally insulating silica aerogel thin film into a new uncooled monolithic thin-film infrared (IR) imaging device. Compared to other technologies (e.g., microbridge), use of an aerogel layer provides superior thermal isolation of the pyroelectric imaging element from the relatively massive heat-sinking integrated circuit (IC). This results in significantly higher thermal and temporal resolutions. In addition, use of aerogels results in an easier, less expensive fabrication process and a more robust device.

We developed and refined a number of deposition processes including ambient-temperature/-pressure sol-gel deposition of the aerogel, sputter deposition of the electrodes, and solution chemistry deposition of the lead lanthanum zirconate titanate (PLZT) imaging elements for fabrication of these monolithic devices. We achieved uniform pyroelectric response across the devices by use of appropriate planarization techniques involving the aerogel, electrode, and imaging element layers. In addition, we characterized the individual layers and monolithic structure using scanning electron microscopy (SEM), atomic force microscopy (AFM), thermal conductivity measurements, and Byer-Roundy techniques.

In our integrated uncooled IR sensor projects in FY97, our most important achievements were (1) development of methods to deposit and measure the pyroelectric response of monolithic PLZT devices, (2) determination of the effect of anneal temperatures and stress on pyroelectric response, (3) development of a multiple-layer, solution chemistry

deposition technique to produce low-stress, thick pyroelectric imaging elements, (4) modification of an ambient-pressure/-temperature aerogel deposition process to optimize porosity and thickness while providing a smoother, more homogeneous surface for subsequent electrode deposition, (5) measurement of the thermal conductivity of aerogels used in these devices (results pending), (6) development of a deposition technique for lead scandium tantalate (PST) imaging element using solution chemistry techniques, and (7) submission of a U.S. patent application on the technology developed under this project.

Overall, this project was a great success because our team built a monolithic thin-film structure for uncooled IR imaging on an aerogel insulation layer for the first time. The noise-equivalent temperature difference for our monolithic devices was typically 0.05° – 0.10° C for f/1.0 optics and a thermal conductance of 5×10^8 W/K. This represents twice the signal-to-noise ratio available from competing technology. In addition, we anticipate the use of aerogels as the scratch protection layer in the final integrated device to provide thermal isolation in the lateral directions, resulting in an even higher signal-to-noise ratio.

Publications

Refereed

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Recognizing Atoms in Atomically Engineered Nanostructures: An Interdisciplinary Approach

A. M. Bouchard, K. M. Horn, J. S. Nelson,
R. M. Biefeld

Scanning-tunneling microscopy (STM) is a powerful tool for both characterizing and manipulating the atomic topographies of surfaces. However, STM has typically been unable to provide unambiguous chemical recognition of atomic sites in many technologically relevant, but chemically heterogeneous, systems. Sandia will develop the theoretical and experimental underpinnings necessary to enable unambiguous, computer-based identification of atomic sites in multivariate STM imagery, focusing on heterogeneous III-V semiconductor materials and atomically engineered nanostructures. The project will have several subtasks: (1) develop the first "database" of multivariate STM spectral features, (2) study the effects of different tip states on the STM spectral features and attempt to establish procedures for computationally removing or minimizing variable-tip effects, and (3) use pattern recognition (PR) of STM spectral imagery, based on the results of tasks (1) and (2), to map out the atomic-scale chemical structure of selected cleaved (110) III-V surfaces. We will specifically attempt to understand the alloy ordering and interfacial structure of III-V structures of current programmatic interest for IR device applications.

We demonstrated the capability to unequivocally distinguish elemental

species on, and in, an atomic surface, the ability to discern different bonding configurations of a given species, and the ability to image foreign atoms in the substrate surface. Furthermore, classed images depicted clear distinctions between regions of differing electronic structure that are indistinguishable in the corresponding topograph, and conversely, identified similar electronic structure among features that appear dissimilar on the basis of the topograph alone.

In this last year we focused on the use of Sandia's STM facilities to collect multispectral data from a variety of Group IV surfaces and to classify this data. In this way, we achieved a very tight "feedback loop" between STM experiment and classification that permitted us to examine and understand a number of basic issues concerning the effect of experimental parameters on the subsequent classification; this information will have direct impact on the classification of III-V multispectral data.

On the Sandia STM system, we examined and classified intrinsic defects in Si(001), Si-deposited Si(001), Ge-deposited Si(001), Si/Ge-deposited Si(001), and highly B-doped Si(001). We showed classed images of a kink in a Si(001) step edge, vacancies and c-defects in Si(001) surfaces, and 0.1 ml Ge-deposited Si(001) surfaces, to cleanly discriminate between surface features that are often, at best, indistinct in the topograph. Adatoms exhibiting motion on the surface (such as rotating dimers) have classed as distinctly different structures from their stationary counterparts—reflecting this technique's ability to distinguish different bonding conditions. Features hidden, or only vaguely

represented, in the topographic images of many surfaces were clearly revealed in the classed image. Thus, the application of the visually empirical region of influence (VERI) clustering algorithm to the analysis of multispectral STM data succeeded in exemplary fashion for all Group IV systems examined.

We transferred two sets of Sandia-fabricated III-V samples to our university collaborators for multispectral imaging in their recently completed low-temperature STM. These samples span a range of designs and include InAs/InAsSb quantum wells, InGaAs/InAsSb superlattices, and layered InGaAs/InAs samples. The layer thickness and periodicity of each sample was characterized with x-ray diffraction. We chose these samples to provide a variety of binary/ternary mixtures, as well as varying the Group V (anion) and Group III (cation) elements, to give a broad representation of the types of intermixing that might be encountered. We anticipated the multispectral data to be ready for classification at Sandia at the end of the summer. A third STM system with cleaving capabilities, five deposition sources, replaceable STM tip, and tip-conditioning capabilities, and if necessary, a field ion microscope for *in situ* tip characterization were to become operational in the fall for use in III-V measurements.

We completed first-principles, plane-wave electronic structure calculations for a selection of Si(001) surface structures, including the idealized, relaxed 2x1 surface, dimer vacancies on that surface, and Ge dimers in the surface layer of Si(001). We calculated the local density of states for each system and are formatting them for image classification to facilitate comparison to experiment.

Modeling Electrodeposition for Metal Microdevice Fabrication

S. K. Griffiths, R. W. Bradshaw, W. D. Bonivert, R. H. Nilson

LIGA, an acronym from the German words for lithography, electroforming, and molding, is a promising new process for producing metal microdevices having micron-to-millimeter features. Currently under worldwide development, this process offers a means to manufacture high-resolution, high-aspect-ratio devices including microscale valves, motors, solenoid actuators, and gear trains. Most research in LIGA has focused on the lithography process used to produce LIGA molds. Filling these molds by electrodeposition has received much less attention, despite several serious problems. Device-scale voids in the deposited metal occur frequently and often without apparent cause. These problems are likely due to the depletion of metal ions and the accumulation of hydrogen in the stagnant layer between the top and bottom of the mold. The presence of this diffusion layer distinguishes LIGA electrodeposition from traditional electroplating and electroforming processes.

To help understand and optimize the electroforming portion of the LIGA process, Sandia is developing a 1-D numerical model describing the electrodeposition of metal into high-aspect-ratio molds having lateral dimensions on the micron scale. To guide model development, and later to validate this model, we are also conducting a series of 1-D and 2-D laboratory experiments.

We developed a 1-D model describing the quasi-steady electric field and multispecies ion transport within the LIGA mold. This model includes the eight ion species important to the deposition of nickel or iron alone, and to the co-deposition of nickel-iron alloys. We obtained electric potentials by solving an elliptic field equation, taking into account variations in electrolyte conductivity with ion concentration. We incorporated the kinetics of the electrode reactions through Butler-Volmer equations relating current density to electrode polarization. We computed metal ion and hydrogen concentrations by solving a multicompo-

nent system of implicitly coupled, quasi-steady conservation equations describing simultaneous transport and reaction of ions diffusing from the bath to the deposition surface.

We also designed and built a laboratory apparatus for simulating LIGA electrodeposition in deep molds having high-aspect ratios. Experiments performed over a range of total currents show a strong influence of the current on the morphology of deposited metals.

We compared calculated currents and deposition rates with the measured values over a range of mold depths, mold aspect ratios, bath chemistries, and electrode potentials. These comparisons show that natural convection plays an extremely important role in plating high-aspect-ratio molds, even when feature sizes are very small.

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3502.190

The Initiation and Propagation of Nanoscale Cracks at an Adhesive/Solid Interface

M. S. Kent, M. J. Stevens, E. Reedy, Jr.

Sandia is investigating submicron debonding processes at polymer/solid interfaces with a combination of continuum stress analysis, molecular dynamics (MD) simulations, and a new experimental approach. Each component of this program is designed to provide complementary information with the goal of bridging the gap between molecular and continuum descriptions. Our objective is a validated, molecular-to-continuum fracture theory. Despite significant progress made in recent years in the fields of fracture mechanics and adhesion science, it is still not possible to predict the lifetime of a polymer/solid interface from

first principles. On the continuum level, we made considerable headway in an interfacial fracture mechanics approach for preexisting macroscopic cracks between linear elastic materials. Little is known, however, about modeling cracks on a micron or submicron level, how microcracks develop into macroscopic cracks, or about length-scale limitations on the use of a continuum analysis. Furthermore, there is an interphase region with property gradients between the two bulk materials. The effect of interphase structure and molecular properties on fracture mechanics parameters, needed for a fundamental understanding of failure criteria, is unknown. On the molecular scale, much is known about polymer dynamics, the origin of viscoelastic behavior and relaxation phenomena, and the behavior of polymers near surfaces. Yet it is not clear how stress concentrations develop on a molecular scale in an imperfect thermoset polymer, or how nanoscale inhomogeneities grow into microcracks under stress. An understanding of the link between the molecular and the continuum levels is required before the goal of a truly comprehensive model of fracture can be approached.

We used neutron reflection to probe *in situ* the degradation of interface structure in model epoxy/silicon samples subjected to a cyclic stress. We obtained quantitative information regarding the density and crosslink density of the epoxy within 5-2000³ of the substrate surface as a function of cure temperature, strength of bonding to the surface, and number of stress cycles. For most of the work thus far, the stress has been imposed by thermal cycling (a very low-frequency deformation, ~ 3 hours per cycle). We also initiated a study of mechanical methods for imposing the stress field. In particular, we prepared double-beam samples using beams cut from polished silicon wafers. We subjected these samples to a three-point bend deformation. Such a method will allow us to explore a larger range of frequency and strain amplitude than can be achieved by thermal cycling.

We developed an MD code to produce a (glassy) network polymer between two parallel plates. This geometry allows various stress fields to be imposed (tensile and/or shear). The network is formed by creating a melt of

linear chains and then allowing them to crosslink. To accomplish this, we added bond creation as a dynamical feature to the code. We realized early in the year that special attention to network formation is essential to accurately capture the stress localization and energy dissipation mechanisms that lead to molecular-level chain scission events. We also added bond breaking for the crack initiation simulations.

We carried out detailed finite-element (FE) stress analyses for the micron-length scales of our test geometry (a 2-micron-thick epoxy film cast on a relatively thick silicon substrate). We determined the variation of energy release rate and mode mixity with interfacial crack length and film thickness for a variety of thermal and mechanical loadings. We developed a temperature, strain rate, and hydrostatic pressure-dependent constitutive relation for the epoxy so we can model the highly nonlinear, time-dependent, yield-like behavior found within the fracture process zone. We are now assessing this initial material model and refining it as further test data become available. In collaborative work with the University of Arizona, we measured epoxy yield strength data for strain rates varying from 1E5-s to 1E3-s. An extensive suite of epoxy characterization tests currently being conducted at Sandia will soon be completed.

To couple the MD simulations and the continuum stress analysis, we use a continuum mechanics analysis to calculate the stress field for a small enough length scale (~ 1 micron) that it can be used as a boundary condition for the MD simulation. An important first point of contact is the comparison of stress-strain curves. We accomplished an initial comparison, and further work is in progress.

To make contact with experiment, we compared the structure obtained in the MD simulation (density and crosslink density variations) qualitatively with that resulting from the neutron reflection experiments (obtained in 1-D only, normal to the interface) before cyclic loading. The main result of the experiments is the observation of an elevated density and a decreased crosslink density within ~ 20° of the interface. Direct quantitative comparison with the structure of the network in the simulation

requires an accurate simulation of the crosslinking process.

We developed a test of mechanical strength for the thin-film test geometry. We applied self-assembling monolayers (SAMs) to the bare silicon prior to coating with epoxy in order to vary the number of bonding sites per area. We measured adhesive strength for a wide range of SAM densities.

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3502.210

Monolithic Structures for Nanoseparation

T. J. Shepodd, A. Martino, M. E. Warren, D. S. Anex

Miniaturization in detection and separation technologies requires easily built, rugged devices based on materials that have well-understood interactions with analytes at the molecular level. The goals of this project are to design such materials for state-of-the-art separation science, understand their structure/function relationships, and fabricate them into useful devices. Sandia is utilizing their expertise in the synthesis of micro- and nanoporous materials to develop continuous, high-surface-area polymers as

monolithic nanoporous supports for ultra-efficient separations. We evaluated these materials using capillary electrochromatography (CEC) as a test-bed. We will quantify the interaction of functionalized surfaces of these supports with analytes, propelled by the electroosmotic flow (EOF), in terms of separation efficiency and selectivity. Our goal is to engineer an open and interconnected network where every nanopore functions as a CEC column. The ideal pore-size range (for EOF-supporting materials) is in the 0.5–10-micron size range. Inverse emulsion technology produces open-celled continuous structures in this size range and is amenable to different chemistries to introduce functionalities and selectivities. We will integrate these new solid supports, which are cast as fluids and cured to monolithic polymer structures, into micromachined grooves as pre-prototype devices for ultra-efficient separations.

Our work in the project will make a dramatic impact on the understanding of analyte/support interactions as influenced by engineered materials. Besides impacting Sandia's proven expertise in capillary electrophoresis (CE) and CEC, the rugged pre-prototypes that we construct will demonstrate applicability to all areas of chromatography and, correspondingly, to the sensors and devices that take advantage of separation science.

We successfully designed and synthesized monolithic polymer supports that function as CEC columns. We demonstrated that these columns support EOF and showed baseline separation of analytes in simple chromatography experiments. We developed efficient synthetic routes to organic and inorganic monolithic supports. We discovered a way to use inverse emulsion polymerization to simultaneously create the chromatography medium, the species to support EOF, and the bonds connecting the support to the substrate (capillaries in these studies). Thus we avoid time-consuming and logistically difficult surface modification chemistry. Our first-generation supports demonstrate modest efficiencies, but the results of our initial experiments suggest new synthesis schemes. We synthesized a second generation of supports for immediate testing. We are preparing a patent technical advance to protect the intellectual property associated with this project.

Fundamental Aspects of Micromachine Reliability

M. P. De Boer, J. M. Redmond, M. R. Tabbara, T. M. Mayer, J. J. Sniegowski

A fundamental basis for designing micromechanical devices with high-yield, reliable performance and long life is lacking. Mechanical design tools for macroscale machines relate reliability to inertial forces. However, the performance of micron-scale structures of high-aspect ratio is dominated by surface forces. The technical goal of this project is to use experimental reliability results obtained directly from micromachined test structures to develop and verify mechanics models containing interaction terms appropriate to the micron scale (e.g., capillarity, van der Waals forces, electrostatics, etc.). Issues to be addressed include auto-adhesion (stiction), friction, and wear. Beginning with auto-adhesion, Sandia will design and build microbridge structures with varying geometry and surface properties (roughness, chemical coatings, etc.). We will monitor deformations by interferometry in an environmental chamber. We will develop finite-element (FE) models incorporating new surface elements and verify and refine them by comparing against experimental results. Next we will investigate friction and wear using smart micromachined structures that enable self-diagnosis by electrical monitoring of capacitance and Q-factor changes. We will also explore optical detection technique. We will verify dynamical response models incorporating internal friction terms as well as damping and will refine them using experimental results. We will then extract friction due to energy loss at rubbing surfaces.

This project will develop a new tool set based on an experimental and theoretical foundation. We will use the tool set to calculate and characterize reliability of micromachines for integrated microsystem applications.

(1) *Designed and fabricated a test chip incorporating auto-adhesion and friction structures.* We completed fabrication of the test chip. We showed most test structures to work; a few had design errors that we will correct in a new design, and some structures are still being tested (friction, fracture). Parts successfully fabricated include single- and double-cantilever beam structures that we used to measure mechanical properties such as Young's modulus, strain gradient, and residual tension. The devices are electrically connected by a narrow poly fuse so they can be operated in unison, which makes testing more efficient. However, the fuse can be blown to obtain isolated device data. We also used the beam devices to measure auto-adhesion of beams with various coatings in controlled relative humidity (RH) environments from 0% to 87% RH.

(2) *Built an environmental chamber to apply electrostatic forces and monitor deflections by interferometry; measured adhesion lengths for various RHs and surface properties.* We built an automated environmental interferometric microprobe station as schematically represented. We demonstrated that the method would give 10-nm z-deflection resolution (out of plane). We used this to quantify deflections of adhered beams. Measurements and analytical modeling led us to realize that a beam adhered over a long length gave an improved fracture mechanics situation compared to a beam adhered only at its tip. A linescan from the interferometric image is deconvolved by a program to obtain z-deflection versus x-position data. We can obtain an adhesion measurement from a single beam. This improves over the previous method of finding the shortest adhered beam for two reasons. First, it is an equilibrium fracture situation in which beam mechanics apply. It is doubtful that beam mechanics apply to the shortest-beam adhered beam, as only one or two asperities are in contact. Second, each adhered beam gives a measure of adhesion, which takes up much less area than the array of beams required in the previous method.

Confident that we had an improved adhesion measurement method, we proceeded to seal the system using a latex seal around the interferometric attachment. We also automated the testing and image taken with LabView. Finally, we added a simple humidified nitrogen gas delivery system and interfaced a humidity meter to the test apparatus. We also made progress in automatically analyzing the data, although work remains in this area. Preliminary data show a very interesting result—beams coated with a highly hydrophobic coating of FDTS (a perfluorinated molecule) remain adhered at 90% humidity. We will explore this important result in more detail in the coming months.

(3) *Simulated theoretical behavior of beam deflections subject to electrostatic, capillary, van der Waals, and adhesive forces; compared to measured adhesion lengths.* As an example of our modeling/experimental synchronization, we brought a beam 600 μm long into contact with the substrate by electrostatic forces. As we increased voltage, the beam continuously pulled in. To model the problem, an iterative approach is required because deformations affect forces that in turn affect deformations. We obtained close agreement between experiment and theory (lines) by assuming an insulator thickness of 14 nm.

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Enabling Science and Technology for Cold-Spray Direct Fabrication

M. F. Smith, J. E. Brockmann, R. C. Dykhuizen, R. A. Neiser, Jr.

Cold-spray processing (CSP) is a recently discovered, poorly understood, Russian coating technology that can rapidly deposit (mm/sec) metals, polymers, and composites at temperatures < 200°C by accelerating powder particles up to 600–1000 m/s in a supersonic compressed gas jet. Sandia envisions a radical new direct fabrication technology in which we combine a highly focused CSP particle beam with a robotic motion system to spray-fabricate a single- or multimaterial component directly from a computer model. Compared to alternative processes, because CSP particles are never melted, superior surface finishes, microstructures, and properties might be achieved (finer grain size, no brittle phases, minimal oxidation, less residual stress, etc.). With CSP, one might also deposit functionally graded or layered materials at low temperatures, thus eliminating joining operations, simplifying design/fabrication,

reducing part counts, and decreasing stress cracking. CSP may also be a cost-effective green alternative to electroplating, soldering, and painting. A primary technical barrier to cold-spray direct fabrication (CSDF) is focusing the particle stream. Theory indicates major technical challenges. But a recently developed, noncontact particle stream-focusing technique known as an aerodynamic lens might provide a solution. This technique, originally developed with submicron particles at low pressures, shows promise for focusing larger particles at higher pressures. In our first year, we modeled the focusing process, established a new cold-spray capability, and successfully demonstrated a basic degree of aerodynamic focusing. We are currently one of only two labs in the U.S. with cold-spray capability, and in this first project year, we have already begun to attract interest from both government and industrial customers.

In the first nine months of this project, we computationally modeled gas and particle flows in single-stage aerodynamic lens systems. We then designed and built an experimental lens system. Next, we brought a basic cold-spray capability on-line and, for the first time ever, we experimentally demonstrated that aerodynamic focusing works for large particles (up to 60 microns) in

subsonic flows at pressures above one atmosphere. This major technical breakthrough may be a key enabling technology for CSDF. It is also a scientific breakthrough since no one has previously demonstrated that aerodynamic focusing works for large particles at high pressures. With the single-stage lens experiments, we reduced a 1-cm flow width to a collimated beam approximately 5 mm in diameter. We believe even smaller particle beams are possible with multistage lens designs. Our new cold-spray capability has already attracted funding from two external sources.

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Atomic-Level Studies of Surfactant-Directed Materials Growth

P. J. Feibelman, J. C. Hamilton, N. C. Bartelt, J. A. Floro, G. L. Kellogg, B. S. Swartzentruber

Sandia identified a pre-nucleation arrangement of Ge adatoms on Si(001), at low T and very low coverage, characterized by a significant buckling of the substrate dimers; these Ge-induced chain structures are likely precursors to formation of stable Ge islands. Using our new low-energy electron microscopy (LEEM), we discovered a dramatic effect of (B) on step motion on Si(001), and lesser effects of O: B causes the rough SB-steps on the Si(001) surface to facet into triangles, which then evolve into stripes spanning the terraces between the SA-steps. We developed a simulation tool to interpret our LEEM observations and used it to explain the modifications in step structure induced by B. Using multiple optical beam stress sensor (MOSS) and various microscopies, we evaluated stress effects in island formation on SiGe alloys, both qualitatively and quantitatively. We discovered theoretically that H stabilizes reconstructions on all Al surfaces, leading to faceting and rough H-covered Al surfaces, and that H adsorption changes both Al diffusion mechanisms and rates on Al surfaces. Experimentally, we discovered that chemisorbed H can increase the hopping self-diffusion rate, on Rh surfaces, by orders of magnitude, depending on coverage. For Pt on Pt(001), we found that H can change the diffusion mechanism from substitutional to hopping. We computed diffusion barriers for Pt at clean Pt steps, proving that concerted interlayer transport dominates at low temperatures. We developed a qualitative understanding of O-adatom bonding to Pt and a heuristic picture of how the O surfactant effect on Pt(111) growth may work. Via simulations for Si(001) we showed that hopping over an edge and substitutional exchange can lead to very different surface morphology evolution; we thus inferred the interlayer diffusion mechanism for Si/Si(001) from LEEM observations. To model film growth realistically, we developed a way to derive

the parameters of a 2-D Frenkel-Kontorova model from arbitrarily realistic interatom force laws.

(1) Scanning-tunneling microscopy (STM) revealed low T and coverage, pre-nucleation arrangement of Ge on Si(001), with significant buckling of the substrate dimers that form chains. We developed a model for atom arrangement: paired monomers between substrate rows—likely precursors of stable Ge islands.

(2) With LEEM, we saw B and O effect on step motion on Si(001). B facets rough SB-steps into triangles. They evolve into terrace-spanning stripes. 1-D roughening explains measured changes of step stiffness versus T , angle of the triangular-shaped facets, aspect ratio of elliptical islands. O affects step motion, but less. Larger O-effect, stressed-Si(001) surfaces return to domains of equal area upon exposure to O_2 , which is evidence for O-induced stress relief.

(3) MOSS with *ex situ* imaging shows no big difference in Si-Ge alloy surface morphological evolution versus strain. $Si_{0.8}Ge_{0.2}/Si(001)$ (strain = 0.8%) and $Ge/Si(001)$ (strain = 4.0%) evolve similarly, except island length scales differ by an order of magnitude. Both systems first grow layer-by-layer, then transition to 501-faceted islands that relax 20% of the stress.

(4) We developed an interpretation of observations of surfactant-modified step motion. We applied it to step-structure changes caused by B-segregation to Si(001). LEEM shows B-induced faceting begins with big random thermal fluctuations. Simulations show facets form because segregation lowers step energy in one orientation. We concluded that step-faceting is likely needed to understand surfactants.

(5) We did total energy calculations to explain detrimental effect of H in Al epitaxy. We were surprised to find that H stabilizes reconstructions on all Al surfaces. H reduces surface vacancy and adatom formation energies and makes steps favorable. This leads to faceting and rough H-covered Al surfaces. Important feedback was that extra roughness slows Al diffusion, producing yet rougher growth morphologies. We found that H sits on top of adatoms with mobility change depending on valence and coordination. Too, H suppresses

exchange diffusion, and thus, intermixing in heteroepitaxy.

(6) We studied H-influence on diffusion on metals with field ion microscopy (FIM). We found that it depends on diffusion mechanism. On Rh, ad-H increases rate up to several orders of magnitude, depending on coverage; thus we can use H to control diffusion. For Pt/Pt(001), H slows diffusion. More importantly, H can suppress substitutional displacements on Pt(001) enough that hopping becomes energetically accessible. Thus ad-H controls both adatom displacement rate and transport mechanism.

(7) We computed Pt-diffusion on flat Pt(111) terraces and at type-B steps of Pt(221); 0.33 eV hop-barrier on flat terrace is in reasonable agreement with 0.26 eV of FIM data. At B-steps, results prove concerted interlayer transport dominates at low T ; barrier for exchange is 0.30 eV, and 0.57 eV for hopping. We discovered "frustration" that repels ad-O from quasi-*hcp* sites and explains O's location on surfaces vicinal to Pt(111). To explain why experiments show ad-O weakens surface Pt-Pt bonds, we calculated O-induced stress; results agree with observation. We also completed simulations showing for steps on Si(001) that hopping over an edge and substitutional exchange can lead to very different time evolutions of surface morphology. Comparing simulations to LEEM observations of step motion on Si(001), we showed that Si adatoms are ~ 40 times likelier to descend a step edge without being incorporated than with. This "permeability" is a necessary starting point to learn how surfactants modify step-edge barriers to diffusing Si adatoms.

(8) We developed a 2-D Frenkel-Kontorova model with few Fourier components, adatom-substrate interaction and two adatom interactions from embedded atom method (EAM) calculations of dislocation structure energies. We used it to compute prefactors and activation energies in excellent agreement with full 3-D calculations. Thus, we can use this method with first-principles calculations to allow accurate treatment of many surfactant effects.

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3502.250

Intelligent Polymers for Nanodevice Performance Control

G. M. Jamison, J. A. Shelnutt, R. J. Martinez, R. S. Saunders, D. R. Wheeler, D. A. Loy

The purpose of this project is to develop organic materials systems that can be predictably manipulated to alter the fundamental optical, electrical, and rheological properties of the materials. Molecular modeling of a family of metal porphyrin-terminated polyenes provided theoretical insight into the steric consequences of attaching olefins to the pyrrole rings of the porphyrin ligand; these results will aid in determining the spatial extent of the electronic interaction between two porphyrin chromophores through a conjugated polyene.

The first thermal cycloadducts derived from addition of dienophiles to quadricyclane yielded azo-bridged ring opening metathesis polymerization (ROMP) monomers, which we took on to the first macromolecules bearing a substituted azo bridge; we are evaluating the polymers, which are characteristically monodisperse, for thermal and/or chemical susceptibility to form diazo derivatives as potential polyacetylene precursors. Other work toward polyconjugated systems includes the development of a new family of bidentate ligands and new electrophilic catalysts derived from chelation of the ligands to Group VI metal alkylidenes.

We demonstrated thermal sensitivity in carbonate-bridged polysiloxanes. High-molecular-weight materials undergo thermal depolymerization with the liberation of CO₂ and hydroxy-terminated nonvolatile residues. Trace acid can direct the thermolysis products to a single, recyclable oligomer.

We demonstrated photolytically initiated depolymerization of acid-sensitive polyacetals using sub-stoichiometric amounts of photoacid generator additives. We are evaluating this chemical amplification approach for its applicability to base-sensitive polymer systems as well.

Research in intelligent polymers for nanodevice performance control has been productive beyond expectations in modeling, and especially in synthesis of

smart materials systems and their utility in stimulating customer interest. These polymeric systems feature thermally-, redox-, or photochemically sensitive functionalities, which alter the rheological, chemical constitution, or electrical properties of the system. We incorporated sensitive groups covalently and as sub-stoichiometric additives. Computer modeling techniques are guiding the design of these systems for selection of suitable sensitive residues per their thermodynamic, optical, or redox characteristics.

Chemical amplification. We successfully demonstrated the photocatalytic initiation of acid-sensitive polyphthalaldehyde depolymerization by photoexcited organic nitrates in the presence of a photoacid generator source. The production of large numbers of monomer molecules for each original analyte molecule will result in the chemical amplification of the analyte signal. We showed that a dilute solution of TNT reacts with benzyl tosylate under ultraviolet (UV) irradiation; this liberates tosic acid, which initiates depolymerization of dissolved polyphthalaldehyde as determined by spectroscopic and chromatographic means.

Further, we synthesized polychloral as a representative base-sensitive polymer; we showed it to be susceptible to violent base-initiated depolymerization with sub-stoichiometric amounts of organic bases (very strong exotherm, with partial vaporization of monomeric chloral, a powerful anesthetic/sedative). We invested a wealth of effort in identifying photobase generators with sensitivities suitable for light-initiated polychloral degradation. A lack of sensitivity with known (2-nitrobenzyl)carbamate esters led to the preparation of novel nitrated carbamates, whose light sensitivity is under evaluation.

Molecular modeling. The molecular modeling component of the project initially focused on potential organic conductors whose properties can be manipulated by their redox characteristics. Modeling these systems, as opposed to the thermal properties of diazo-containing sites, will allow us to investigate intelligent photo-, thermal-, and redox-controlled manipulation of organic systems.

One type of polymer of interest combines a conducting polymer with a photoactive redox center. We are using molecular simulation to design such a light-responsive polymer using photoactive metal porphyrins linked by polyacetylene (PA). PA serves as an initial model for computer simulations of other, more interesting polymers. All-carbon conjugated systems with an increased degree of 2-D structure should offer the best prospect of maintaining interesting electrical and optical properties.

As a first step in the computer design of light-responsive polymers, we are investigating the molecular and electronic structure of metal porphyrin linked by PA segments of varying length. We designed our initial calculations to determine the spatial extent of the electronic interaction between two porphyrin chromophores through a conjugated polymer linker. Toward this end, we computationally examined the conformational properties of a series of polymers in which two nickel(II)-porphine molecules are linked by polyacetylene (PA) molecules of differing lengths and conformations. We showed this year that nickel porphine is a planar molecule. However, we find that attaching a vinyl group destabilized the porphyrin macrocycle enough to cause a significant out-of-plane deformation (ruffling angles), which is affected by the spatial proximity of the other Ni-porphine within the same molecule. For two or more bridging ethylene groups, the deformation of the porphyrins is nearly constant.

PA precursors. We prepared soluble, electrically insulating precursors to conductive PA and characterized them for baseline thermal studies. These include both feast-like PA prepolymers and soluble polysulfoxides.

Publications

Refereed

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3502.270

Quantum Dot Arrays

J. E. Martin, D. R. Jennison, M. T. Anderson, P. Provencio, J. P. Wilcoxon, R. A. Anderson

The goals of Sandia's research are to investigate methods of forming quantum dot arrays (QDAs)—superlattices of nanoclusters—and to understand the properties of these novel materials. It is well known that nanoclusters have many unusual properties, including anomalous optical properties, size-dependent bandgaps, high catalytic activity, low melting temperature, anomalous magnetic properties, etc. However, the formation of cluster-based materials requires that these nanoclusters be isolated in a matrix to prevent the spontaneous sintering of clusters to form a bulk material. This can be accomplished by forming these clusters into periodic arrays where clusters are separated by an isolating matrix. These periodic arrays may exhibit coherent effects, or may simply be efficiently close-packed materials.

We synthesized narrow dispersity nanoclusters using the Sandia-patented inverse micellar synthesis method to form "quantum dots" with novel properties, including large catalytic activity, room-temperature photoluminescence (PL), size-dependent bandgaps, etc. We then stabilized these nanoclusters with a variety of hydrophobic and hydrophilic capping ligands and quantitatively extracted the nonionic surfactant used in the synthesis, along with residual ions, to form highly purified and extremely stable solutions of quantum dots. We then found appropriate conditions for the crystallization of these nanocrystals to form superlattices in the form of large twinned crystals, the so-called QDAs. X-ray diffraction measurements and transmission electron microscopy (TEM) show that these 3-D QDAs consist of 42³ particles with an 18³-thick isolating layer. In a parallel effort, we inserted hydrophobically capped nanoclusters into micelles of a quaternary ammonium surfactant with a cosurfactant. Adding a silica source and reaction catalyst should then incorporate these clusters into a mesoporous structure.

Freeforming of Ceramics and Composites from Colloidal Slurries

J. Cesarano, III, M. L. Griffith, R. P. Schunk, L. D. Harwell, D. J. Schmitt

Sandia proposed to develop a model-based direct freeform fabrication technique for ceramic, metal, or graded composite components. These components are fabricated by computer-controlled dispensing of colloidal suspensions through an orifice. Any conceivable 2-D pattern may be "written" layer by layer into a 3-D shape. Our goal is to develop model-based processing rules that will aid in the development of slurries with the appropriate rheology, density, and drying kinetics to ensure process success for a variety of ceramics and composites. Software and equipment development is also essential for precise control of layer thickness and feature resolution.

Development of this technique into a manufacturing process requires computer simulations of the relevant physical phenomena, materials expertise for tailoring colloidal slurry properties and processing dissimilar materials, software and equipment expertise for computer-aided design (CAD) model conversion, and robotics expertise for process optimization and incorporation of knowledge-based processing capabilities with closed-loop, sensor-based control.

We developed a new technique for freeform fabrication of ceramics. It provides near-net-shape fabrication of components with simple or complex shapes. The technique, called *robocasting*, uses robotics for computer-controlled extrusion of ceramic slurries through an orifice. We deposit the ceramic slurries in sequential layers. Any conceivable 2-D pattern may be "written" layer by layer into a 3-D shape. Orifices range from tenths of a millimeter to over one millimeter. The slurries are typically aqueous-based with ceramic loadings of

40–65% vol. and organic contents less than 2%. Robocasting is analogous to slip casting and gel casting; however, robocasting is moldless, and fabrication times are quicker. To maintain structural integrity while building a component, robocasting relies on the rheology of the extruded slurry and on drying of the individual layers. In contrast, gel casting and other freeform fabrication techniques require organic polymerization reactions or solidification of a polymeric melt to maintain the shape of components. Since the organic content of fabricated components is so low, direct-casted parts can be fabricated, dried, and sintered to complete density in less than 24 hours.

To control the shape of dispensed beads, the slurry rheology must be extremely pseudoplastic so that the material can flow smoothly during dispensing but then solidify in place once shear stresses are removed (similar to paint). If the slurry is too fluid, beads will spread uncontrollably. If the slurry is too viscous, beads lie down like rope and maintain rounded tops. When the proper rheology is obtained, beads yield nearly rectangular cross-sections with relatively straight walls and flattened tops. Perfectly rectangular cross-sections would be optimal for filling space when additional layers are sequentially dispensed.

Models that we developed to study the progression of bead shape with time as a function of viscosity and drying rate also show that close to rectangular cross-sections may be obtained when the properties are properly tailored. Controlled drying between subsequent layer deposition is important for the minimization of cracking and warping. Under optimal drying conditions, the moisture content of a previously deposited bead is low enough to induce the permeation of fluid into its structure from a wet, freshly dispensed bead. The fluid transport naturally drags some powder particles with it and creates a finite interpenetrated region between the two beads

that is free of defects or delaminations. If the drying rate is too fast, warping, cracking, and delamination may occur. When the drying rate is too slow, the built-up weight from several layers can induce slumping and the creation of nonuniform walls.

In summary, we demonstrated robocasting for making intricate aluminum oxide bodies that sinter into relatively strong, dense, defect-free parts. Upon drying, the consolidated densities of aluminum oxide bodies are routinely greater than 60%. Upon sintering, crack-free components have sintered densities greater than 95%. Components may be fabricated into bulk solids with large thicknesses unobtainable using slip casting, or into thin-walled pieces made with aspect ratios greater than 20 and wall thicknesses less than 1 mm. Also, we designed, fabricated, and assembled a platform and five-axis workcell capable of multimaterial deposition.

Publications

Refereed

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Other

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3502.280

Laser-Assisted Arc Welding for Aluminum Alloys

P. W. Fuerschbach, F. M. Hooper

A strong need exists in the defense programs and the automotive, aerospace, and transportation industries for a rapid, robust, high-quality process for welding aluminum alloys, especially for relatively thin-gauge product. While laser beam welding is widely applied in these industries, it has not proved valuable for aluminum because of problems with reflectivity and weld joint variability. Sandia intends to develop a new welding process by combining a fiber-optic-delivered materials-processing laser with a small arc-welding heat source. The new laser-assisted arc-welding (LAAW) process will couple the process advantages of the two heat sources and will also enable process capabilities never before envisioned in arc welding. The project is a System of Laboratories (SOL) collaboration among Oak Ridge National Laboratory (ORNL), Idaho National Electrical Engineering Laboratory (INEEL), and Sandia. The team combines their welding expertise to develop the scientific understanding and engineering methods required for the novel process. We anticipate that the team established through this SOL interaction will allow the U.S. to successfully compete with international entities in developing (and hence owning) advanced joining technologies for commercially critical markets.

Sandia's efforts in laser-assisted arc welding this year centered on developing an end-effector to collocate a high-current tungsten arc and a focused pulsed Nd:YAG laser beam. We fabricated a

hollow tungsten electrode and transmitted and focused the laser beam just below the tip of the electrode. Initial weld trials on aluminum alloys revealed that the arc could be consistently started by the transmission of the laser beam through a hollow tungsten electrode. Subsequent welds with the combined process also revealed that solidification cracking in the aluminum alloys was eliminated by the addition of the continuous-power arc to the pulsed-laser beam. The hybrid process was successful in removing the tenacious surface oxide on aluminum without the aid of reverse polarity. These experiments also indicated that the hollow electrode would quickly become contaminated with aluminum vapor. We started a redesign and reconstruction of the end-effector to shield the tungsten from the laser keyhole vapor by directing an internal flow of inert gas around the electrode. We recently tested this design in the laboratory, and it appears to be successful in preventing electrode contamination. We achieved broad welds with enhanced weld penetration as anticipated.

Several collaborative technical exchanges between the SOL participants have taken place. ORNL furnished both Sandia and INEEL with two automotive aluminum alloys for testing. Sandia pulsed-Nd:YAG laser-welded these materials with a matrix of process conditions.

Publications

Other

Fuerschbach, P. W., and F. M. Hooper. 1997. "Laser-Assisted Non-Consumable Arc-Welding Process Development." Paper to be presented to the 79th Annual AWS Welding Convention, Detroit, MI, 27 April 1998. SAND97-2015C.

System Studies in Electrochemical Processing

J. W. Braithwaite, R. G. Buchheit

Corrosion is the leading material degradation mode observed in the nuclear weapons stockpile. Sandia established this project to gain a better understanding of some important electrochemical aspects of two distinct and relevant degradation modes: environmentally assisted cracking (EAC) of aluminum alloys and corrosion in moist salt. The specific tasks addressed the effect of aluminum microstructural variability on the susceptibility to EAC and the development of experimental and analytical techniques that can be used to identify the processes that most influence the corrosivity of moist salt mixtures. These capabilities and understanding then form part of the basis needed to ultimately predict component reliability and/or possibly to identify techniques that could be useful for controlling corrosion in critical weapon components. We formulated a physical model and related understanding for the relevant degradation processes. The principal result was the identification of a reasonable set of experiments we can perform to characterize the potential corrosivity of moist salt mixtures.

The first task in this project involved studying the role microstructural and environmental interactions have on EAC of engineering aluminum alloys, specifically Al2024 (aluminum alloy 2024). Work focused on advancing two particular technical aspects: (1) identification of the key interactions and (2) determination of microstructurally-based anodic dissolution mechanisms.

We used standard electrochemical techniques (i.e., electrochemical impedance spectroscopy and potentiodynamic/static polarization) as the principal experimental control and analysis methodologies. That is, we identified the

behavior of the key microstructural elements involved in the cracking process and controlled it using electrochemistry. We conducted stress corrosion cracking tests under fixed displacement conditions using specially designed stressing jigs.

Because the objective of this task involved characterization of EAC response, the cracking experiments focused on electrochemical conditions (applied potentials) under which rapid cracking might be expected—that is, those environments where localized attack occurs at grain boundaries that are populated with precipitates of a particular second phase along with an associated Cu-depleted zone. We performed two sets of potentiostatic exposures: (1) at a value more positive than the breakaway potential of second-phase precipitate, but more negative than the breakaway pitting potential for both the Cu-depleted zone and the matrix phase, and (2) same as Set 1 except that we increased the potential to a value more positive than the breakaway potential for the Cu-depleted zone.

None of the samples in Set 1 exhibited evidence of corrosion or mechanically failed during the five-day stress exposure period, and we identified no evidence of any loss of mechanical properties. Conversely, in all of the Set 2 samples, relatively large amounts of electrochemical corrosion damage occurred, and the samples mechanically failed during the five-day exposure period. Fractographic analysis indicated that severe intergranular and secondary cracking had occurred. These results provide a correlation between the microstructural variations and their role in the susceptibility of Al2024 to EAC.

In the second project task, we designed methodologies and qualitatively validated them for determining the corrosivity of salt mixtures. Dry oxidation

of most engineering metals at or near ambient temperatures is a very slow process. For the degradation rate to become appreciable, an aqueous or adsorbed water phase along with an effective oxidant is required. Their presence enables classical electrochemical processes to become functional. Then, depending on the extent of the moisture, its physical nature, and the existence of other contributors (such as agents that destroy passivating layers), corrosion can proceed at measurable rates.

We used simple hydration/dehydration experiments with selected salt materials to determine how any water present in the system would distribute. We showed aqueous DC polarization techniques to be an effective way to quickly identify the role of the nonaqueous constituents in the corrosion process (e.g., passivating agents, oxidants). However, the absolute rate of steel corrosion in the salt compositions studied is relatively low. As such, we will require long-term exposure to actual conditions to characterize and then validate the response. A positive feature in this regard is that the apparent activation energy for this process is much higher than occurs in aqueous systems. As such, temperature could be an effective age accelerant.

Publications

Other

Braithwaite, J. W., and R. G. Buchheit. 1997. "Aspects of Two Corrosion Processes Relevant to Military Hardware." Sandia Technical Report SAND97-2899, October. Sandia National Laboratories, Albuquerque, NM.

C

omputer Sciences projects improve high-performance computing and develop simulation technologies that work on systems levels.

Computer Sciences consists of three research areas: (1) developing technologies that address key science and engineering challenges related to

massively parallel computing, algorithms, systems software, virtual environments, and advanced simulations; (2) advancing the modeling, analysis, and control of complex systems; and (3) developing revolutionary ideas in computational and computer sciences and mathematics.

Projects that address the DOE Accelerated Strategic Computing Initiative are an important area of emphasis. Defense, energy, and environmental remediation projects are also pursued.

Researchers are developing computer codes that can construct realistic, three-dimensional models of physical environments. Sandia's scannerless range imager furnishes the data for these models. Invented and patented at Sandia, the imager is a unique camera system that provides distance- and reflected-light intensity to each pixel in a field of view. Computer images of terrain are developed from camera data. Terrain images could facilitate remote security systems, plan clandestine activities, and rapidly assess hazardous environments.

Data transfer to and from disks as well as data storage and networking lag behind the computational power of massively parallel computers. Scientists are developing new tools and codes to allow these important resources to work more efficiently. A new code will permit massively parallel computers to solve more complex problems faster than they did before. This work supports the DOE Accelerated Strategic Computing Initiative and will have impact on all massively parallel computing.

A laser radar measures a calibration target from a distance of 500 meters. Aboard an unmanned spacecraft, this technology could enable the craft computer to autonomously search for an acceptable site and execute a landing.

COMPUTER SCIENCES

Parallel Quantum Chemistry for Material Aging and Synthesis

C. F. Melius, E. J. Friedman-Hill, E. T. Seidl, J. L. Durant, Jr.

Massively parallel (MP) computers offer the promise of predicting the aging of materials and optimizing the synthesis of new materials. Sandia is developing a new hybrid quantum chemistry procedure for accurately calculating the thermochemical properties of these materials. The procedure incorporates a combination of density-functional-based methods (DFT) and Hartree-Fock-based methods (HF, MP2) using various basis sets for each calculational step. We are implementing the methods to run on MP machines as well as on distributed shared-memory machines. This effort will provide the computational quantum chemistry methods necessary to treat chemical degradation processes occurring during the aging of the nuclear stockpile, including polymers, energetic materials, adhesion, and corrosion. It will also aid in the processing of new materials, such as semiconductors, protective coatings, and ceramics. The thermochemis-

try will also aid in other areas, such as demilitarization, environmental cleanup, and waste minimization.

The objective in the second year of this project was to develop the formal procedure for determining the thermochemical heats of formation using bond-additivity corrections (BACs), incorporate these procedures into an object-oriented chemistry database, demonstrate the procedure for a large molecule on the MP machine, and modify the MP quantum chemistry code (MPQC) to treat open-shell molecules at the MP2 level of theory. We developed a procedure that involves performing a geometry optimization of the molecule using a hybrid Hartree-Fock/Density Functional Theory (HF/DFT) quantum chemistry method using a split-valence basis set with polarization functions on nonhydrogen atoms followed by a frequency calculation using the same method and basis set. We then performed single-point energy calculations at the Möller-Plesset second-order perturbation theory level using a triple-zeta basis set with diffuse functions and multiple polarization functions. In addition, we carried out another single-point HF/DFT energy calculation using

the same large basis set. We then processed these electronic energies through a BAC procedure to correct for the systematic omissions to the electron correlation energy. We modified the BAC procedure to include both atom-based and molecule-based correction terms in addition to the bond-based terms. To demonstrate the usefulness of the ASCI (Accelerated Strategic Computing Initiative)-red machine, we performed an 1123 primitive basis function/834 contracted basis function MP2 calculation on the energetic material PETN ($\text{C}(\text{CH}_2\text{ONO}_2)_4$). This calculation represents the key single-step energy calculation in the new BAC procedure.

Publications

Refereed

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Modeling Complex Turbulent Chemically Reacting Flows on Massively Parallel Supercomputers

J. N. Shadid, S. P. Burns, A. R. Kerstein,
R. C. Schmidt, R. J. Cochran, K. D.
Devine

This project is to develop a massively parallel (MP), adaptive, unstructured finite-element (FE) code for simulating 3-D high-Reynolds-number (HRN) and turbulent chemically reacting flows in complex geometries. Important applications of such flows include the "crash-and-burn scenario" for safety calculations for nuclear weapons transport and storage (Accelerated Strategic Computing Initiative [ASCI]-related); jet-mixed chemical reactor design; high-performance compact heat exchanger design for aircraft, automobiles, and chemical process plants; and high-temperature combustion process modeling for the destruction of hazardous waste. Currently, these large, multiple length- and time-scale problems can be solved only in 2-D for a limited number of species due to the required computational resources. These difficult problems strongly couple turbulent momentum, thermal energy, and mass transfer with chemical reaction kinetics, making current 2-D models unsuitable. The simulation code is constructed on the foundation of an existing, successful, 3-D MP chemically reacting flow simulation code (MPSalsa). We will add state-of-the-art engineering models for reaction kinetics in turbulent flow, thermal radiation in participating media, and advanced turbulence models for fluid flow and heat and mass transfer to MPSalsa. We will also add MP adaptive mesh methods, dynamic load-balancing techniques, high-order convection stabilization methods, and subgrid turbulent reaction models to enable the sharp resolution of steep gradients and multiple length scales in the flow. With the proposed

code development, MPSalsa will be capable of solving very large strongly coupled multiphysics turbulence problems with multiple time and length scales. This tool will be immediately useful for Sandia's weapons program responsibilities (ASCI) as well as many advanced engineering technology problems for U.S. industry.

In the second year of this three-year project, we accomplished the following:

- (1) The full implementation of the two-equation (k- ϵ) model in both a HRN and low-Reynolds-number (LRN) form.
- (2) The full implementation of the Spalart-Almaras turbulence model. This is a robust one-equation (RANS)-type turbulence model comparable to a LRN k- ϵ model but having better numerical properties.
- (3) Benchmark studies on two important turbulent internal flow problems (turbulent channel flow and turbulent flow over a backward-facing step). The results show agreement between our implementation, previous numerical studies, and experiments.
- (4) The successful implementation of a low-order-species mixing model.
- (5) The initial implementation of a large eddy simulation turbulence model.
- (6) The completion of an initial participating media radiation library (SYRINX) based on the discrete ordinate method.
- (7) The implementation of the underlying dynamic data structures for mesh adaptivity and dynamic load balancing.
- (8) The selection of a turbulent non-premixed flame and a coupled fluid-flow-participating media radiation benchmark problem.

Publications

Refereed

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Scalability of Cryptographic Algorithms and Protocols

K. S. McCurley, P. S. Gemmell, Y. Frankel, S. V. Spires

The goal of this two-year project is to research and develop techniques for encryption and authentication that maintain system efficiency in the case where one or more system parameters increase. Some such parameters are the numbers of signers and verifiers in authentication systems, the number of shareholders in threshold protocols, and the accuracy that needs to be given to signed information.

(1) *Approximate authentication and biometrics.* We investigated the area of approximate authentication. In this model, signatures applied to a piece of data should verify for that data as well as other data that are in some sense "close" to the original piece of data. Put another way, signatures are applied to and are valid for sets of data. Because the original signed data might be any of the possible data elements in a set, the signature must somehow reflect the whole set given only one (or possibly several) set elements. This aspect of the research involved varying techniques from the theory of error correcting codes and probability theory. One application area is that of the authentication of biometric (inherently

approximate) data. In this application, an individual might carry with him or her a digital signature based upon the set that corresponds to his or her biometric data (such as retinal scan or fingerprint). That signature must be recognized as valid by verifiers who need to ascertain either the identity or authorization privileges of the individual.

(2) *Proactive RSA function sharing.*

We developed new techniques for scaling proactive RSA function-sharing protocols as the number of shareholders increases.

(3) *Shared RSA key generation.* We investigated the area of shared RSA key generation. It is devoted to making robust the protocols of Boneh and Franklin that allow for distrusting parties to generate an RSA modulus N and a public key e . The improvements to shared key generation made under the scalable cryptography project are to make the Boneh-Franklin protocols robust in the presence of anonymous Byzantine shareholders whose goal is to prevent surreptitiously the proper creation of the shared key. The new protocols use cryptographic program-checking techniques to reveal such cheating shareholders.

(4) *Scalable authentication and heterogeneous certification.* New scalable authentication techniques for time-varying data were developed that potentially may have great impact on the areas of Internet certification, electronic commerce, and database security.

Developers investigated efficient, flexible, multi-authority certification systems, cryptographic tools that enable two otherwise unacquainted parties on the Internet to establish the trust needed for business and/or personal transactions.

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Computer-Designed Molecular Memory and Switching Elements

J. A. Shelnutt, C. M. Rohlfing, D. J. Hobbs

Sandia's goal is to develop the computational methods necessary to engineer photophysical properties of molecules for optical-switching and memory applications, with the primary purpose of developing the basic physical and chemical understanding. Specifically, we are developing electronic structure and molecular dynamics (MD) calculations needed for modeling these complex systems. We are also extending massively parallel (MP) quantum and classical molecular modeling methods and using them to tailor the magnetic, optical, and/or structural properties of materials for molecular-scale memory devices. By using conformational trapping mechanisms and by modifying the structure of the organic part of the molecules, we are controlling to an unprecedented degree the photophysical properties (e.g., state lifetimes, magnetic and optical properties) of a class of organometallic compounds. We are synthesizing some of the designed molecules and characterizing their optical and magnetic properties for validation of the theoretical predictions. We are using MP computational methods to develop materials for nanoscale optoelectronic device applications. We identified nanoscale bioelectronic devices as having the highest value and probability of success for both near-term and future commercial and defense needs. These materials offer significant advantages in access speed, radiation hardness, and weight relative to metallic systems for emerging ultra-high-density memory technologies. Primary interest is for applications in monolithic optoelectronic integration, sensor fusion, molecular architectures for bio-optics, optical-switching windows, optical communications, and computing. High-information-density devices offer opportunities for quantum improvements in information storage.

The need for high-density data storage is growing, and memory materials that are size-scalable to the molecular level provide a promising solution. For a molecular-scale optical memory device, the optical material must (1) possess

distinct "on" and "off" states, (2) possess states that can be set and read optically, and (3) provide precisely accessible small-area/-volume elements. We computer-designed and synthesized a porphyrin, nickel(II) tetra(tert-butyl)porphyrin (NiTtBuP) that has these photodynamic properties. This new class of optical-storage materials enables a variety of ultra-high-density, ultra-fast, radiation-damage-resistant devices. Besides memory applications, the materials have uses as fast optical switches for Q-switching, cavity dumping, and mode locking/intercavity modulation for vertical-cavity surface-emitting laser (VCSEL) technology. This diverse range of applications results from the ultra-fast optical-switching properties and wide variability of the switched-state lifetime ($> 10^{12}$).

We completed a computational investigation of NiTtBuP using molecular simulations and found that it has the required optical properties for many optical-switching applications. The work focused on designing the optical media by using electronic structure and molecular mechanics calculations. We also successfully synthesized NiTtBuP and characterized the optical properties of the new molecule to validate the simulation results. We verified the proposed conformational trapping mechanism by which the optical media functions. The experimental results are promising enough to warrant a strong development effort aimed at creating a prototype optical storage device using NiTtBuP. We also computer-designed several new optical media (and next-generation analogs) and made significant progress in their synthesis. The results already obtained strongly point to the possibility of optical materials with greatly enhanced properties. Specifically, orders-of-magnitude increases in memory retention times, ultra-high densities (Terabits/cm² or Exabit/cm³), ultra-fast switching (< 10 ps), and parallel access are all enabled by the new optical media.

We completed the calculations for electronic and vibrational energies of NiTtBuP to improve classical mechanics. We established the mechanism of NiTtBuP photophysical behavior using temperature-dependent, time-resolved absorption spectroscopy. These experi-

mental results suggested new candidate materials. We computer-modeled these and synthesized one new memory molecule. We performed QUEST calculations of metal interactions in metal-porphine crystals. We calculated structures and energies of new candidates and determined which would be synthesized.

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Refereed

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3504.060

A Massively Parallel Sparse Eigensolver for Structural Dynamics Finite Element

G. M. Reese, D. M. Day, J. R. Red-Horse, R. S. Tuminaro

This project focuses on the development of a massively parallel (MP) eigensolver for structural dynamics analysis. Solving large-scale Accelerated Strategic Computing Initiative (ASCI) problems, however, requires not only parallelization techniques, but also the replacement of the traditional direct linear solver (used within the eigencode) by an iterative technique.

Within this project, Sandia successfully developed an initial version of an MP structural dynamics eigensolver code. This new code fundamentally advances Sandia's structural dynamics eigenvalue capabilities by allowing us to solve systems that are an order-of-magnitude greater than previously possible.

In this last year, we propose to improve the robustness of the iterative solver so it can be applied to more complex structural dynamics problems (e.g., different types of elements, floating substructures, and constraints). Additionally, we will solve much larger systems by reducing memory usage and computation time within certain key kernels.

A major stumbling block in developing a large sparse eigencode is the linear systems solver. Direct methods are traditionally used for structural dynamics problems, but for applications with over one million unknowns, e.g., ASCI, direct linear system solvers are not at all viable. Unfortunately, the application of iterative solvers to structural dynamics problems is nontrivial due to severe ill-conditioning. In fact, standard iterative techniques usually do not converge at all.

We implemented one of the most promising iterative techniques for solving structural dynamics systems. This

method, finite-element tearing and interconnecting (FETI), uses a very sophisticated coarse grid preconditioner to overcome the notorious ill-conditioning problems. We implemented an initial version of the solver on both the Intel Paragon and TFLOP machines. We devoted a substantial part of this effort to the algorithmic improvement of a number of key FETI subtasks. That is, the overall performance/robustness of the method depends fairly heavily on the quality of a number of nontrivial kernels. For example, we significantly accelerated the preconditioning of the FETI equations by incorporating scaling techniques that properly weight different constraint equations used within the algorithm. We also implemented a parallel sparse coarse grid linear solver based on the conjugate gradient (CG) method with a stable reorthogonalization scheme. The reward for using the stable algorithm is a costly matrix decomposition that can now be computed once and reused. Overall, these improvements dramatically improved the run time and robustness of the eigensolver.

(1) *Incorporation of FETI solver with Arpack.* We integrated the MP linear solver with the MP eigensolver developed last year. This required development of an eigenvalue driver that allows for shift-and-invert capabilities. We can use the combined code to solve either a single structural dynamics linear system (statics) or an eigenvalue problem that invokes the linear solver many times. In addition to standard code integration tasks required to merge two sophisticated codes, a number of important efficiency improvements were critical to reducing memory usage per processor and computation time. Most of these correspond to using information from previous FETI solvers. That is, many expensive quantities are computed only once and then saved for subsequent invocations.

(2) *Eigensolver integrated with new finite-element (FE) structural dynamics code.* A new parallel FE code, called SALINAS, is being developed at Sandia.

Though the initial version of SALINAS is not complete, the fully integrated product is a major milestone for this project. Structural dynamics developers can define/partition models (CHACO/Nemesis/Exodus) and then invoke SALINAS to assemble these models in parallel to compute eigenvalues or solve linear systems. The SALINAS code fundamentally advances Sandia's structural dynamics eigenanalysis capability by providing a scalable tool for analysis of large Defense Program (DP) applications. We will be able to analyze models more than 100 times larger than those addressable today. This increased capability is due not only to parallelism, but also to algorithm improvements (i.e., the replacement of the direct solver with an iterative one). Parallelization of the previous algorithms would have provided some improvements, but would not have allowed such large problems to be solved.

(3) *Application to structural dynamics problems.* We evaluated a number of structural dynamics models using this eigensolver. We solved simple brick models with up to 800,000 equations (requiring 1/2 hour of computation) and confirmed the scalability of the overall algorithm. Larger and more complex models are currently under development.

Publications

Refereed

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3504.050

Automated Geometric Model Builder Using Range Image Sensor Data

C. F. Diegert, J. T. Sackos

Sandia's goal is to develop algorithms that automatically construct realistic, 3-D models of physical environments based on range and optical reflectance information collected with Sandia's Scannerless Range Imager (SRI). The SRI is a unique camera system invented and patented by Sandia that provides distance and reflected light intensity to each pixel in a field of view (FOV). We will design algorithms to analyze and reduce the complexity of the data collected from multiple range images taken from different perspectives, recognize and eliminate redundancies in the images, and integrate them into a simplified geometric model. The resulting model will be compatible with virtual reality (VR) and computer-aided design (CAD) software. The algorithms will be flexible enough to accommodate massively parallel (MP) processing for national security applications involving large volumes of data. The resulting capabilities could be used to rapidly survey unknown terrain or hazardous environments, monitor remote sites for security, plan clandestine activity, and enhance the ability of robotic systems to move about an environment based on a 3-D model.

Our field experimentation work demonstrates our greatly improved SRI instrument and visualization algorithms and our new ability to achieve a quick-turnaround 3-D data rendering on a

transportable system. The 0.1-inch range accuracy established in this experiment generated a lot of excitement, and in the context of reaching our automatic model building goals, it demonstrated our new statistical fitting capabilities. We could not have established the 0.1-inch accuracy without first fitting the planar surface models of the test calibration targets. Beyond simple fitting tasks are the automatic model building capabilities we obtain by applying fitting and segmentation algorithms together. We produced both fitted plane models and trimming curves. While the considerable extra trouble of obtaining trimmed models was unnecessary for establishing a simple accuracy measure, it did allow us to present computer-generated imaging of the fitted models and of the residuals about the model. Adding the trimming summarizes the raw range-imaging information in a manner that helps us obtain insight from these data. We need the trimming information to produce fully formed models that load into a CAD or VR system. During the past year we also added the capability to write summary models to DXF-format files.

Publications

Refereed

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Density Functional Theory for Classical Fluids at Complex Interfaces

L. J. D. Frink, F. B. van Swol, A. G. Salinger, K. D. Devine

The primary goal of this project was to complete a general finite-elements (FE) code for solving nonlocal density functional theory (DFT) for 2-D and 3-D problems. Sandia completed this task for a uniform fluid mesh and tested the 2-D geometries extensively. We parallelized the new code (TRAMONTO) and ran it on platforms ranging from desktop workstations to the massively parallel (MP) Intel Paragon. TRAMONTO applies the collocation method for solving the integral equation of the DFT and Galerkin's method to solve Poisson's equation where charged systems are of interest. We currently can use the code to model hard-sphere fluids, charged systems (in the restricted primitive model), and Lennard-Jones fluids. We extensively tested surfaces such as charged and neutral planar surfaces and cylinders. In addition to the code development efforts, we pursued several applications. These include the forces between rough surfaces, adhesion, osmotic stress measurements, solvent templating and microporous media, integrating molecular detail into continuum modeling of sol-gel films, and the forces between charged cylinders.

Most important was the development of a general FE code for solving the nonlocal DFT in two and three dimensions. This new capability is a significant advance in the state of the art for DFT calculations and will allow the study of complex fluid-solid interfaces. The second accomplishment involved parallelization of the new code TRAMONTO, allowing the code to run on Sandia's MP computers. Finally, we applied both the 1-D code and TRAMONTO to a variety of applications.

(1) *Development of TRAMONTO.* We had planned to generalize the 1-D code that we developed in FY96; however, after considerable discussion, we decided to abandon the 1-D FORTRAN code in favor of a new C code that could use the libraries developed under the AZTEC project for solving systems of linear

equations in parallel. The new code solves the DFT on a regular mesh and can therefore use one set of stencils to fill the Jacobian and residual at each point on the mesh. This minimizes the memory overhead for each node and utilizes the structures of C. In addition to solving the integral equations of the DFT, we designed TRAMONTO to simultaneously solve Poisson's equation in its differential form for charged (electrolyte) systems. TRAMONTO can also solve for Lennard-Jones fluids confined by hard surfaces. Finally, we implemented periodic, reflective, and bulk boundary conditions (BCs) at the domain boundaries. These different BCs may be applied to eliminate redundancies in the calculation.

(2) *Parallelization of TRAMONTO.* We initially developed TRAMONTO on workstations, but we also completed generalization of the code to run on distributed memory parallel architectures. The two major components of the code that contribute to the performance are the fill of the Jacobian and the solve of the linear system $Ax=b$. In most cases, the Jacobian fill is the most expensive step. As a result, we developed a successive bisection routine that performs load balancing based on the time required to fill the Jacobian for each row of the matrix (or node in the mesh). Our parallelization efforts resulted in a code that achieves nearly perfect speedup over a wide range of numbers of processors for the Jacobian fill and the AZTEC solve. In addition, the load balancing improved code performance between 30% and 50%, depending on the run conditions.

(3) *Application of 1-D DFT and TRAMONTO.* In addition to code development efforts, we undertook several applications of the DFT code. Several of these resulted in manuscripts in progress or submitted. Briefly, the results of the applications were as follows:

- *Rough surfaces.* We showed surface roughness to change character of solvation forces, but not destroy them altogether.
- *Adhesion.* We demonstrated the importance of capillary condensation in surface forces pull-off measurements.
- *Osmotic stress.* We demonstrated the separate roles of chemical potential and osmotic pressure in experiments.

- *Solvent templating.* We established the role of solvation forces in causing formation of micropores during drying.
- *Bridging length scales.* We incorporated solvation forces from DFT into continuum models of drying.
- *Charged cylinders.* We resolved a controversy concerning attractions between like-charged cylinders.

Publications

Refereed

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Sensing and Compressing 3-D Models

J. C. Krumm

After intensive investigation, Sandia changed the technical approach of this project. Instead of trying to generate a 3-D range image from stereo, we chose to measure 3-D positions of objects based on a new object-recognition algorithm. The object-recognition algorithm that we developed tolerates partial occlusion, background clutter, and illumination variations. It is automatically trained based on a sequence of training images of the part. A probabilistic analysis of the algorithm helps optimize some of its operating parameters (e.g., detection threshold). On a test of 1000 images of a part, the algorithm successfully found the part 99.3% of the time.

Our new object-recognition algorithm addresses deficiencies of commercially available algorithms for object recognition to use in factories. The goal of these algorithms is to recognize an object before it is picked up or inspected by a robot. Commercially available solutions require careful engineering of the scene to present a "clean" image to the computer. In addition, these systems must be programmed by engineers skilled in computer vision.

Our system is robust to various image problems and trains itself to recognize new parts. The algorithm starts with a sequence of training images of an object. These training images show the object in different, known orientations and are used to build efficient, yet expressive, appearance-based models of the object. We match these models to images to find the object. Since the algorithm uses discrete visual features to match appearance, the algorithm tolerates partial occlusion, background clutter, and illumination variations. Thus, our new algorithm addresses the major deficiencies of commercially available software for this task.

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3504.090

Gradient-Driven Diffusion of Multi-Atom Molecules Through Macromolecules and Membranes

G. S. Heffelfinger, A. Thompson, D. J. Hobbs

The goals of this project are threefold: (1) to develop a method for modeling diffusion of multi-atom molecules through macromolecules under conditions of a chemical potential gradient, (2) to develop a companion parallel algorithm, and (3) to apply the new method to three sample problems. Currently, no such method exists; therefore, many important industrial and technological materials problems where gradient-driven diffusion of multi-atom molecules is the predominant phenomenon are beyond the reach of today's molecular simulation, including the three that we plan to study. These are (1) diffusion in polymers, (2) chiral polymer membranes for separating ceramic mixtures, and (3) the permeation of drug analogs through lipid bilayers. The first problem is directly applicable to one of the three Accelerated Strategic Computing Initiative (ASCI) polymer degradation projects: oxidative degradation of O-ring elastomers via a diffusion-limited reaction mechanism.

We added the ability to model gradient-driven diffusion through bonded (macromolecular) systems. We did this by combining parts of the original LADERA code with the molecular dynamics code LAMMPS, thus leveraging the considerable work done in LAMMPS to include bonded force fields. We tested and verified the new hybrid

code LADERA-B on several systems, including binary Lennard-Jones fluids permeating through bead-spring polymers. We are currently applying it to the permeation of He and a He/H₂ mixture in polyisobutylene; this application is relevant to the ASCI polymer degradation project mentioned above and is running on the ASCI teraflop machine. We did a literature survey and determined parameters for CHARMM-type force fields for several polymers (polyisobutylene, ethylene-propylene-dimer-monomer [EPDM]) and penetrants (O₂, H₂O) of relevance to ASCI. We are also developing chiral polymer models. Although any type of bonded interaction supported by LAMMPS can be used to model the host matrix (polymer), LADERA-B is currently limited to single-site models of penetrant molecules (inserted/deleted species).

Publications

Refereed

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An Easier Way? An Attempt to Tightly Couple Complete Grid Generation with the Flow Solver for Discretized Governing Equations

D. W. Barnette

Sandia examined the first two truncation error terms resulting from finite differencing the convection terms in the 2-D Navier-Stokes (N-S) equations for the purpose of constructing 2-D grid generation schemes. We constructed these schemes such that the resulting grid distributions drive the error terms to zero. Two sets of equations result, one for each error term, that show promise in generating grids that provide more accurate flow solutions and possibly faster convergence. One set results in an algebraic scheme that drives the first truncation term to zero, and the other a hyperbolic scheme that drives the second term to zero. The equations reveal the possibility of using the schemes in sequentially constructing a grid in an iterative algorithm involving the flow solver. In essence, we envision the process to generate a flow-field solution and grid simultaneously.

We presented a mathematical basis for automated grid construction that is tightly coupled to the flow solver. We derived the method from equations whose solutions drive the first two leading convection truncation error terms to zero. We also discussed an algorithm whereby the equations may be used to automate grid construction that is tightly coupled with the flow solver. We envision that nothing is specified about the grid being generated by the coupled flow solver other than the user-generated surface grid; hence, the number of points as well as their distribution is not predetermined. This approach differs substantially from the multigrid or adaptive methods in that the grid is "grown" in increments away from the relevant geometry. We added grid points, and relocated old points, by utilizing feedback from the flow solver on the previously constructed, coarser grid.

This approach is novel. However, if successful, the proposed algorithm will be extremely significant to computational algorithms for solving discretized governing equations. We need to work through many details, including the development of the approach in three dimensions, the effect of various flow-solver differencing schemes on the form of the grid generation equations, and exactly how grids that drive truncation error terms to zero affect the flow solver's convergence rates and solution accuracy. The foundation of the analysis appears strong.

Publications

Refereed

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3504.120

Fast and Easy Parallel I/O for Efficient Scientific Computing

P. Chen, S. W. Attaway, R. A. Haynes, D. E. Womble, J. P. Noe

The performance of I/O subsystems on massively parallel (MP) computers lags the computational power of these machines. New algorithms and approaches to input/output (I/O) are necessary to compensate for the imbalance between I/O and computational performance. In this project, Sandia developed new tools and algorithms that allow application programmers to use I/O resources easily and efficiently. We focused on collective I/O, i.e., coordinated requests from many processors, because of the increased potential for efficient use of disk and tape systems. Programs that require out-of-core computation or frequent checkpointing should see significant performance improvement due to lower I/O overhead. Moreover, new I/O capabilities developed in this project will allow larger simulations to be run, reduce the computer

time required for these simulations, eliminate the long file-recombination process prior to visualization, and reduce programming time to develop new applications. In sum, the Accelerated Strategic Computing Initiative (ASCI), model simulation-based life-cycle engineering (MSBLCE), and warhead protection program (WPP) codes will be able to solve bigger problems than would otherwise be possible, and they will run faster while doing so.

We achieved a number of results toward the ultimate goal of having a scalable parallel I/O (PIO) library that simulation and visualization applications can use to transfer massive amounts of data among memory, disks, and tape archive:

(1) Designed a new file format for efficient PIO with customer inputs from unstructured grid applications, visualizations, and tape archive.

(2) Designed and implemented a low-level collective disk I/O library PIO that supports efficient transfers of locally permutable data arrays with flexible compression options and minimal buffering requirements.

(3) Designed and implemented a mid-level parallel data set (PDS) management library that supports collective, random access of primitive finite-element data arrays.

(4) Adapted a visualization package (Griz) to read the new file format.

(5) Demonstrated library functionalities with an unstructured grid application (Gila). Observed from a 253-node run a preliminary fivefold I/O speedup relative to the current one-file-per-node model, in addition to eliminating any file-recombination process prior to visualization.

(6) Implemented the parallel file transfer interface to the high-performance storage system (HPSS) archival storage system on the research platform.

(7) Experimented with the scalability of HPSS TCP/IP (transmission control protocol/interest protocol) transfers in an asynchronous transfer mode (ATM) network environment.

Novel Load-Balancing for Scalable, Parallel Electromagnetic and Plasma Physics Simulation Software

M. L. Kiefer, M. F. Pasik, S. J. Plimpton

Sandia uses fully 3-D, electromagnetic particle-in-cell (EM-PIC) simulation techniques to address many Navier-Stokes (N-S) applications. These include neutron generators, weapon radar systems, Z-pinch (x-ray) accelerators, radiography systems for weapon primaries, inertial confinement fusion (ICF) accelerators, and high-power microwave devices. EM-PIC simulates the time-response of EM fields and low-density plasmas in a self-consistent manner (the fields push the plasma, and the plasma self-current modifies the fields). Sandia's QUICKSILVER code is currently used for these applications, but it does not have the scalability required to perform full system-level simulations on thousands of processors as required for the Accelerated Strategic Computing Initiative (ASCI). The chief obstacles are load-balancing the computations due to the nonuniform, time-dependent density of particles on the grid and the use of different numerical algorithms and cell types in various grid regions. We propose to test and implement novel methods to achieve a fully parallelized, scalable version of QUICKSILVER and have devised potential candidates.

The first is a static method that divides the grid into many more subdomains than processors and assigns them to processors so that, on the average, each processor has nearly equal computation. The second is a dynamic method that is an extension of the first—weighted subdomains will migrate as needed to new processors to address the changing workload due to particle motion. A third method is to use fewer grid subdomains than processors, replicate each grid subdomain on multiple processors, and distribute the particles equally between processors that have a copy of the grid

subdomain. All methods should have some level of success since EM-PIC is compute-limited rather than memory-limited, and the only data exchanged between processors are on the surface of the 3-D subdomains. Hence, low communications will allow small subdomains, and low memory will allow grid data to be replicated.

QUICKSILVER is now running in parallel on Sandia's massively parallel (MP) computers using two static decomposition schemes on purely rectilinear grids. The first method allows only a single-block rectilinear grid and uses a 2-D decomposition. We implemented this method mainly to study parallel communication overhead and the lower limit of the number of cells per node. The second method allows a general, multiblock rectilinear grid (an assembly of multiple, 3-D rectilinear grids), then partitions that using an arbitrary 3-D decomposition. We implemented the first method in both a linear EM mode (no plasma present) and full PIC mode (with plasmas present). We have implemented the second in only the linear EM mode.

Detailed study of the parallel efficiency of the first method (linear EM mode) showed that acceptable (75%) efficiency is possible with a very low number of cells (6000) on each node of the RED machine. These algorithms are the worst-case test of parallel efficiency since they are 10x–20x less computationally intensive per cell than full plasma simulations. With the more computationally intensive PIC algorithms, we can maintain the efficiency with many fewer cells per node. This demonstrated that our decomposition approach (many small subdomains on each processor) is sound. Further, we now know that complex, asynchronous communications are not necessary and will not be pursued.

An unanticipated result of this excellent efficiency is that linear EM simulations can now be turned around rapidly. In our first test on the RED machine against a previous run on a high-end workstation, we reduced the "CPU-time" by nearly a factor of 100.

The full PIC version will soon allow large-scale studies of power flow systems for the proposed X-1 accelerator and neutron-tube ion-source effects on ion-beam focusing.

We implemented a rudimentary parallel version of QUICKSILVER that allows for an arbitrary decomposition into 3-D subdomains. This provides a critical partitioning capability that is necessary for scaling realistic simulations to large numbers of subdomains. This method uses QUICKSILVER's inherent serial capability to break a simulation into multiple user-defined grid blocks, then sets each subdomain to be a single grid block. At this point, the rudimentary version has no PIC capability, and its key advance is that it performs the complex message-passing necessary to "seam" the irregular subdomain connections in an optimal way on any number of processors. We also implemented several of the boundary and initial conditions within this context, though to complete a fully functional fields-only parallel tool, we must automate the preprocessing tasks that partition the simulation geometry.

To support the setup and analysis of MP simulations, we improved the automation of the simulation setup. This entailed adding dynamic memory management to QUICKSILVER (it had to be recompiled for each new simulation previously) and reading and processing the text input file in an MP manner. We also developed a method to initialize inlet boundaries by reading data from an external file, rather than using an internal 2-D Poisson solver that was difficult to parallelize. In addition, we revamped the internal particle data structures and methods from their original, Cray-optimized version. Further, we improved portions of our data output method for parallel operation so that the files produced are compatible with those produced by the serial version of QUICKSILVER. Note that these files are binary, do not need to be translated when moved to different machines, utilize highly optimized I/O, and employ 16-bit numerical precision.

Parallel Computational Chemistry Using Constraints

T. D. Plantenga, J. C. Meza, C. H. Tong,
C. F. Melius, S. J. Plimpton

This project seeks to create and study a constrained energy minimization capability for the Sandia parallel computational chemistry code LAMMPS. Energy minimization is important for studying polymer materials, chem/bio sensors, and protein-protein docking. However, minimization of large covalently connected molecules is difficult and expensive because of numerical ill-conditioning. The use of flexible distance constraints greatly improves the numerical properties and performance of minimization algorithms. We successfully demonstrated the power of constrained minimization on molecules with 1000 atoms running on a single workstation. The goal of this project is to create a similar code for parallel computers and to compute energy minima of covalent structures with up to a million atoms on the teraflop machine.

A by-product of this work includes implementation of an improved unconstrained minimization algorithm in LAMMPS. Originally intended as a first step toward constrained minimization, this algorithm has already proved important in Accelerated Strategic Computing Initiative (ASCI) work on estimating O-ring diffusion coefficients.

Progress toward a full constrained minimization capability satisfied the original milestones. We obtained preliminary results on small molecules using a shared-memory SGI (Silicon Graphics, Inc.) Power Challenge. We procured data for large polymers and are currently porting the code to the Teraflop and Intel Paragon machines.

We studied the 14,000 lines of source code in LAMMPS to understand how data objects are distributed and how parallel communication is orchestrated. Constrained minimization requires two new distributed objects: a vector of distance constraints, and the Jacobian matrix of constraint gradients. We designed both objects and coded them to follow the spatial partitioning of atoms that LAMMPS uses to distribute its data objects. Matrix-vector multiplication with the constraint Jacobian (and its transpose) required a special design for mapping distributed n -vectors into distributed m -vectors, and vice versa. We coded the constrained minimization algorithm in C as a set of routines (75 functions, 8000 lines of code) that can be embedded in general applications. We wrote the algorithm with a reverse communications interface and data abstraction of all vector and matrix objects. As a result, we can easily reuse the routines used in the distributed computing context of this project in other applications on other architectures.

The current version of the code solves least-squares subproblems by a

conjugate gradient (CG) method. The CG method needs a preconditioner for improved performance. Our plan is to use the preconditioner suite available in AZTEC; however, some modification of AZTEC is needed because LAMMPS modifies the distribution of matrix elements after every iteration of minimization.

We added an unconstrained minimization algorithm to LAMMPS. Originally intended as a first step toward constrained minimization, this algorithm proved to be immediately useful to the ASCI goal of estimating O-ring diffusion coefficients.

Publications

Other

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Accurate Numerical Methods for Wave Propagation

C. C. Ober, L. Romero, D. E. Womble

Accurate modeling of wave propagation is a critical kernel in the simulation of many physical systems, including shock propagation, electromagnetic and acoustic scattering, and computational fluid dynamics. In wave propagation simulations, numerical errors, however small, are magnified as the wave propagates, until eventually the simulation contains no useful information. The general problem is to minimize the numerical errors and analyze the numerical process to determine the limits of the simulation.

The goal of this project is to develop innovative, accurate, numerical methods for numerical simulation of acoustic-wave propagation. A classical approach to achieving high accuracy is to increase the number of grid points in the simulation, which increases the computational time. Sandia's approach will be to focus on high-order finite-difference (FD) methods and phase corrections. The use of multigrid methods is of particular interest because of the ability to extract wave behavior at various scales.

During the first year of this project, we focused on multigrid methods in FD wave propagation. The preliminary target equation was the paraxial approximation to the scalar wave equation, which is used to model acoustic-wave propagation through the earth for oil and gas exploration and wave propagation in thin-lens optics.

We were able to develop a relationship involving the wave propagation angle, the wave speed in the medium, and the desired number of grid points

per wavelength that enabled us to select a different computational grid for each frequency in the simulation. Combining this with the use of a phase correction filter, we accurately modeled wave propagation in homogeneous and mildly heterogeneous media with as few as four grid points per wavelength (reduced from approximately twenty grid points per wavelength for second-order FDs). The reduction in the number of grid points resulted in a substantial savings in computational work for the actual wave propagation. There was some additional computational work required to transfer information between the different grids used, and the overall computational savings was approximately 20%.

3504.160

Massively Parallel Ab Initio Validation for ASCI Materials Aging

C. F. Melius, E. T. Seidl, C. H. Tong

The transition from an experimental test-based lab to a lab based on predictive computational modeling will entail a detailed model-based understanding of the aging of weapon components. This understanding requires the simulation of large molecular systems with an accuracy beyond the current state-of-the-art for small molecules. Sandia is developing the computational tools necessary to validate the large-scale ab initio quantum chemistry Hartree-Fock (HF) and density-functional (DFT) methods. The new methods involve developing massively parallel (MP) versions of highly accurate electron-correlated ab initio methods. We will develop the codes using object-oriented programming. During this project, we will

apply these parallel methods to several problems related to the chemical aging of high-energy weapon components. These benchmark calibrations will constitute some of the largest highly correlated quantum chemistry calculations ever performed and will take full advantage of the teraflop-scale parallel computing.

We implemented a working prototype of an object-oriented coupled cluster singles and doubles (CCSD) method. We developed over a half dozen C++ classes that provide the multidimensional array operations needed to perform the coupled cluster calculations. We contracted to develop local-correlation methods. We wrote a prototype code for calculation atom-centered functions spanning the occupied space for the local-correlation methods as well as a prototype local-correlation MP2 energy code. The computationally dominant task in coupled cluster theory is the "contraction" of arrays with one another. The key tasks in parallelizing coupled cluster theory are to distribute the memory requirement for the arrays across the processors and to distribute the computation of the contractions. Given the number of contractions that must be evaluated and the complexity of each contraction, our approach was to use a general C++ class to store all arrays and a single routine to handle all contractions, thus making it possible to rapidly implement and assess the performance characteristics of the code. Furthermore, by isolating the contractions to one function, making improvements to this function immediately affects the entire code. The current prototype multidimensional array (MA) implementation permits use of both point group and index permutation symmetries. The principle C++ classes that make up the implementation include MAContext, MARange, MASuperIndex, MASymOffset, and MMArray.

Dynamically Coupled, Massively Parallel Simulation of Grain Growth and Aging/Degradation

E. A. Holm, T. E. Buchheit, G. A. Knorovsky, M. R. Tabbara, G. W. Wellman, M. K. Neilsen, R. J. Bourcier, R. M. Fye, J. S. Glass, H. E. Fang

Computational materials simulations have traditionally focused on an individual phenomenon: grain growth, crack propagation, plastic flow, etc. However, real materials behavior results from a complex interplay between phenomena. We will explore methods for coupling mesoscale simulations of microstructural evolution and micromechanical response. In one case, we will dynamically couple massively parallel (MP) simulations for grain evolution and microcracking in brittle materials. In the other, we will iteratively link MP codes for domain coarsening and plastic deformation. We will extend Sandia's MP PARGRAIN code to simulate microstructural evolution in both systems. To model microcracking, we take a three-tiered risk approach. Initially, PARGRAIN will couple with the parametric GLAD model, later with a more costly finite-element (FE) model with death elements, and finally with a newly developed Element-Free Galerkin (EFG) model. Plastic flow is amenable to a conventional FE modeling approach; we will extend the constitutive relations used in the JAS 3D-based crystal plasticity model to incorporate the appropriate flow mechanisms. Coupling microstructure and mechanics codes will require time synchronization, mesh matching, and information-passing algorithms. We will validate microcracking in brittle materials in the context of alumina used in stronglinks. We will study

plastic deformation response in a Ag-Cu eutectic braze alloy used in weapon components. This project achieves the first experimentally validated model for plastic deformation and fracture in realistic, evolving microstructures. Moreover, this project provides the first full spatial and dynamic integration of computational models for coupled materials response phenomena. This project will support efforts in materials selection and processing requirements to predict degradation and failure of current stockpile components.

We extended the microstructural evolution model to include phenomena appropriate to each material system studied. We implemented grain boundary energy anisotropy and boundary blocking by cracks in the serial code for grain growth in alumina. We implemented long-range diffusion of solute and strain-free coarsening of a second phase in the serial evolution code for CuSi. To make tractable the 10^6 – 10^9 volume elements required to represent a unit of material, we ported the 2-D and 3-D versions of the MP PARGRAIN microstructure code to ASCI Red. We realized per-node speedups of about three over the Paragon for test runs, and the speedup with the number of ASCI Red showed close to perfect scaling. In addition, we implemented a new, fast PARGRAIN algorithm, yielding an additional two-orders-of-magnitude increase in tractable system size.

To simulate brittle fracture, we developed and tested a 3-D GLAD model. GLAD takes the 3-D microstructures generated by PARGRAIN as input and performs mesoscale cracking simulations under user-specified deformations and thermal expansion. This code is the first lattice mechanics code capable of modeling inter- and transgranular

cracking in a 3-D grain structure under quasi-static thermomechanical deformations. We completed an MP implementation of GLAD. As a complement to GLAD, we formulated a 2-D EFG model and used it to examine the effective Young's modulus of microcracked materials. We found the effective modulus of microcracked systems to be substantially lower than previous analysis predicts.

We modeled plastic flow of CuSi using a conventional FE modeling approach (JAS 3D) with PARGRAIN supplying the grain structure and mesh. We implemented cubic anisotropic elasticity and cyclic hardening into our continuum micromechanics constitutive model, and periodic mechanical boundary conditions (BCs) into the JAS 3D FE code. We successfully simulated the quasi-static room-temperature deformation response of single-phase and multiphase equiaxed polycrystals with subgrain-size spatial resolution. These are the most detailed and computationally intensive 3-D crystal plasticity calculations ever performed.

We validated these models on stockpile materials. To study microcracking, we procured, processed, and characterized alumina with various purities and textures using orientation imaging microscopy (OIM). We used the National Institute of Standards' (NIST's) object-oriented finite element (OOF) code to evaluate the effects of crystallographic orientation and external loads on the residual stress distribution in a polycrystalline alumina microstructure. To validate plastic flow simulations, we procured a set of silver- and copper-based alloys. We prepared and annealed specimens to obtain large-grained, strain-free polycrystals. We isothermally annealed and metallographically characterized a series of samples to

examine strain-free grain growth and coarsening. We performed uniaxial and fully reversed cyclic tests to allow extraction of microstructural and continuum constitutive parameters.

The critical step in this project is coupling microstructural evolution codes to mechanical response codes. Work in the first part of this year focused on developing and refining the individual response models. In addition, we defined PARGRAIN/GLAD and PARGRAIN/JAS 3D coupling interfaces. Because of the interdisciplinary nature of this work, we made substantial efforts to involve all relevant investigators in each step of the project, with our accomplishments attesting to the success of our approach.

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An Investigation of Wavelet Bases for Multiscale, Grid-Based Simulation

M. A. Christon, J. R. Weatherby, T. E. Voth, D. E. Womble, T. G. Trucano, R. S. Baty

The primary objective for this work is to establish the foundation for optimal wavelet formulations for grid-based simulation based upon numerical performance, computational efficiency, parallelism, and the ability to exploit the hierarchical adaptive nature of wavelets. Wavelets are a new mathematical tool that dissects data, functions, and differential operators into components of different frequency and wave number with a resolution matched to the scale of each component. Wavelet bases constitute a significant shift from traditional grid-based simulation methods because the multiresolution character of wavelets enables the development of hierarchical solutions—a critical requirement for simulation-based design. Compact support wavelets are localized in space, permitting the solution to be refined without local or global remeshing to resolve regions of high gradients without causing overshoot phenomena (ringing) in adjacent regions where the solution is smooth. In addition, preliminary studies indicated that wavelet formulations can deliver spatial convergence rates superior to finite-element (FE) and finite-difference (FD) methods. This effort seeks to develop a rigorous technical framework for the evaluation and application of wavelet bases to the solution of wave propagation, advection, and diffusion problems. These physical processes are characteristic of more complicated applications such as turbulent

flow where the solution accuracy and computational requirements depend directly upon the numerical errors (i.e., numerical dispersion) associated with the computational method. The algorithms developed as a result of this research will find direct application to multiple Accelerated Strategic Computing Initiative (ASCI) problems and to applications that demand accurate far-field solutions such as counterproliferation and environmental characterization. This effort will greatly enhance Sandia's recognized leadership role in large-scale, multiphysics simulation.

Over the course of the past year, the wavelet team investigated and reviewed the five wavelet formulations. These include the Wavelet-Galerkin (WG), Wavelet-Collocation, Wavelet Optimized Finite Difference, Discrete Element Wavelet, and Reproducing Kernel (RK) methods. Based upon the preliminary scoping efforts, we selected the WG and RK methods because we can use these methods as generalized discrete frameworks with a variety of approximating bases; they demonstrated application to realistic physical problems. We concluded that multiwavelets in a Galerkin formulation should be explored further because the "squeezeable" bases promise the ability to treat boundary conditions (BCs) and complex geometry. We developed a series of model problems and baseline comparison data for the FD, FE, and RK methods in terms of dispersive characteristics, truncation error, and rate of convergence for hyperbolic, parabolic, and elliptic partial differential equations (PDEs). In addition, we developed a general theoretical framework for the evaluation of wavelet solution methods for elliptic PDEs. We demonstrated a detailed dispersion analysis of the RK method that excellent dispersion characteristics may be obtained when a consis-

tent mass matrix is used with the proper choice of dilation parameter, i.e., there are essentially no phase or group velocity errors up to a wavelength of approximately $3Dx$. In contrast, we found the influence of row-sum lumping the mass matrix to introduce severe lagging phase errors. A "higher-order" mass matrix improves the dispersion characteristics relative to the lumped mass matrix but delivers lagging phase errors relative to the fully integrated, consistent mass matrix. Based upon the numerical analyses, we developed several 1-D codes using RK and WG methods to compare to FE and FD solutions, and gained experience with numerical quadrature, BCs, and implementation strategies.

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3504.190

Integrated Quantum/Classical Modeling of Hydrogenic Materials

F. B. van Swol, R. M. Fye, J. G. Curro, S. J. Plimpton

Sandia's work this past year focused on the modeling of quantum fluids using path integral (PI) techniques. The PI technique consists of mapping a quantum mechanical path integral onto a ring polymer connected via harmonic springs, a classical system. This project is aimed at implementing this technique into a molecular simulation code and extending existing integral equation techniques (i.e., Polymer Reference Interaction Site Model [PRISM]) to ring polymers, i.e., quantum fluids. This report describes the algorithm chosen to simulate the ring polymers and reports preliminary molecular simulation

results obtained for a pure hydrogen fluid. In addition, we outline the issue of deciding on a closure for PRISM.

(1) *Imported parts of LAMMPS code to model a ring polymer.* The choice fell on using a predecessor of LAMMPS, namely POLY. This code is best suited for our project because it was written specifically for a bead-and-spring model of a polymer chain. We will take care to ensure that the newly added features are portable to the LAMMPS code. The PI formalism maps the quantum mechanical system onto a classical system of interacting ring polymers. The intermolecular interaction between two ring polymers is peculiar in that a particular bead on ring 1 interacts only with its counterpart on a neighboring ring 2. Thus, the number of interactions between rings is equal to the first power of the number of beads, not the second power.

(2) *Implemented multi-timestep algorithm.* We implemented and thoroughly tested the multi-timestep method. The essence of this method is the separation of the stiff harmonic intramolecular forces from the more slowly varying intramolecular forces. We used the velocity Verlet algorithm to integrate the equations of motion.

(3) *Implemented hybrid Monte Carlo scheme.* We implemented the hybrid Monte Carlo scheme and tested it for fluid hydrogen. In this scheme, we replaced the traditional Monte Carlo displacement step by a small number (order of ten) of oversized molecular dynamics (MD) timesteps. Due to the oversized nature, the total energy change was nonzero along the trajectory. The displacement step was then accepted with a probability given by the Boltzmann factor of the total energy change. We then drew new velocities from a Maxwell-Boltzmann distribution centered on the specified temperature.

(4) *Applied PIHMC code to liquid-vapor hydrogen mixtures.* We successfully applied Path Integral Hybrid Monte Carlo (PIHMC) to simulate liquid hydrogen

and used it to determine the liquid-vapor coexistence properties, including densities and vapor pressures. The simulations allowed an assessment of two sets of potentials that are due to Buch, Silvera, and Goldman. The overall agreement with experiments was excellent.

(5) *Decided on an optimized closure for PRISM.* We performed PRISM calculations with a variety of closures, including Percus-Yevick, Hypernetted Chain, Molecular MSA (Mean Spherical Approximation), Molecular Percus-Yevick, and Laria-Wu-Chandler closures, in an effort to determine the most accurate one for use with polymers having short-range repulsive and long-range attractive potentials. We found the Laria-Wu-Chandler closure to be the most accurate formulation of self-consistent PRISM theory. We obtained evidence of the accuracy from comparing PRISM predictions for the root-mean-square size end-to-end distance R of polymers in solution, interacting with a screened coulombic, with full Monte Carlo simulations as a function of concentration.

(6) *Performed preliminary calculations with PRISM.* We performed preliminary PRISM computations on polyelectrolyte solutions to demonstrate that the polymer structure can be found self-consistently for both the intra- and interchain structure.

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The Next Generation of Teraflop Density Functional Electronic Structure Codes

M. P. Sears, A. F. Wright, P. A. Schultz, A. A. Quong

The purpose of this project is to develop algorithms for a new generation of codes, with primary emphasis on the development of density functional methods. Competitive algorithms must scale linearly with system size; this is true for both the standard energy/force computation as well as the linear response calculations. Sandia plans to combine a real-space variable grid method with innovative linear scaling algorithms, testing the resulting code against existing codes and against experiment. The result will be a tool useful for a wide variety of materials research applications and will keep Sandia in the forefront of this area.

Work proceeded on several fronts:

(1) We developed a code to solve for the electronic structure in a curvilinear grid representation. Here the grid is curvilinear in real space but is a logically regular grid. We are involved in studying the main algorithmic and numerical issues, including the implementation of nonlocal pseudo-potentials, the finite-difference (FD) form for the Laplacian operator, and the method for solving Poisson's equation on the curvilinear grid.

(2) We developed a code to generate the desired curvilinear grids. The code solves for the inverse transformation while determining the Jacobian and metric and third-rank tensors needed in the electronic structure code. There are a number of possible atom-centered weighting functions that could generate useful grids; the code implements parameterized versions of several of these, and we derived some interesting tests for determining which is best before the actual grid is generated. Combined with the code described in (1), we demonstrated substantial improvements in efficiency.

(3) We evaluated most of the $O(N)$ algorithms described in the literature for several figures of merit. Many of the variational energy functionals proposed can be unified, and we discovered that certain rigorous constraints are being compromised and that commonly used gradient expressions are incorrect. We additionally demonstrated on paper that a new concept for computing second derivatives and linear response will scale linearly with system size, much better than existing algorithms.

3504.220

Methodology for Characterizing Modeling and Discretization Uncertainties in Computational Simulation

K. F. Alvin, W. L. Oberkampf, B. M. Rutherford, K. V. Diegert

To meet the goals of the scientifically-based stockpile stewardship program, the U.S. must build significantly improved confidence in a variety of numerical simulations. The goal of these simulations is to accurately characterize the response of the complete system with high-fidelity, three-dimensional, unsteady, coupled physics, together with uncertainty bounds on the predictions. Quantifying uncertainties in computational physics-based simulations is also critical to the verification and validation of these simulations; without uncertainty quantification, validation is highly subjective. Nondeterministic methods seek to quantify response uncertainties by propagating uncertainties due to stochastic inputs and variability or uncertainty in the geometric, constitutive, and manufacturing parameters through the simulation. There remains a pressing need, however, to address the question of whether the proper physics have been modeled, both mathematically and numerically. The objective of the present research is to develop methods to quantitatively estimate the errors or uncertainties due to the mathematical form of the partial differential

equations (PDEs) and errors due to the discretization of the equations. This work complements, but is distinct from, nondeterministic methods for numerical simulations.

Sandia is developing a general methodology for characterizing the effects of modeling on computational simulation. This methodology is intended to apply in all numerical simulations of continuum mechanics and heat transfer, assuming that the mathematical formulation of the physical model is given by a system of differential equations that are solved by discretization methods. The present research effort focuses on three strategies for characterizing computational simulation errors and uncertainties: (1) identification of error sources and interactions, (2) parameterization and survey of the model structure, and (3) methods for evaluating model uncertainty and its contribution to global uncertainty.

We made significant progress in the following areas: (1) characterization of applicable current research in operations research, statistics, and computational mechanics, (2) development of a framework to categorize all sources of errors and uncertainties in computational simulations, (3) identification of candidate methodologies for assessment and propagation of model uncertainty, and (4) preliminary work on simple example problems in structural dynamics and flight dynamics that consider uncertainty in model assumptions and problem discretization. The candidate methodology for model uncertainty quantification is the use of a discrete expansion of models to approximate the model space and the application of Bayesian statistics and inference to that set of models. This approach leads to the use of multiple models with associated probability weights that we can use to estimate prediction variances due to model uncertainty. We also applied this Bayesian model averaging approach to structural dynamics modeling. Finally, we initiated work to study the application of response surface methodology to uncertainty quantification.

A Critical Evaluation of Algorithms for Global Optimization

W. E. Hart, C. A. Phillips, J. S. Wagner, L. Swiler

A wide variety of scientific and engineering problems can be posed as optimization problems in which the desired solution to the problem corresponds to an optimal set of parameters for an objective function that measures a solution's quality. Sandia has begun to develop a library of robust and efficient optimization algorithms that can be used to find globally optimal solutions to complex optimization problems. Our work will lead to a critical evaluation of standard global optimization algorithms (e.g., genetic algorithms, simulated annealing) as well as new, innovative methods that are inspired by our analysis. This analysis will focus on a variety of algorithmic factors that fundamentally affect the practical application of these methods, including (1) the combination of global sampling and local optimization, (2) termination rules that provide practical confidence guarantees, (3) the appropriate design of constrained optimization methods, (4) the effective use of all function evaluations, and (5) the role of parallelism (for large-scale optimization problems). This research has the potential for high impact on a wide variety of existing Sandia programs. Our research will have immediate impact on three application domains: (1) problems relating to scheduling, (2) system design optimization, and (3) chemical-biological warfare defense (counterproliferation). This effort will develop new expertise in global optimization techniques as well as build on Sandia's current expertise in parallel algorithms.

This year we surveyed standard global optimization algorithms, which enabled us to target specific methods to include in our future work. We began

including these methods in stochastic global optimization algorithms (SGOPT). We also extended the capabilities of SGOPT to provide a generic optimization facility that allows users to easily perform optimization on a new search domain. We identified three test applications that we will use to evaluate our applications, and we began to develop these applications and apply global optimization methods to them.

We made a variety of related algorithmic developments this year. We identified several ways in which genetic algorithm hybrids can improve their use of local search and began experiments to confirm our predictions. We also proved a stationary point convergence theory for a new class of evolutionary algorithms that adapt the mutation operator in response to the success of prior iterations. We developed a simple thread management tool that we used to implement a simple parallel branch-and-bound algorithm as well as a parallel genetic algorithm. Finally, we began developing techniques for optimizing neural networks when a very large number of training examples are needed.

In addition to the algorithmic issues addressed in our original proposal, we targeted constrained optimization methods as an area where further algorithmic developments are needed.

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Dynamic Simulation of Mechanical Systems with Intermittent Contacts

C. L. Lewis, G. A. Laguna, R. A. Lafarge

Sandia is developing an efficient dynamic simulator to accurately predict probabilistic distributions of motions for arbitrary numbers of bodies experiencing multiple applied forces and intermittent contacts. Current simulators employ either weak or computationally expensive contact models and frequently cannot handle complex time-varying contacts. Our approach utilizes a compliant surface model to account for the fact that macroscopically rigid bodies are not absolutely rigid at contacts. The model is much less computationally intensive than full finite-element (FE) methods. Our simulation results will be verified through comparison to data from extensive physical experiments.

We are working closely with Mechanical Dynamics, Inc. (MDI), the developers of ADAMS, acknowledged to be the world's most widely used mechanical system simulation software. Within the automobile industry, ADAMS is the standard for motion simulation. Since MDI is willing to tailor their application programming interface (API) to accommodate the implementation of our models, we can ensure the long-term availability of our results and avoid re-engineering an already mature user interface.

We will develop custom software modules to predict the statistical robustness of mechanisms such as strong-links, trajectory-sensing signal generators (TSSGs), and small smart machines, as well as robustness of the assembly, disassembly, and maintenance procedures that contribute to their life-cycle cost. Our simulation software will provide force histories for critical tasks and predict the success of inherently stochastic processes such as part feeding.

Our first task was to evaluate commercial dynamic simulation software, ADAMS and DADS (data acquisition and display system), regarding intermittent contact analysis. We constructed a problem consisting of a simple object free to tumble inside a rotating dryer drum. We found that both DADS and ADAMS were quite limited. DADS was constrained to analyze contacts only between extruded bodies and a collection of spheres, while in ADAMS, the user must write a subroutine to define the contact modeling.

During our evaluation, we started discussions with the developers of both ADAMS and DADS. The developers of DADS indicated that they had no plans to implement automatic contact detection and analysis; however, the developers of ADAMS were working on the implementation of this critical functionality for release.

We were able to concentrate our efforts on the central issue of contact analysis. From our evaluation process we concluded that we could minimize our user interface by simply parsing the model definition files and communicating through a documented API. We intend to provide three stand-alone modules: (1) fast collision detection, (2) contact analysis, and (3) eventually a module for statistical analysis.

Sandia's fast collision-detection module is part of a more general code, the Configuration Space Toolkit (CSTk). We extended the CSTk to meet the needs of multibody simulation. The main extension enables efficient tracking of interference, bounded-distance, and closest/contact features among all members of a system of moving rigid bodies.

Although modularity and encapsulation of distinct codes has advantages, we still require a stand-alone simulation capability from which we can both develop and demonstrate the individual modules. For this purpose, we developed a test-bed that has a very limited user interface and simplistic numerical integration routines and processes only a limited class of constraints.

A key component to our simulation goals is to be completely interfaced with a computer-aided design (CAD) system. Within the CAD system, the user should be able to assemble mechanisms and define joints and other constraints, and to perform an analysis of the system's performance. We were able to rely on published commercial interfaces for this purpose. ADAMS integrated its software with Pro/E and CADSL. We plan to use this utility within ADAMS.

Simulation to first collision requires that our test-bed couple a six-degree-of-freedom (DOF) trajectory capability with collision-detection software, the CSTk, under a recent project. The test-bed's design permits us to take a Pro/E description, convert it to our internal geometric description to determine the trajectory evolution, and use the CSTk to determine contact information. The approach we are using for addressing the collision analysis problem is to relax the rigid-body assumption and to model the contact with nonlinear lumped elements. This method is simple to implement and captures phenomena like wedging or press fits. This is not possible with rigid-body models. Additionally, this method does not require reformulation of the governing equations with changes in contact states. A unified approach applies to both impacts and persistent contacts. We can currently simulate multibodies through the first collision using a naive impact model without friction.

Publications

Refereed

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esearch that ensures the supply of Sandia components supporting the DOE mission of stockpile stewardship is supported through Electronics and Photonics funding.

Electronics and Photonics projects comprise six categories: (1) silicon-based microelectronic devices for defense, energy, and industrial uses; (2) research on low-power microsensors; (3) studies of microelectromechanical systems that are small, affordable, reliable, low-power, and immune to shock and vibration; (4) research to advance existing hardware and software projects; (5) development of faster, smaller, smarter systems to collect, process, and transmit information; and (6) exploration of rapid prototyping, packaging, and testing.

Micromachines are leading the revolution in faster and smaller technologies. Current research is combining Sandia expertise in micromachine sensors with experience in rapid prototyping. The ability to test new concepts in a relatively short period of time will make Sandia's microsensors widely available to the manufacturing community for both defense- and nondefense-based technologies.

Keeping microelectronic systems cool enough to operate at higher speeds in smaller volumes is key to success in these systems. Engineers are developing a new method of providing microelectronic cooling. The method uses Sandia's micro-heat-pipe design combined with a metal base. The result is a robust, low-cost, and efficient cooling technology that will support the smaller, faster microelectronics of tomorrow.

Photo-patterned nickel, wick structures are plated on a Kovar substrate for a new type of heat-pipe. The structures with overplated cap areas enhance heat-pipe performance in microelectronic cooling applications.

ELECTRONICS & PHOTONICS

High-Speed Modulation of Vertical-Cavity Surface-Emitting Lasers

K. L. Lear, H. Chui, K. D. Choquette, V. M. Hietala, M. G. Armendariz

Sandia continued to develop high-speed vertical-cavity surface-emitting lasers (VCSELs) for multigigabit-per-second optical data communications applications. The program resulted in VCSELs that operate with a bandwidth of 2x0 GHz. We obtained this large bandwidth simultaneously with a DC-to-light-conversion efficiency of about 20%. We pursued two approaches to realize this very high-speed-frequency response. First, we developed conventional VCSELs in a form suitable for high-speed operation, including adaptation to microwave probing, and demonstrated them with 20-GHz bandwidth. We explored the second approach, polarization modulation, which offers the promise of much higher bandwidths, with some limited static results. This high-risk approach was not successfully demonstrated at high speeds and therefore remains an intriguing future possibility.

We demonstrated VCSELs with 20-GHz bandwidths. This speed was the primary goal of this program. We obtained this record large bandwidth simultaneously with a very high conversion efficiency (about 20%).

To obtain this record performance, a number of design/process/test iterations were necessary. We required several novel process and material variations, including careful design of the epitaxial mirrors for minimization of resistance; *n*-type VCSEL design to lower the effective contact resistance; selective thermal oxidation for improved mode confinement; and thick polyimide under contact pads along with an additional proton implantation to lower parasitic device capacitance.

We performed small-signal on-wafer measurements of the VCSEL up to 30

GHz. These included both impedance and response measurements. We performed measurements over a temperature range of -50° to +100° C. We developed a detailed small-signal RF model of the VCSEL that accurately describes the electrical and optical characteristics of the VCSEL.

We demonstrated and characterized large-signal operation of the VCSEL by using two-tone (third-order intercept) and bit-error-rate testing to 12.5 Gbps (gigabits per second). The devices appear suitable for operation in communication links to speeds in excess of 10 Gbps.

We developed a high-speed package for the VCSEL and packaged 10-GHz-bandwidth VCSELs for testing.

Publications

Refereed

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Micromachined Inertial Sensors (Accelerometer, Gyroscope)

E. J. Garcia, C. C. Barron, J. L. Wilcoxon

The major goals for this project are to develop, fabricate, and test an accelerometer and a gyroscope in surface-micromachining technology. The motivation for this project is the long-term realization of a low-cost inertial guidance "system-on-a-chip." Surface-micromachining technology adapts integrated circuit (IC) fabrication techniques with certain modifications to produce mechanical and electromechanical structures and mechanisms in polycrystalline silicon. Sandia's work completed in FY97 includes further experiments with the silicon micromolding process to create thick accelerometer structures and the design of a free-rotor microgyro, which includes capacitive pick-offs to detect orientation changes of the rotor with respect to the sense platform and torque-producing elements to restore the rotor to the null position as part of a closed-loop feedback control-sensing scheme.

We pursued a force-feedback teeter-totter design with torsional springs at the pivot for the accelerometer portion of the project. Earlier work concentrated on a means for increasing the accelerometer proof mass by deposition of tungsten. Difficulties with the tungsten deposition process led to investigation of the silicon micromolding process, which permits the fabrication of "thick" silicon structures. We used reactive ion etching (RIE) to deep trench into the silicon substrate to produce an array of pillars. After oxidizing the pillars, we deposited chemical vapor deposition (CVD) polycrystalline silicon (polysilicon) on the sidewalls of the oxidized pillars to completely fill the voids created by RIE trenching to produce a thick polysilicon structure. We then dissolved the oxidized pillars, leaving the newly formed polysilicon structure in place. This approach is ideal

for creating substantial proof masses for accelerometers. However, problems with the silicon micromolding process resulted in proof masses becoming stuck to the underlying substrate. We focused on building additional proof mass structures and refining the process to eliminate sticking. A prototype accelerometer incorporating a revised process to eliminate sticking is in fabrication.

We completed the design of a first-ever free-rotor microgyro after overcoming a variety of difficulties related to coupling a rotor with an appropriate driver and developing a suitable suspension. The free-rotor microgyro has the potential to increase sensitivity (torque produced per unit angular rate change of sense platform) up to three orders of magnitude when compared to vibratory or resonator gyro designs. The development of a free-rotor microgyro has never been accomplished because there has not been a suitable microactuator available to turn a rotor. The free-rotor microgyro uses a modification of the Sandia-developed microengine to spin an inertial mass (rotor). The rotor is suspended by two orthogonal sets of torsion bars that permit the rotor to deflect from its original orientation with respect to the sense platform to which the microgyro is mounted. As the platform experiences an angular rate, the spinning rotor will change orientation with respect to the sense platform. A set of three capacitive pick-offs are equi-spaced about the rotor perimeter to determine rotor orientation. We use another set of three similarly spaced capacitive pick-offs to apply an electrostatic torque to restore the rotor to its original orientation. Since the magnitude of the restoration torque is directly proportional to the angular rate experienced by the sense platform, we can determine the angular rate. We fabricated the free-rotor microgyro using the four-level polysilicon surface-micromachining process; it is capable of being integrated with complementary metal oxide semiconductors (CMOS).

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3506.030

Red-to-Blue-Wavelength Photonic Devices

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Sandia proposed to develop broad-spectrum visible photonic devices, covering the wavelength range from red to blue, using III-V materials. The initial phase of the work will focus on extending the wavelength of lasers and light-emitting diodes (LEDs) based on the AlGaInP alloys and heterostructures from the deep red (690 nm) to shorter visible wavelengths. Sandia has extensive experience in the growth of these materials, so we anticipate that the primary issues in the development of the devices will be associated with their design. We will place particular emphasis on the development of novel vertical-cavity surface-emitting lasers (VCSELs). Concurrent with this initial phase of the work, we will further develop Sandia's new GaN growth capability for application to blue emitting photonic devices, and process development for the new nitride materials will begin. In the second phase of the work, the primary focus of the device effort will be on building blue light-emitting photonic devices from the nitrides. The main emphasis will be on advancing the growth capability to enable p-type and n-type materials and the fabrication of efficient blue LEDs. At the completion of this work, Sandia will have demonstrated novel photonic devices

including surface-emitting lasers and conventional LEDs from red to blue wavelengths.

This project involved two main thrusts that would advance photonic device technology in the blue and the red wavelengths, respectively. In terms of short-wavelength (blue) devices, our main emphasis was the development of GaN and related alloys to enable the demonstration of *p-n* junction structures for blue LEDs. A critical milestone was the demonstration of controllable *n*-type and *p*-type doping. This involved being able to reduce the intrinsic *n*-type background, which is strongly dependent on growth conditions, as well as to controllably incorporate silicon dopants (for *n*-type material) and magnesium dopants (for *p*-type material). We achieved both silicon and magnesium doping in GaN at levels greater than $1 \times 10^{18} \text{ cm}^{-3}$. These accomplishments enabled us to demonstrate GaN *p-n* junction structures on sapphire substrates. To enable improved performance from the *p-n* junction structures, we developed higher-bandgap AlGaIn alloys with Al fraction up to 40%. We integrated these AlGaIn materials with GaN to form a GaN multi-quantum-well (QW) structure with AlGaIn barriers. These multi-QW heterostructures should enable more efficient carrier confinement and light emission in an LED structure.

Another milestone involving GaN-based materials was the advancement of our processing technology for blue laser diodes. Our focus was on advancing our plasma-etching capabilities to enable sidewall profiles suitable for laser facets. While a number of groups are using reactive ion etching (RIE) to etch laser facets, we focused on using high-density plasma-etch technology, which typically yields higher etch rates with less damage than conventional RIE systems, as well as more anisotropic profiles due to lower process pressures and reduced collisional scattering of the plasma species. Previous work on this project involved using an electron cyclotron resonance (ECR) plasma system; our recent work involves a new inductively coupled plasma (ICP) system. We demonstrated very smooth pattern transfer of GaN over a wide range

of plasma chemistries and conditions. Using $\text{C}_{12}/\text{H}_2/\text{Ar}$ plasmas, we obtained highly anisotropic, smooth GaN etching at rates of 688 nm/min. Our results suggest that ICP etching of the Group-III nitrides in C_{12}/H_2 -based plasmas enables etch profiles and sidewall smoothness, which should improve the yield and performance of etched facet lasers.

The second major thrust in FY97 involved advancing our understanding of the limitations in short-wavelength performance from AlGaInP (red-emitting) laser materials. Our theoretical studies involved improving our laser model to better predict the performance of AlGaInP laser diodes. We developed a consistent treatment of carrier collision effects at the level of quantum kinetic theory in the Markovian limit. We included this analysis in our previously developed laser gain theory and compared our calculations to gain spectra from AlGaInP laser diodes. We found the new treatment of carrier collision effects to be critical in modeling several experimentally observed effects, such as the blue shift of the peak gain with increasing current injection as well as the low energy dependence of the gain spectra.

Our experimental work on AlGaInP VCSELs involved improving the performance of our selectively oxidized devices through optimizing the number of oxide layers and top mirror pairs. These studies enabled the demonstration of continuous wave (CW) lasing up to 85°C (highest temperature to date), threshold currents as low as 0.38 mA (lowest to date), and multimode powers greater than 4 mW. These devices lased in the longer-wavelength visible regime (670–690 nm); we then designed and grew these devices for shorter-wavelength emission (630–650 nm).

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Double Electron Layer Tunneling Transistor

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Quantum transistors based on resonant tunneling have long been of interest due to their multifunctionality and intrinsically high speed. However, the addition of a third gate terminal has typically required lateral quantum confinement for the gate to have any effect. Unfortunately, the stringent lithographic tolerances of such lateral devices render them extremely difficult to fabricate in the numbers necessary for real-world applications.

In this project we investigated, developed, and demonstrated a novel three-terminal quantum device, the double electron layer tunneling transistor (DELTT), which does not require lateral confinement but rather is entirely planar in configuration. Because unlike other devices both electron layers are 2-D, the densities of each 2-D layer can be modulated with surface gates, allowing the tunneling to be easily controlled.

We showed the DELTT to work quite well. At 1.5°K we demonstrated DELTTs with excellent transistor characteristics. These DELTTs also exhibited negative differential conductance and negative transconductance. Both of these characteristics indicate that the DELTT is multifunctional, i.e., capable of performing circuit functions with many fewer transistors than are required with conventional devices.

We also engineered new DELTT structures designed for higher-temperature operation. At 77°K these also exhibited excellent operating characteristics. Indeed, we observed negative transconductance up to ~ 250°K.

To demonstrate the multifunctionality of the DELTT, we also constructed several circuits using the DELTT. These included both n-type and complementary-type static random access memory (SRAM) cells, some at temperatures up to 77°K. Because of the DELTT's multifunctionality, these

circuits used only half as many transistors as conventionally required. We also demonstrated digital logic circuits, including exclusive-or (XOR) and not-and (NAND) gates.

Quantum transistors based on resonant tunneling have long been of interest due to their multifunctionality and intrinsically high speed. However, the addition of a third gate terminal has typically required lateral quantum confinement for the gate to have any effect, e.g., laterally gated double barrier resonant tunneling diodes (DBRTDs). Unfortunately, the stringent lithographic tolerances of such devices render them impossible to fabricate in the numbers necessary for real-world applications.

In this project we demonstrated a novel quantum device, the DELTT, which does not require lateral confinement but rather is entirely planar in configuration. The DELTT operates on the principle of coherent resonant tunneling between the two electron layers in a double quantum-well (DQW) heterostructure. Because unlike DBRTDs both electron layers are 2-D, the surfaces of the structure play a crucial role: the densities of each 2-D layer can be modulated with gates, allowing the tunneling resonance to be easily controlled. While the physics of 2-D/2-D tunneling has previously been explored, the behavior of such structures in the extreme nonequilibrium conditions (i.e., large source-drain bias) required for device applications has received little attention.

We studied several AlGaAs/GaAs DELTTs with various growth structures. The source (top QW) and drain (bottom QW) contacts are formed by diffusing Au/Ge/Ni ohmic contacts to both QWs, then using Ti/Au surface gates to deplete the QW one does not wish to contact. Large-area top and/or back control gates act as third terminals by modulating the density of the nearest QW. We developed and utilized a novel epoxy-bond-and-stop-etch (EBASE) method to place the backgates only ~ 2 μm from the bottom QW. This allows the spacing between the depletion and control gates to be kept at 5 μm , reducing unwanted tunneling leakage current and yielding large peak-to-valley ratios.

At 1.5°K, low-density DELTTs exhibit very strong resonances in the small-signal source-drain conductance G as a function of top-control gate voltage (V_G). The resonance appears when the two QW subband minima line up at -0.12 V and has a peak-to-background ratio exceeding 50:1. In the source-drain current-voltage (I - V) curves at fixed V_G , the peak-to-valley ratios approach 20:1. More importantly, the resonance position depends strongly on V_G , clearly demonstrating gate-control of the tunneling.

At 1.5°K we demonstrated a bistable SRAM cell using a single DELTT and a 1-k-ohm load resistor in series. By controlling the position of the I - V resonance with the gate, we switch the circuit between two different stable operating points. The on-off voltage ratio is ~ 10:1, allowing simple biasing and good relative noise immunity. We also demonstrated a bistable memory using two DELTTs in series, biased so that both stable points of the circuit are in a I - V valley of a DELTT. This acts much like a unipolar complementary metal oxide semiconductor (CMOS) memory cell, with low current in both states. Due to the DELTT's multifunctionality, each of these two memory cells uses half as many transistors as required with conventional devices.

The DELTT's operating temperature is roughly given by the energy difference between the two QW subbands in the ungated regions. DELTTs with a large-density difference exhibited greatly improved temperature performance: At 77°K they exhibited peak-to-background ratios of 10:1 in the small-signal G versus V_G , and peak-to-valley ratios of 4:1 in the I - V curves. Using these devices we also demonstrated bistable memories and XOR and NAND logic gates at 77°K, using only one DELTT. (Larger-density differences and narrower QWs should enable room-temperature operation.) At present the DELTT's speed is limited by parasitic capacitance. We extended the EBASE technique to allow dual-side electron-beam writing for very high speed.

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Subwavelength Diffractive Optics

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Sandia is investigating subwavelength surface relief structures fabricated by direct-write electron-beam (e-beam) technology as unique and very high-efficiency optical elements. A semiconductor layer with subwavelength-sized etched openings or features can be considered as a layer with an effective index of refraction determined by the fraction of the surface filled with semiconductor relative to the fraction filled with air or other material. We can use such a layer to implement planar gradient-index lenses on a surface. Additionally, the nanometer-scale surface structures have diffractive properties that allow the direct manipulation of polarization and altering of the reflective properties of surfaces. With this technology we can use a single direct-write mask and etch to integrate a wide variety of optical functions into a device surface with high efficiencies, allowing, for example, direct integration of polarizing optics into the surfaces of devices, forming antireflection surfaces or fabricating high-efficiency, high-numerical-aperture lenses, including integration inside vertical semiconductor laser cavities.

We fabricated a high-performance lens composed of subwavelength grating structures that modulate the phase of each Fresnel zone of the lens by two pi. We designed these structures by optimizing the efficiency of each zone separately, then combining the gratings into a single pattern. As these structures are strongly birefringent, we had to take care to minimize the polarization sensitivity of the design so it would work with random polarization sources. The lens was similar in design to more conventional diffractive lens designs that we fabricated in the past so that comparison could be made to more conventional approaches. We fabricated the lens in GaAs for operation at 975 nm. We used direct-write e-beam lithography to make the pattern, which we transferred from the e-beam resist to a metal etch mask by lift-off processing. We etched the resulting lift-off pattern into the GaAs structure by reactive ion beam etching (RIBE) with chlorine.

The lens was an off-axis design that focuses the beam at a 20-degree angle to

the normal optical axis of the lens. The lens is 80 microns in diameter and has a focal length of 100 microns. This is a suitable size for integration with bottom-emitting vertical-cavity surface-emitting lasers (VCSELs), as we did with more conventional lenses. Measuring the performance of such a lens is difficult because of the small dimensions required for the setup. The primary measurement of performance is diffraction efficiency, which measures how well the lens actually focuses the light to where it is supposed to go. To do this we used a 20-micron-diameter aperture at the focal point of the lens and measured the light through the aperture, then compared it with the total light transmitted through the lens, whether focused or not. We measured this for both input polarizations, relative to the grating vector of the lens, which was primarily along the off-axis tilt direction. The lens had a diffraction efficiency of 72% for transverse electric (TE) polarization and 59% for transverse magnetic (TM) polarization. This performance compares very well with that of our conventional lenses, which were close to 80%, without as much polarization dependence. We did some preliminary investigation of fabricating these types of structures in fused silica for visible wavelength applications. We were able to demonstrate aspect ratios of 5:1 for fused silica grating structures (compared to 10:1 for GaAs), which should be sufficient for realizing some subwavelength designs. We also did some preliminary design work for beamsplitting and polarizing gratings in fused silica. In addition, we continued our computational development and our work on a modal approach to designing and analyzing these structures that promises to greatly reduce the time required to design new elements.

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Vehicle Exhaust-Gas Chemical Sensors Using Acoustic-Wave Resonators

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A need exists for on-line, real-time monitors that continuously analyze the toxic gases—nitrogen oxides (NO_x), carbon monoxide (CO), and hydrocarbon (HC) species—found in vehicle exhaust. Directly measuring gas concentration simplifies documenting compliance to Environmental Protection Agency (EPA) atmospheric emission regulations. Additionally, we can use such a monitoring system in a closed loop for engine control and performance optimization, leading to better fuel efficiency, lower toxic emissions, and generally higher customer satisfaction. In this project we explored acoustic-wave microsensors consisting of piezoelectric substrates coated with robust thin-film surface layers that have a specific affinity or reactivity to the target gas molecules. Acoustic-wave devices, surface acoustic-wave (SAW) devices, and thickness shear mode (TSM) resonators use quartz substrates for operating temperatures 500°C and below. At higher temperatures, we selected LiNbO₃ substrates for implementation. Significant thin-film coating development investigated pure and doped binary metal oxides (TiO₂, SnO₂, ZrO₂, and CuO), surfactant-templated mesoporous SiO₂ and ZrO₂ with transition-metal ion exchange (Cu, Pd, V, Fe, Cr, Mo), and the noble metal catalytic films.

The most promising sensor configuration consists of a high-surface-area, mesoporous Pd:SiO₂ film on a TSM quartz resonator acting as a trace HC calorimeter.

The TSM resonators and SAW devices sense gas concentration by measuring shifts in electrical resonant frequency, resonance damping, propagation phase delay, or wave attenuation when the chemical species interacts with the sensor coating. Changes in the coating mass, device temperature, surface stress, or film conductivity are mechanisms that can produce a measurable response.

The following are highlights of our major accomplishments over the past year:

(1) We characterized the frequency response and damping magnitude of bare and coated TSM AT-cut quartz resonators over the temperature range 20°–500°C. The frequency shift of these devices has a positive cubic dependence with increasing temperature. Sensor thin-film coatings do not change the response. Similarly, we characterized ST-cut and Y-cut quartz SAW devices. These devices have a quadratic negative temperature dependence. SAWs coated with platinum show added stress dependence in the frequency response.

(2) We implemented several improvements in the high-temperature acoustic device experimental system. We made changes in the gas flow system to add a second target gas to the mixture. We improved temperature control to better than 0.2°C at all points in the 20°–500°C range by implementing a high-current dc power supply. We wrote new HPVee data acquisition and control software. We are now using a new stainless-steel test device enclosure. The test cell can house two SAW or TSM resonators. All devices are fully wire-bonded to ceramic stripline substrates. We control and monitor the TSM resonator sensors using two lever oscillator electronic circuits that are tuned for 6-MHz operation and for the excess capacitance of the stripline conductors.

(3) We spin-deposited surfactant-templated periodic mesoporous SiO₂ thin films on TSM resonators from alcoholic acid-catalyzed sols. We used CTAB surfactant as the templating material. These films have unimodal pores of 2–3-nm diameter with pore spacing of 7–8

nm. Porosities are about 40–50%. The accessible surface area exceeds 1000 m²/g. Film thicknesses are 150–200 nm. The coated devices show good acoustic characteristics and stable thermal properties. We exchanged metal ions of Cu, Pd, Fe, Mo, Cr, and V into the SiO₂ films using metal-salt solutions. Electron parametric resonance (EPR) spectroscopy indicates ion concentrations of ~0.1 atom percent or greater. The ion exchange improves gas measurement sensitivity and provides some species discrimination.

(4) Testing of Cu²⁺:SiO₂ and Pd²⁺:SiO₂ sensors shows both having little sensitivity to CO gas. The response is nonlinear with concentration and exhibits some temperature dependence. Interaction in the sensor film occurs only in an oxygen-deficient environment, indicating that the reaction mechanism is CO oxygen stripping from the silica matrix, producing a slight, but measurable, mass decrease. Pd²⁺:SiO₂ sensors exhibit a large sensitivity to HC simulants (propylene and ethylene) and hydrogen but only in the presence of oxygen. The sensor response to propane is much smaller. Sensitivity to propylene is ~0.07 ppm DF/ppm propylene; minimum detectable concentration levels are ~20 ppm at 500°C. The interaction mechanism for the HCs is primarily calorimetric, producing an enhanced measurable temperature change as gases and oxygen combine at the sensor surface. Because the catalytic reaction occurs in the sensor film, it appears to stress the surface of the acoustic device, shifting the resonant frequency more than expected from simple heating.

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GaAs PIC Development for High-Performance Communications

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Sandia is establishing a foundational technology in photonic integrated circuits (PICs) based on the (Al,Ga,In)As material system for optical communication, radar control and testing, and network switching applications at the important 1.3- μm /1.55- μm wavelengths. We are investigating the optical and electrooptical performance characteristics of the fundamental building-block PIC elements designed to be as simple and process-tolerant as possible, with particular emphasis placed on reducing optical insertion loss. We are building relatively conventional device array and circuit designs using these PIC elements to establish a baseline performance standard; to assess the impact of epitaxial growth accuracy and uniformity, and of fabrication uniformity and yield; and to resolve the requisite optical and radio frequency (RF) packaging issues. We are exploring more novel and complex PIC designs and fabrication processes, viewed as higher payoff but higher risk, in a parallel effort and will mesh them into our baseline higher-yield capability as they mature. The first application focus targeted the design and fabrication of packaged solitary modulators meeting the requirements of future 10-Gb/s digital links and 60-GHz analog links. We expect successfully prototyped devices to feed into more complex PICs, solving specific problems in high-performance communications, such as optical beam-forming networks for phased-array antennas (PAAs). Possible candidate circuits are 1x32-switch matrices, millimeter-wave linearized modulators, and parallel arrays of high-density multi-Gb/s baseband modulators.

On our baseline effort, we demonstrated record low-loss optical waveguide routing and distribution components for (Al,Ga)As PICs, including (1) single-mode attenuations < 0.5 dB/cm (our best 0.4 ± 0.1 dB/cm), (2) right-angle turning mirror insertion loss of 0.4 ± 0.1 dB, a world-best record, and (3) excess loss of 0.4 ± 0.2 dB for lateral mode interference (LMI) 1X2, 1X4, 1X8, and 1X32 splitters, all with typically ~ 95% on-chip yields. We developed an approach to velocity match (< 10% mismatch) low-loss transmission line electrodes to undoped (Al,Ga)As optical-waveguide modulators with ~ 95% on-chip yields, fabricated wideband electrooptic waveguide modulators, and developed fiber packaging for loss-limited small-signal bandwidth > 50 GHz and fiber-waveguide-fiber-insertion loss of < 6 dB. We theorized and then demonstrated experimentally that the use of highly form-birefringent waveguide designs are a practical solution to obtaining high-extinction-ratio Mach-Zehnder interferometers, thus resolving the longstanding problem of device depolarization in semiconductor PICs. We based our novel approach on high-index-contrast digital alloys. The origin of the otherwise unpredictable lightwave depolarization is associated with uncontrolled strain introduced by residual electrode stresses and submicron misalignment on our deeply etched waveguide features, feature microroughness (especially sidewall roughness), and crystallographic misorientation of the starting substrates. Typical interferometer extinction ratios are now routinely measured to be in the 30-dB range, with a best value of about 43 dB, for devices that exhibit on-chip optical losses of 2-5 dB, and half-wave voltages of 4-10 V, depending on the design specifics. We invented and demonstrated a novel fiber-waveguide coupler to have ~ 1.5-dB insertion loss with substantial misalignment tolerance, a dramatic improvement over the 8-10-

dB range typically expected for very high electrooptic figure-of-merit (FOM) modulators. We demonstrated high FOM modulators with 15.5-dB (VD = 2.6 V) and 14-dB extinction ratios using novel XY combiner and cut-off mesa waveguide designs, respectively, and have on-chip losses of about 7 dB. We invented novel traveling-wave optical photodetectors using high-InAs-mode-fraction absorbing layers on standard low-loss AlGaAs waveguides and are developing them for wideband, high-optical-saturation-power RF applications. We invented a novel 1X32 switch based on LMI splitters, phase-modulated arrayed waveguides, and electrooptic in-plane focusing effects to address optical control problems in phased-array radars.

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Application-Specific Tester-on-a-Resident-Chip (TORCH)

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Manufacturers widely recognize testing as a major factor in the cost, producibility, and delivery of product in the integrated circuit (IC) business. Traditional test techniques are a major cost factor for stockpile electronics, where small production quantities make it difficult to amortize the cost of increasingly expensive testers. Application of multiple ICs in multichip modules (MCMs) greatly multiplies testing problems for commercial and defense users alike. Presently, each new design requires custom test hardware and software and often dedicated testing equipment costing millions of dollars. Also, physical properties of traditional test systems limit capabilities in testing at-speed (> 200 MHz), high-impedance, and high-accuracy analog signals.

Sandia proposes a revolutionary approach to these problems: replace the multimillion-dollar external test system with an inexpensive test system integrated onto the product wafer. Such a methodology enables testing functions otherwise unachievable by conventional means, particularly in the areas of high-frequency at-speed testing, high-impedance analog circuits, and known good die assessment. The techniques apply specifically to low-volume applications, typical of Defense Programs, where testing costs represent an unusually high proportion of product costs, not easily amortized.

Concept definition and verification occupied the tasks associated with Tester-on-a-Resident-Chip (TORCH-1). In this first year we had to determine how to technically reach our goals of miniaturizing and automating the test of ICs. We chose boundary scan as our primary

digital interface because of its low pin count and high clock speed. We developed a four-wire analog bus for measurements and created an on-chip switch matrix for routing signals to the test circuits. In addition, we attempted to create IC test building blocks such as the boundary scan test access port (TAP), analog-to-digital converters, digital-to-analog converters, timing circuits, and counters. We had mixed success in these areas. The control software and hardware were all custom built and were therefore not easily configured, which made them difficult to use. We adopted an antiquated scripting language as the control software, which made testing the part difficult. In addition, the IC was not designed with ease of use in mind, making it difficult to set up and use.

In year two of this project we redesigned the application-specific TORCH IC and applied it to a real, functional design by applying it to a quiescent current I_{DDQ} test function. The new design featured die-to-die communications more appropriate for MCMs, an improved boundary scan interface, improved timing measurements, and programmable faults for testing I_{DDQ} measurements. We added a method of measuring impedance of an IC pad and simplified or improved analog functions. An MS Windows-based hierarchical software system (LabView) controls the TORCH chip and collects data from internal registers. Control of the TORCH chip is a simple and portable system, involving a personal computer, commercial-off-the-shelf (COTS) boundary scan controller cards, and an open software control system that allows complete freedom of design while adhering to the IEEE standard 1149.1 boundary scan conventions. We developed a logarithmic auto-ranging analog-to-digital converter as part of TORCH-2. We also put this technology to use in other applications.

In year three of this project we compiled the learning from years one

and two and created a functional, simplified, and portable IC reliability and parametric test system. We created TORCH-3 using existing boundary scan interface technology from TORCH-2 and analog switching technology from TORCH-1 and TORCH-2. We created an automated reliability and parametric test system that automatically configures and tests ganged transistor and capacitor structures. We used boundary scan protocols to set up the test structures and the analog bus to collect the parametric data from the structures under test. The IC control and data analysis system is based on COTS software and hardware. LabView is an open software development system that permitted us to develop custom user interfaces that allow a hierarchical assembly of software modules to be developed. The end result is that the boundary scan protocols, key to the operation of the system, become transparent to the user, allowing the tester to concentrate on testing the part versus operating the IC. We reused the COTS boundary scan controller from TORCH-2 and used external source-measurement units (SMU) for ease of prototyping. Future derivatives of TORCH technology should focus on replacing the external SMU units with on-chip SMUs derived from the logarithmic auto-ranging analog-to-digital converter developed in TORCH-2.

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Ultra-Low-Power Microwave CHFET Integrated Circuit Development

D. F. Dubbert, R. J. Shul, D. Greenway, Jr., L. R. Sloan, A. G. Baca, V. M. Hietala, P. G. Muyschondt

Microwave-active devices such as gallium-arsenide (GaAs) metal-semiconductor field-effect transistors (MESFETs) and silicon bipolar-junction field-effect transistors (BJTs) typically do not exhibit low-power dissipation characteristics when optimized for high-frequency, low-noise applications. Logic functions implemented with GaAs MESFETs and BJTs also require relatively high operating power. Many high-frequency applications such as portable global positioning system (GPS) receivers, miniature tagging and monitoring devices, cellular phones, pagers, and personal status monitors (PSMs) would greatly benefit by the availability of a high-frequency amplification device that requires a low-voltage, low-current, single-ended supply. The activities proposed here are to develop the microwave devices. The goal is to realize high-gain, low-noise, low-power, positive-threshold devices for high-frequency and microwave applications. The emphasis will be on the lowest-power operation achievable.

We accomplished the following in FY97:

(1) Fabricated 2.4-GHz microwave monolithic integrated circuit (MMIC) amplifier based on junction field-effect transistors (JFETs).

(2) Fabricated a 200-MHz microwave hybrid IC based on 0.25- μ m pseudomorphic high-electron-mobility transistors (pHEMTs). At 50 μ W power, we obtained

7.5-dB gain and 7-dB noise figures. At 100 μ W, the gain was 9.5 dB and the noise figure was 7 dB.

(3) Wrote SAND report detailing MMIC performance and test results, pHEMT circuit test results, and all prior year results.

We revised some of the goals from those set at the beginning of the year due to evolving understanding of what the future system needs will be. Long battery life is the driver for ultra-low-power microwave circuits. We deemed a goal of 100 μ W to be feasible for this year with an ultimate goal of 10 μ W; thus the emphasis changed from further development of the 0.3- μ m JFET toward a 0.25- μ m pHEMT due to superior gain at 50- and 100- μ W power dissipation. The lower limits of usable gain for the JFET were at 250 μ W. For this reason we abandoned a second MMIC based on JFETs and developed pHEMT circuits instead. These pHEMTs are the lowest-power microwave circuits ever developed.

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Wafer Fusion for Integration of Semiconductor Materials and Devices

K. D. Choquette, S. H. Kravitz, M. H. Crawford, D. M. Follstaedt, O. B. Spahn

Sandia continued the development of wafer fusion to achieve integration of semiconductor materials and heterostructures with widely disparate lattice parameters, electronic properties, and/or optical properties for novel devices not now possible on any one substrate. Using our simple fusion process, which uses low-temperature ($\sim 500^\circ\text{C}$) anneals in inert N_2 gas, we will extend the scope of this technology to include such materials systems and devices as AlGaAs-based (infrared) and AlGaInP-based (visible) vertical-cavity surface-emitting lasers (VCSELs) on transparent AlGaAs and GaP substrates and fusion of III-V semiconductors to Si substrates. With an emphasis on the materials processes responsible for the atomic-scale fusion, we believe that mixing and matching a broad spectrum of materials will be feasible, enabling novel devices to be pursued. As a baseline fabrication technology applicable to many semiconductor systems, wafer fusion will revolutionize the way we think about possible semiconductor devices and enable novel device configurations not possible by epitaxial growth.

We established a simple, yet novel, wafer fusion process and fabricated numerous samples and optoelectronic devices as detailed in the following:

(1) Developed a reproducible and robust wafer-fusion process that uses low-temperature (300°–500°C) anneals in inert N₂ gas (rather than > 500°C in H₂).

(2) Established the wafer fusion parameter space for temperature (>500°C) and pressure (< 30 in./lb).

(3) The wafer-bonding process produces fused interfaces with intimate atomic contact with a 2–4-monolayer-thick disordered region.

(4) Examined the bonding achieved between GaAs/InP, GaAs/AlGaAs, GaAs/GaP, and InP/Si, including the case of patterned substrates, by cross-section transmission electron microscopy (TEM).

(5) Wafer-fused GaAs-based VCSELs to AlGaAs substrates to fabricate the first wafer-fused 850-nm bottom-emitting VCSEL arrays.

(6) Fused VCSEL heterostructures to GaP substrates to form novel bottom-emitting lasers on transparent substrates.

(7) Fused InP/Si and are pursuing the fusion of GaAs/Si for integrated microsystems applications.

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3506.120

Highly Parallel, Low-Power, Photonic Interconnects for Inter-Board Signal Distribution

P. J. Robertson, K. D. Choquette, V. M. Hietala, I. A. Erteza, B. H. Rose, D. C. Craft, B. T. Meyer, L. G. Pierson, M. E. Warren, C. J. Helms, L. Dean

The transmission of digital signals has become ubiquitous in Sandia applications that range from weapons interconnections to secure parallel computing and signal processing. Many of these digital interconnects occur at the board or connector level and require low-power communication of data in formats that allow for (1) electromagnetic interference (EMI) immunity, (2) scalability to large numbers of parallel channels, and (3) large data throughputs over serial links at moderate (< 3 m) distances. Performance of such connectors is typically limited by crosstalk, electrical impedance matching, contact area, and repeatable connections. Another factor that limits data throughput density is the need for equal numbers of signal and ground lines to prevent crosstalk and ground bounce effects. These difficulties can be alleviated with photonic interconnections that provide noncontacting separable connections, if the photonic interconnections can be realized at a sufficiently low-power consumption. We are combining Sandia's high-efficiency vertical-cavity surface-emitting laser (VCSEL) technology with appropriate optics or optical fibers and optimized photoreceivers to produce high-density, scalable interconnections that are separable, but that consume much less power than previous optical links using light-emitting diodes (LEDs) or edge-emitting laser sources.

We investigated and developed applicable devices and breadboards to allow further exploration of the three interconnection concepts. We developed a breadboard version of the high-isolation power and data transmission connector. The connector module uses VCSELs with external lenses and large-area detectors to transmit data bidirectionally across the isolation interface. Power is transmitted across the interface using a laser and a six-junction, center-tapped photovoltaic cell to generate the +3 V and –3 V power in the interior of the Faraday cage. We measured power-conversion efficiency at 13 percent.

We designed and fabricated applicable drive and receiver circuitry and performed initial tests of the circuitry. We designed and fabricated an integrated detector/receiver circuit based on heterojunction bipolar transistors (HBT) technology. We expect this circuit to operate at up to 3 Gbps. We completed a new low-power design using complementary HBT technology that will be directly compatible with complementary metallic oxide semiconductor (CMOS) circuitry at 100 Mbps. We simulated power dissipation for the 3-Gbps transimpedance amplifier to be only 50 mW at 3.3V.

At the breadboard level, we investigated the applicability of free-space external lensing and fiber-optic interconnections for board-level interconnections. In addition, we completed applicable binary lens designs and fabricated an integrated receiver design by Georgia Tech in a GaAs field-effect transistor (FET) technology.

Achromatic Nonlinear Optics for Sensing and Process Control

R. P. Trebino, M. G. Mitchell, B. A. Richman, S. E. Bisson

Sandia performed extensive and more detailed and precise modeling of several achromatic phase-matching (APM) designs and experimentally tested two superior designs, achieving a tuning range of 85 nm with a six-prism APM design (150 times the range of the nonlinear crystal without APM), and 100 nm with a "grism" (a transmission grating on the surface of a prism) design.

As in the previous year, we model our APM designs precisely by using the exact refractive-index-versus-wavelength curve of the nonlinear crystal beta barium borate (BBO) and of the prisms. We very accurately calculated all beam angles and the second-harmonic-generation (SHG) efficiency versus wavelength. We optimized the overall efficiency with respect to all prism incidence angles to find prism arrangements that have good phase-matching over very large tuning ranges.

We need a minimum of six prisms to obtain sufficient dispersion without large incident and exit angles (for which antireflection coatings are difficult to make) such that all beams cross in the crystal. We use the many degrees of freedom (DOFs) to adjust the dispersion to high order.

This year, we experimentally demonstrated two arrangements, the better being a six-prism arrangement with a 4-mm-thick type-1 BBO crystal. We used an optical parametric oscillator between 600 and 700 nm as input to the APM apparatus and achieved a tuning range of 85 nm. The six-prism device uses an additional six prisms after the crystal to align all of the second-harmonic beams.

The use of diffraction gratings, which have greater dispersion than prisms, may soon be possible because of progress in the production of highly efficient gratings. In anticipation of such availability, we also demonstrated a design based on a grism, which produced a 100-nm tuning range.

In the past year, we performed extensive, detailed, and precise modeling of specific APM designs. Based on the results of these calculations, we experimentally tested two designs, achieving a tuning range of 85 nm (150 times the range of the same crystal without APM) using a device consisting of six prisms and a 4-mm-long type-1 BBO crystal, and 100 nm using a "grism" device. The six-prism device uses an additional six prisms after the crystal to align all of the second-harmonic beams.

We continued to use our extremely precise computer model to examine possible APM designs. We optimized the overall SHG conversion efficiency with respect to all prism incidence angles. We found that nonlinear terms yield complex behavior in the tuning curve. We also found that three-, four-, and five-prism arrangements generally do not suffice. Such simple designs lack sufficient dispersion, require large incidence and exit angles that cause excessive reflective loss, or cannot make the beams of all wavelengths cross in the crystal. At least six prisms are needed to overcome these problems. However, the need for as many as six prisms is not problematic because prisms are inexpensive, compact, and easy to work with. The use of many prisms also yields more DOFs, which is helpful for adjusting the APM dispersion to match the BBO crystal phase-matching-angle tuning curve to high order, just as the use of several lens elements achieves more achromatic performance in a camera lens.

We experimentally demonstrated one six-prism arrangement. Our arrangement used SF-11 glass Brewster prisms, Littrow prisms (and one F-2 glass Littrow prism), and a 4-mm-thick type-1 BBO crystal. We used the output of a Nd-YAG-laser-pumped optical parametric oscillator (which is used in Lidar experiments) between 600 and 700 nm as input to the APM apparatus. We obtained a tuning range of 85 nm. For comparison, the tuning curve for the crystal without an APM apparatus is less than 1 nm. The improvement due to APM is approximately 150. We took care in the design to prevent the divergence of each monochromatic beam from exceeding the angular acceptance of the crystal, which would compromise conversion efficiency. We chose and arranged the first two prisms in the apparatus specifically to accomplish this.

Another six prisms (all fused silica) after the crystal align all of the second-harmonic beams onto a single path. The position at the device output varies by only one-quarter of a beam spot diameter as the wavelength is tuned over the entire tuning range, and the output angle varies by only 200 microradians.

The use of a diffraction grating (previously considered undesirable due to inefficiency) may soon be feasible because of rapid progress in the production of highly efficient gratings. Gratings have the advantage that their dispersion can be much greater than that of a prism. We tested a simple design using a grism. Both our model and our experimental measurements produced a tuning range of 100 nm with a 4-mm-long BBO crystal, 200 times the range of the crystal without APM. We also modeled output designs using grisms.

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3506.140

Virtual Reactor for the Semiconductor Manufacturing Plant of the Future

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Drummond, K. C. Baucom, C. P. Tigges, J. F. Klem

This project will develop a sophisticated system to enable model-based agile manufacturing in the critical metalorganic chemical vapor deposition (MOCVD) and molecular beam epitaxy (MBE) materials growth processes essential to high-speed microelectronic and optoelectronic components. This effort is founded on a modular and configurable process automation system that will serve as a backbone allowing integration of process-specific models and sensors. Sandia will develop and integrate both MOCVD- and MBE-specific models in this system and demonstrate the effectiveness of both model-based and sensor-based real-time feedback control in improving the accuracy and reproducibility of semiconductor heterostructure growth on MOCVD and MBE systems. In addition, within this framework we will construct "virtual reactor" models for both growth processes and show how we can use these models to greatly shorten the epitaxial growth process development cycle.

We installed and tested two complete MOCVD reactor automation systems using this scheme, the first on a system used primarily for the growth of antimonide-based materials and the second on a system dedicated to growth of Group-III nitrides. We constructed a

virtual reactor prototype using the LabView software.

The virtual reactor can be driven by the programmable logic controller (PLC) and responds to exactly the same set of electrical signals/commands that the PLC sends to the actual reactor to drive the hardware. The virtual reactor gives a graphical display showing the status of all relevant components of the system (valve positions, flow rates, etc.). The virtual reactor model will find immediate application in developing safety interlocks on our MOCVD systems. We tested the link between LabView and a user-written software module. We began development of chemical models for antimonide deposition and simplified rotating-disk reactor models for incorporation into the virtual reactor.

We installed a single-wavelength reflectance monitor on our EPI (manufacturer) MBE chamber in the past 6 months. We designed a wafer-rotation-synchronous detection system and implemented it to minimize wafer wobble effects in obtaining the reflectance signal. As a test of the MBE reflectance system, we acquired *in situ* data during growth of a series of custom reflectance modulators. We began correlating the *in situ* reflectance measurements with post-growth *ex situ* measurements.

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Integrated Separation and Optical Detection for Novel On-Chip Chemical Analysis

M. E. Warren, J. R. Wendt, P. L. Gourley,
D. S. Anex

The future of advanced chemical detection and analysis is in miniature devices that are able to characterize increasingly complex samples. These attributes are embodied in a "laboratory-on-a-chip." In this concept, chemical operations used to analyze complicated samples in a chemical laboratory—sample handling, species separation, chemical derivatization and detection—are incorporated into a miniature device. By using electrokinetic (EK) flow, this approach does not require pumps or valves, as fluids in microfabricated channels can be driven by externally applied voltages. This is ideal for sample handling in miniature devices, since external voltages can be used to deliver samples and to drive them through separation columns. This is an opportunity for Sandia to develop on-chip electrokinetically driven separation columns integrated with photonic devices for miniaturized chemical-analysis systems. This project will develop a key component of a miniaturized chemical-analysis system—truly miniature on-chip optical systems based on vertical-cavity surface-emitting lasers (VCSELs) and diffractive optics. We will build these into a complete system that also has on-chip EK fluid handling and chemical separation in a microfabricated column. Such an advance is a critical step to full miniaturization, enabling increased portability, analysis speed, and operational flexibility.

Major activities will center on four areas. The first is the design and fabrication of an on-chip separation column with fluorescence sources and detectors that, utilizing EK flow, we can use as the basis of an automated chemical-analysis system. The second involves investigation of an advanced technique, developing a dispersed fluorescence module that we can use

to extend the versatility of the basic system. The third is investigation of on-chip, intracavity laser absorption as a high-sensitivity detection technique. The fourth part of the project will be a concurrent testing and characterization program.

A major part of this project is the use of VCSELs to excite tag dyes that we separated in an etched capillary channel by electrophoresis. We fabricated VCSELs for this project, but have not yet produced any exactly matched to a dye that can be used for an actual analysis by being tagged to a specific molecule of interest. Our current choice for this is a dye for DNA sequencing that can be pumped at 750–760 nm. We now have a full wafer with epitaxial growth of a VCSEL structure that will give us 760-nm emission, which should work well with the tag dyes that we will use for a separation and detection demonstration.

We performed the electrophoretic separation of the fluid in capillary channels. Part of this project is to demonstrate such separations in planar channels etched in a fused silica substrate. We are continuing to fabricate flow channels in fused silica for capillary separations. This is now a well-established, high-yield process. Last year we demonstrated use of such channels for chromatographic separations with a simple channel sealed to a cover plate with an ultraviolet (UV) photostetting adhesive. To improve on that result, it is necessary to fabricate and seal more complex flow channel patterns.

Sealing the capillary channels etched into the fused silica substrates was a much more difficult challenge than originally anticipated. We worked on a polyimide sealing layer between the channel substrate and the cover, which was unsuccessful. We were able to use silicone adhesives to seal channels for preliminary testing, but are continuing to work on other sealing techniques on related projects.

Another important aspect of this project is the use of microoptical elements, such as diffractive lenses, to route the light for the fluorescence spectroscopy system through the transparent flow

channel system in a planar interconnect architecture. We designed the diffractive optical elements for the planar, folded-path, optical layout envisioned for this project. We are fabricating the collection optic for the fluorescence emission from the flow channel.

We accomplished the final assembly of the microanalysis system by a combination of adhesive bonding of some components and, in the case of active electronic components, a process called *flip-chip bonding* that simultaneously provides mechanical placement and attachment of the die and electrical connections to the die. This is the method we will use to attach the VCSEL or VCSEL array to the analysis module. We acquired a new flip-chip alignment and bonding capability that we have been applying to this project. The system is capable of aligning the chip to the substrate with a precision of ± 2 microns, far better than what we could achieve before.

Due to the delays we encountered in addressing the channel sealing issues, we were not able to complete an assembled analysis module on time. However, we demonstrated the fabrication and performance of the various subsystems that are needed which substantially demonstrated the feasibility of such a system.

We also investigated light-emitting semiconductor/glass microcavities filled with simple fluids for use as sensing devices. Specifically, we examined surface tension for transporting liquids into the intracavity space and studied the influence of the liquid on the spectral emission of the microcavity. This transport mechanism is not electroosmotic flow as in the previous description, but pressure-driven or capillary flow. The microcavity laser studied here is formed by bringing semiconductor and glass surfaces together. The intracavity space between these surfaces is a critical parameter for the operation of the laser. It is typically a few microns. Larger spacings create more diffraction loss, lower-cavity Q, and higher pumping threshold.

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3506.170

High-G Accelerometer for Earth-Penetrator Weapons Applications

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This project focused on the development of a new micromachined silicon accelerometer capable of surviving and measuring high-G shocks. Sandia employed surface-micromachining fabrication technology to develop an accelerometer that was both cheaper and more reliable than currently available sensors.

Initially we modified, fabricated, packaged, and tested a diaphragm pressure sensor. This design demonstrated inadequate frequency response and high failure rate.

We developed a second design using a suspended proof mass and reference capacitor as the sensing elements of the sensor. We integrated microelectronics

signal sampling and signal conditioning circuitry on the same substrate as the sensor elements. We fabricated, packaged, and tested the second design. We limited acceleration measurements using this design to 15,000 Gs due to the saturation of the microelectronics. Excessive gain in the on-chip amplifiers and a rail bias limited electronic output to a single polarity and reduced the sensing dynamic range-caused saturation.

We developed a third design that incorporated residual stress relief in the mechanical structures as well as lower electronic gain and greater signal conditioning in the on-chip electronics. We also fabricated, packaged, and tested these devices. We obtained acceleration levels of 25,000 Gs, but we expect higher levels (exceeding 50,000 Gs) when testing is completed. We addressed several issues related to packaging (die attach adhesion due to release treatments and cracking of the packages at high-G loads); additional testing is forthcoming.

Results of a failure analysis performed on an Endevco 7170A accelerometer device using hermeticity testing, delidding, optical microscopy, scanning-electron microscopy (SEM), and internal impact damage analysis showed chipping and complete breakage of the proof mass at high-G levels. Failures in the piezo-resistors also occurred, which caused a resistance shift and eventual open condition to occur. Both the resistor bridges and wire bonds contributed to the failures.

Results of diaphragm pressure sensor testing showed that the design demonstrated inadequate frequency response and high failure rate. We identified several packaging issues, including bond wire breaking and lid seal failures. These devices did perform up to 50,000 Gs in some cases with low-noise output; however, the frequency response was inadequate.

Results of the second design, which incorporated a suspended proof mass and reference capacitor as the sensing elements of the sensor, demonstrated that modifications to the on-chip electronics were necessary to obtain a sufficient dynamic range. We limited acceleration measurements using this design to 15,000

Gs due to the saturation of the microelectronics. Saturation was caused by excessive gain in the on-chip amplifiers and a rail bias that limited electronic output to a single polarity and reduced the sensing dynamic range. We also detected significant signal noise with this design and incorporated plans to filter it on-chip into later designs.

We developed a third design, based on the suspended proof mass and reference capacitor sensor, that incorporated residual stress relief in the mechanical structures as well as lower electronic gain and greater signal conditioning in the on-chip electronics. We also fabricated, packaged, and tested these devices. We obtained acceleration levels of 25,000 Gs, but we expect higher levels (exceeding 50,000 Gs) when testing is completed. We addressed several issues related to packaging (die attach adhesion due to release treatments and cracking of the packages at high-G loads), and additional testing is forthcoming. Die adhesion failures at 20,000- to 25,000-G accelerations occurred due to the surface treatment used during fabrication. We modified the surface treatment to preclude future die adhesion problems. We undertook modifications in the chip clamping bracket (including equal distribution of mechanical stress) to minimize stress concentrations to the package during shock loading. Significant reduction in package body failure resulted.

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Selective Oxidation Technology and Its Applications Toward Electronic and Optoelectronic Devices

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Sandia developed a robust, manufacturable oxidation process, resulting in the design, fabrication, and testing of high-power, high-speed, oxide-confined vertical-cavity surface-emitting laser (VCSEL) structures. Furthermore, extended lifetime tests prove that reliability of the oxidized VCSELs is comparable to commercial implanted devices. Studies of oxidation of Al(Ga)AsSb indicate that separation of the metallic Sb layer can be controlled by the thickness of the cap layer and inclusion of a small percentage of Ga. Also, it appears that As/Sb mole fraction plays a significant role in the oxidation process, with at least some amount of As necessary for oxidation to proceed. Discovery of rapid oxidation of AlAsSb lattice matched to InAs allowed for fabrication of environmentally sealed edge-emitting lasers emitting in the 3–5-mm region. Furthermore, we fabricated and characterized edge-emitting lasers using AlAsSb on InP, where the metallic Sb layer aids current injection. Another device structure that utilizes the peculiar nature of oxidized AlAsSb is a collector up p-n-p heterojunction bipolar transistor (HBT) fabricated and characterized during the past year. Finally, research on the nature of and the means for removal of the interfacial As, which is a product of oxidation of AlGaAs, indicates that the problem may be fundamental in nature, due to unfavorable thermodynamics. Thus utility of oxidized AlGaAs for metal-semiconductor field-effect transistor (MESFET) application is questionable, and other approaches are needed.

We developed a robust oxidation fabrication process for optoelectronic devices. We characterized the influence of gas flow, gas composition, and layer thickness on the oxidation rate to establish a reproducible oxidation fabrication process. We improved the uniformity of the oxidation system to $\pm 2\%$, which for oxidation of $\text{Al}_{0.98}\text{Ga}_{0.02}\text{As}$ corresponds to an AlAs mole fraction variation of ± 0.001 .

This year we designed and demonstrated long-lived VCSELs. At an ambient temperature of 80°C , the current required to maintain 1-mW output power remains relatively unchanged for nearly 10,000 hours, which is comparable to the reliability of commercial ion-implanted VCSELs. Devices employing oxidized AlAs current confinement layers instead of $\text{Al}_{0.98}\text{Ga}_{0.02}\text{As}$ degraded quite rapidly.

We designed and characterized high-power and single-mode selectively oxidized VCSEL structures. We designed a reduced confinement and low-loss oxide aperture to promote high single-mode power. We demonstrated a record 3.5 mW of single-mode power at 850 nm. In addition we achieved 20-mW maximum output power from an oxide-confined VCSEL with $20\times 20\text{-}\mu\text{m}$ aperture.

Selectively oxidized 850-nm VCSELs demonstrated a record high 21.5-GHz small-signal modulation bandwidth. These devices employ a combination of selective oxidation and ion implantation to achieve optical and electrical confinement with reduced capacitance.

We determined the role of As/Sb ratio in oxidation AlAsSb. We found that oxidation of $\text{AlAs}_x\text{Sb}_{1-x}$ for $x=0.16$ proceeds more rapidly than for any other x , while for $x=0$, oxidation does not take place. This enabled fabrication of ridge waveguides for long-wavelength (3–5 micron) edge-emitting lasers, which use $\text{AlAs}_x\text{Sb}_{1-x}$ with $x=0.16$ as a cladding layer.

Location of the metallic Sb layer formed upon oxidation can be controlled by the thickness of the cap layer above

the AlAsSb layer to be oxidized. Another method of controlling the Sb separation is the inclusion of cladding layers around AlAsSb that contain 2% Ga. We also designed, fabricated, and tested an edge-emitting laser utilizing oxidized AlAsSb and the metallic Sb layer. Active region consisted of InGaAs/InAlGaAs multiple quantum wells that emitted at 1.5 μm . In addition, we fabricated identical lasers without oxidized AlAsSb cladding.

We designed, fabricated, and tested a collector-up, p-n-p HBT incorporating oxidized AlAsSb. Partially oxidized AlAsSb layer served to define an emitter that we aligned to a top InGaAs (GaAsSb in another structure) collector. The metallic Sb layer that protruded into the base region contributed to the increased conductivity of the base region. We measured gains of 20 in the larger devices.

We identified the source for the high "interface state density" at oxidized Al(Ga)As/GaAs interfaces and developed a new interpretation for the interface electrical properties that has serious implications for electronic applications of AlGaAs- or AlInAs-derived wet oxides. High-As-content aluminum-oxide/GaAs interfaces show little or no capacitance modulation, while samples with low As exhibit some capacitance modulation, indicating partial Fermi-level movement. Large spatial variation of the potential within the semiconductor near the oxide interface under conditions of accumulation result from the spatially nonuniform pinning of the Fermi level at the low-As interfaces. The resulting collapse of the 2-D electron gas into isolated patches of high electron density with a large activation barrier for transport between patches impedes electron transport parallel to the oxide interface. We found the conductivity parallel to the interface, the transconductance, to be surprisingly low in AlGaAs-derived FETs, consistent with our model.

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Agile Prototyping of Microelectromechanical Systems (MEMS)

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Under this project Sandia is developing an agile prototyping capability for microelectromechanical systems (MEMS) sensors and actuators based on Sandia's state-of-the-art four-level polycrystalline silicon micromachining process, Sandia Ultra-Planar Multilevel MEMS Technology (SUMMiT).

Making the Microelectronics Development Lab's (MDL) state-of-the-art surface-micromachining technology more widely available will vastly increase its impact. The agile prototyping capability will make available to a variety of both Defense Program (DP) and non-DP programs the ability to test new concepts in this advanced manufacturing technology in a relatively short period of time. Sandia's capability to manufacture MEMS structures with four levels of polysilicon and integrated electronics will be unique among the micromachining facilities.

We completed several lots of wafers in SUMMiT using a reticle that includes designs by designers from outside Sandia as well as designs from Sandians outside the MDL. We made the manufacturing process more robust and began correlating performance data with process control data. We also made good progress on design tool development—this year we integrated design-rule checking into our computer-aided design (CAD) environment. Finally, we far exceeded our goals in developing training materials for new designers: We developed an information-packed three-day short course to train designers and gave this very popular course seven times to over 150 designers within 13 months.

In the coming year, we will continue to run lots on new customer reticle sets, including RS-117, RS-122, and subsequent customer reticles. We will continue to perfect the fabrication process and add new experimental process modules to the baseline process technology (such as a fifth layer of structural polycrystalline silicon and integrated electronics). In addition, we will be formalizing our statistical process control (SPC) methods by using the computerized tracking system in the fab (COMETS and RS-1) to generate for our MEMS process SPC charts similar to those used in the integrated circuit (IC) industry. We will also be redesigning our performance data collection test structures to facilitate automated testing.

A number of structures using the SUMMiT process were designed by short-course participants. Their design efforts resulted in several new devices not previously possible using other MEMS fabrication technologies.

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Advanced Concepts for High-Power VCSELs and VCSEL Arrays

K. D. Choquette, G. R. Hadley, W. W. Chow

Sandia continued to investigate and develop vertical-cavity surface-emitting lasers (VCSELs) for operation at high continuous-wave (CW) single-mode output power and pulsed high-power operation. The high-power CW approach focused on "leaky-mode" concepts using lateral modification of the cavity resonance to provide the lateral refractive index difference. VCSEL heterostructure designs for high-power operation, particularly pulsed high power, are generally not appropriate for efficient CW operation. Thus, examining pulsed high-power VCSELs could open up an entirely new opportunity for VCSEL applications. In this area, we are pursuing both new cavity designs and heterostructure active regions optimized for high-power pulsed operation. We are also exploring 2-D individually addressable VCSEL arrays for high-power operation. This effort entails characterization of thermal management issues in the VCSEL array. The overall project objective is to develop high-power single-mode or multimode sources appropriate for many applications leveraging the many inherent advantages of VCSELs.

We accomplished all of the goals established last year and added three extra milestones:

(1) Triggered photoconductive semiconductor switch using high-power selectively oxidized VCSEL.

(2) Achieved record high-power (3.5 mW) single-mode operation in 850-nm VCSEL using novel three-fourths-wavelength-thick buried oxide with tapered profile designed for low optical loss and optical confinement.

(3) Demonstrated high CW power (15 mW) from each element of 8x8 selectively oxidized VCSEL array.

(4) Demonstrated 300-mW CW power from an 8x8 selectively oxidized VCSEL array.

(5) Fabricated metalorganic vapor phase epitaxy (MOVPE)-regrown VCSELs with cavity resonance modification via epitaxial regrowth of the top mirror over the patterned substrate.

(6) Developed dynamical model for gain-switched VCSEL operation to support the experimental effort.

(7) Measured 13-psec pulsewidth and 80-mW peak power from gain-switched VCSELs.

(8) Experimentally determined the optimum output mirror reflectivity for various quantum-well active regions within high-power selectively oxidized VCSELs.

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3506.210

Midwave-Infrared (2-6 μm) Emitter-Based Chemical Sensor Systems

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Long-wavelength (2-6 μm) diode emitters are desirable for many applications, including monitoring of chemical species in the environment and manufacturing, long-wavelength fiber-optic communications, lidar, and infrared (IR)-detector countermeasures. No practical diode lasers are available for any of these applications because the band structure of bulk III-V, II-VI, and IV-VI semiconductor alloys results in large Auger recombination rates at these wavelengths. Experimental and theoretical work at Sandia has resulted in new understanding of the electronic properties of narrow-bandgap III-V heterostructures, and we found methods of reducing the Auger rates in certain InAsSb superlattices and quantum wells (QWs). These devices enable us to begin chemical-sensing demonstrations of important species such as CO-CO₂ and numerous other compounds. This project will involve developing chemical-sensing systems and determining the sensitivity and limitations of these systems. Concurrently, we will improve upon IR emitters used in these systems.

The long-range focus of this project was to develop superior IR emitters (lasers and light-emitting diodes [LEDs]) and to utilize these new IR devices for

high-sensitivity chemical-sensor systems.

In the last year, we made significant progress toward this goal.

We developed LEDs producing record powers at 300°K. We grew InAsSb multiple QW LEDs covering the 4.0-5.0- μm -wavelength range and InAsSb/InAsP strained-layer superlattice, 3.5-4.5- μm LEDs by metalorganic chemical vapor deposition (MOCVD). At 300°K, both devices produce > 100 μW , and they are approximately 10x brighter than commercially available midwave-IR (MWIR) LEDs. We recently developed the InAsSb/InAsP strained-layer superlattice active region, used in one of the LEDs, for our MWIR device program. InAsSb/InAsP strained-layer superlattices promise to have lower Auger recombination rates than alternative, metalorganic chemical vapor deposition (MOCVD)-grown active regions. Initial results for LEDs and lasers with InAsSb/InAsP strained-layer superlattice active regions show state-of-the-art performance. We achieved record-setting operating temperature (240°K) for an Sb-based, 4- μm laser with an InAsSb/InAsP strained-layer superlattice, active region device.

Publications

Refereed

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Microelectronic Biosensors

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In the second year of the project, Sandia focused on the development of a class of microelectronic biosensors called bioFETs. BioFETs are biologically modified ion-sensitive field-effect transistors (ISFETs) in which an enzyme is attached to the gate of the ISFET. The enzyme is a biocatalyst for reactions involving a related target chemical. The underlying ISFET detects the ionic reaction products, providing information about the presence and concentration of the target chemical. For the direct detection of chemical weapon (CW) agent, we demonstrated single-chip integrated bioFETs based on organophosphate hydrolase (OPH) enzyme. We tested these bioFETs using an organophosphate (OP) pesticide, paraoxon, as a surrogate CW agent. We also investigated use of OPH enzymes in a more robust cross-linked enzyme crystal (CLEC) form. In addition, we investigated photolithographic planar processes for application and covalent attachment of enzymes to the gates of ISFETs. The ultimate goal of the project is a combinatorial bioFET array.

We demonstrated an all-on-a-single-chip integrated bioFET composed of paired ISFETs, one enzyme coated to produce a bioFET, one uncoated to act as a reference ISFET. The pair is referenced to a single pseudo-reference platinum electrode, also on the single silicon chip.

We prepared CW agent-detecting bioFET sensors in two forms: (1) an indirect detecting version using acetylcholinesterase (AChE) enzyme, and (2) a direct detecting version using OPH enzyme. We tested these using an OP pesticide, paraoxon, as a surrogate for the CW agent. In the indirect detecting sensor, the OP inhibits the action of the AChE enzyme upon acetylcholine. Reduced activity is detected as OP exposure. In the direct detecting sensor, the OPH enzyme directly hydrolyzes the OP compound, producing detectable ions in proportion to the OP concentration.

In the area of OPH enzymes, we successfully demonstrated that covalently attached enzymes exhibit significantly better resistance to degradation than the unattached enzyme. To improve sensor lifetime, we have been investigating CLECs. A CLEC is a modified, highly robust form of enzyme that still exhibits true enzymatic activity despite crosslinking and crystallization. They are being developed in the biochemical technology field for continuous reuse in large biochemical reactors. We are

investigating their use in bioFETs. We obtained both the conventional and the CLEC forms of the OPH enzyme through a collaboration with Texas A&M University. Whether the CLEC form will produce longer-lived bioFETs awaits further trials.

We investigated the use of microphotolithography techniques for biocoatings. This capability is required to produce arrays of bioFETs on a single chip. Ordinary microphotolithography techniques are too harsh. We demonstrated that the patterning of bioproteins onto semiconductor substrates can be achieved through stabilization of the bioproteins with disaccharides during photolithography processing. Protective photoemulsion pattern masks facilitate selective removal of bioprotein via exposure to an oxygen plasma, after which the mask layer is stripped and the disaccharide dissolved to yield patterned active bioprotein.

The ultimate goal of this project is a combinatorial bioFET array. On the technical side, our early efforts at producing lanthanum fluoride pF (i.e., fluoride ion concentration)-sensitive ISFET surfaces resulted in only insensitive surfaces. We are currently conducting materials studies to evaluate this result. It appears our early lanthanum fluoride surfaces may be too crystalline. A more amorphous structure is re-

quired. At the end of FY97, we were preparing a new batch of wafers with silicon nitride surfaces. These will be substrates for lanthanum fluoride coatings produced at several commercial companies specializing in ultraviolet (UV)-reflective photonic coatings. Likewise, we developed and tested the circuit for a companion control IC.

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A Novel Nondestructive Silicon-on-Insulator Nonvolatile Memory

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Many commercial and defense systems require nonvolatile memories that can store program and critical data without loss of information even in the harsh environments associated with satellites and nuclear weapons. Silicon-on-insulator (SOI) technology is inherently more resistant to radiation-induced single-event upset and high-dose-rate pulses of ionizing irradiation than bulk-silicon complementary metallic oxide semiconductor (CMOS) technology and operates at lower power. Previous work showed that elevated temperature ($> 500^{\circ}\text{C}$) anneals in ambients containing hydrogen can generate mobile, positively charged protons in the buried oxides of SOI transistors. The protonic transport has potential applications in the design of novel nonvolatile readout electronic and optical memory devices. In this project, Sandia proposes a broad-based program to design, fabricate, characterize, and optimize hydrogen-annealed SOI transistors and simple circuits for the realization of this novel, low-power nonvolatile memory.

The project is divided into three years. During the first year we advanced the nonvolatile field-effect transistor (NVFET) concept from the laboratory stage and demonstrated the proof-of-concept in a fabrication facility at the capacitor level. During the second year, we will refine and optimize methods for protonating SOI buried oxides, and design and begin fabrication of NVFET transistor and integrated circuit (IC) test structures. In the third year, we will conclude the program by demonstrating the proof-of-concept at the transistor and IC levels.

During this first year, we successfully demonstrated the protonic memory concept in a fabrication facility and the feasibility of a SOI NVFET. We designed and fabricated a capacitor mask set that included capacitance-voltage (C-V), point-contact transistor, and electron paramagnetic resonance (EPR) test structures. We wrote software to performing the C-V and point-contact transistor measure-

ments. We fabricated capacitors using SOI substrates with buried oxide thicknesses from 100 to 370 nm. We investigated varying forming gas anneal temperatures and furnace pull rates in the laboratory. We determined the optimum temperature for generating mobile protons to be around 600°C . We also observed the furnace pull rate to have a significant impact on the number of mobile protons. If the total time to pull the wafers from the furnace exceeded 10 minutes, the number of mobile protons decreased significantly. For the some of the capacitors, we pulled the wafers at the fastest rate possible for the horizontal furnaces used for the anneal (total time ~ 5 to 10 minutes).

The largest voltage hysteresis (1.13 ± 0.17 V) was for separation by implementation of oxygen (SIMOX) substrates using a low-dose implant with a buried oxide thickness ~ 100 nm. Although this shift is smaller than that expected based on laboratory forming gas anneals (~ 5 V) where extremely high pull rates were used, it demonstrates that we can successfully protonate SOI buried oxides in an IC fabrication facility. We determined the cause of the smaller shifts to be the longer pull rate.

We also characterized capacitors for the change in the number of mobile protons before and after irradiation, voltage cycling (fatigue), and long-term storage (retention). We irradiated capacitors using a 10-keV x-ray source with no bias (floating), positive polarity bias, or negative polarity bias during irradiation. With no bias applied during irradiation, we observed a negligible decrease in the hysteresis for total doses up to 1 Mrad (SiO_2). Irradiating capacitors with a negative polarity bias also resulted in little or no change in hysteresis voltage shift for doses up to 200 krad (SiO_2). However, irradiating capacitors to 100 krad (SiO_2) with a positive top silicon polarity bias resulted in nearly 100% of the protons being trapped near the bottom Si/ SiO_2 interface, reducing the hysteresis voltage shift to near zero. In actual device operation, irradiating under a positive bias corresponds to irradiating a memory transistor while writing it to the "off" state. Most of the time, memory transistors will be unbiased during irradiation. To investigate the fatigue properties, we stressed some capacitors (370-nm gate

oxide) with a 20 V AC signal for up to $1\text{E}4$ cycles. We observed no loss in hysteresis voltage shift during the cycling. To investigate the retention characteristics, we characterized some capacitors with the protons poled at either the top or bottom interface and periodically characterized using point-contact transistor I-V measurements. We observed no change in source-to-drain current for capacitors poled with the protons at either the top or bottom interface for times up to $1\text{E}5$ seconds (the last measurement point) at 200°C . This provides a proof-of-principle demonstration of the retention capabilities of the devices.

During the course of this work, we also observed that moderate-temperature hydrogen anneals have a significant effect on the quality of SIMOX buried oxides. Annealing SIMOX substrates in forming gas substantially reduced the number of high leakage current capacitors and the number of capacitors that broke down at low electric fields. Thus, we can use a moderate-temperature hydrogen anneal to significantly increase buried-oxide integrity for improved circuit yield and reliability.

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3506.240

Integration of Optoelectronics and MEMS by Free-Space Microoptics

M. E. Warren, M. H. Crawford, G. A. Vawter, J. R. Wendt, J. H. Smith

Combining microelectromechanical systems (MEMS) with optoelectronic components is a means of realizing compact optomechanical subsystems. Some examples are laser beam scanning, switching and routing and active focusing, and spectral filtering or shuttering of optical sources. A major obstacle to realizing these types of systems is the difficulty of integrating the two technologies. The devices use dissimilar materials with significant problems for a common process line. Another major difficulty with direct integration is providing the optical path for the MEMS components to interact with the light source. Simply stacking one device on top of another is not compatible with many optical wavelengths. Sandia proposes to use folded optical paths in a transparent substrate to provide the interconnection route between the components of the system. We will surface-mount the components by flip-chip bonding to the substrate. We can fabricate microoptics

into the substrate to reflect and refocus the light at precise angles so it can propagate from one device to another and then be directed out of the substrate into free space. The MEMS components do not require the development of transparent optics and can be completely compatible with the current three-level polysilicon process. The optoelectronics devices will be vertical-cavity surface-emitting laser (VCSEL) arrays that are ideally suited for surface-mounting. This technology will enable the combination of two very successful activities, silicon MEMS and III-V optoelectronics, to address applications in weapons systems, sensor systems, and other areas. Optical systems that can be miniaturized include beam scanning for sensing, communications or displays, active focusing for motion sensing or tracking, and 2-D arrays of phase shifters for real-time reconfiguration of optical systems or miniature displays.

We devoted much of the first year of this project to developing the equipment and processing infrastructure needed for the integration of optoelectronics and MEMS. Several of the key technical people funded on this project participated in the MEMS short course at Sandia to quickly become familiar with the polysilicon MEMS processes. We transferred some recent MEMS designs for layout of contact photomasks that would allow for post-processing of MEMS structures.

An important requirement for implementing optical functions in MEMS is the ability to make good mirrors on the polysilicon surfaces. We demonstrated a shadow mask technique that is applicable to released MEMS parts. Flip-chip bonding is also a key technology in this project for assembling the dissimilar parts together, or onto common substrates, for building subsystems. In the spring we flip-chip-bonded visible-wavelength VCSELs to fused silica substrates (which had etched microlenses) with our old flip-chip system. This indicated the need for a more precise system to achieve the alignment tolerances of a few microns that we require. We began process development with a new flip-chip alignment system with gold thermo-compression bonding, which is a very flexible technique for small quantities of

prototypes. Initial results are very encouraging.

A final key processing goal is fabrication of high-efficiency diffractive optical elements in the polysilicon MEMS structures. The granular nature of polysilicon was cause for some concern as to whether our dry-etch processes could provide surfaces smooth enough after etching to make high-efficiency diffractive optics. The most promising approach is to use polysilicon surfaces smoothed by chemical-mechanical polishing. Etching a diffractive optical pattern into the polished surface resulted in very little surface roughness. The chemical-mechanical-polished (CMP) polysilicon samples had initial root-means-square (RMS) roughness values of 4–5 nm. After etching, the etched surfaces showed comparable to slightly less surface roughness of 3–4 nm. We should be able to realize very high-efficiency diffractive elements in polysilicon with this process.

Recent developments in longer-wavelength VCSEL technology made it possible to consider use of the silicon substrate as a transparent medium, at least over short paths. The surface-emitting VCSEL sources are optimum for surface-mounting on dissimilar substrates by processes such as flip-chip bonding. We measured transmission of the 1.07- μ m light through the Si substrate. More than 30% of the incident light can be collected after traveling through 675 μ m of doped Si substrate if the substrate is polished on the back side. Continued development of longer-wavelength VCSELs will increase the amount of light transmitted through the silicon substrates and holds promise for use of the silicon substrate as an optical interconnect structure with light routed internally through the substrate. The shadow-masked gold coating mentioned in the processing section was effective in blocking the light, allowing for opaque shutters, gold mirrors, and reflective diffractive optics. With these longer-wavelength sources, we can use the polysilicon layers to make transmissive as well as reflective optical elements. This will greatly increase the freedom of the designer trying to make optical systems in MEMS.

3506.250

Advanced Laser Structures for Short-Pulsed Power in Active Optical Sensor Systems

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To address the technological needs of Sandia customers in DOE and DoD for high-power, low-cost, reliable, pulsed lasers in the 0.01–100.0-ns regime, Sandia proposes to develop diode lasers for short-pulse duration and high peak pulse power. Our goal is up to 10 W, while maintaining good far-field beam quality and ease of manufacturability for low cost. We will achieve high-peak-power picosecond pulses by gain switching of flared geometry waveguide lasers and amplifiers. In the longer pulse-length regime, we will obtain 1- to 100-nsec pulses using conventionally pumped ridge waveguide lasers of unique design. We will use novel very large optical cavity (VLOC) lasers to achieve high saturated output power, and we will use lasers with passive optical mode expanders (TRAFFiC) to push the output facet damage limit above that of a standard device.

We finished 2-D waveguide modeling and design of VLOC, TRAFFiC, and multisection Q-switched and flared waveguide lasers, and generated mask sets to be used in the fabrication process. We upgraded our laser diode test system for generation of high-current (10 A) pulses and pulsed-mode measurement of

near- and far-field laser diode emission patterns. We fabricated and tested the first VLOC, TRAFFiC, multisection, Q-switched, and flared waveguide lasers. The peak output power of VLOC lasers was 190 mW/facet with 60% slope efficiency and 78% differential quantum efficiency. Testing of TRAFFiC lasers demonstrated $\sim 7^\circ$ full-width half-medium (FWHM) far-field emission divergence and 55-mW output power. We demonstrated 6-W peak pulse power from flared-waveguide, multisection, Q-switched lasers. We completed modeling of selectively oxidized TRAFFiC laser and evaluated the concept for viability. We developed coupled optical, carrier, and thermal models, and used these models to create improved VLOC laser designs. We also developed dynamic gain models and preliminary gain-switched laser models.

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3506.260

Metal Micro-Heat-Pipe Substrates for High-Power-Density Electronics

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As electronic system requirements move toward higher processing speeds and ever smaller weight and volume requirements, electronic cooling capabilities increase in importance. We find that a major advance in cooling is now possible using an efficient Sandia micro-heat-pipe design combined with a metal substrate. A metal substrate such as Kovar matches the coefficient of thermal expansion of semiconductor die while the micro-heat-pipe gives very high effective thermal conductivity. The result is a robust, potentially low-cost and efficient cooling technology. In the first year of this project, we developed processes and made and tested an initial prototype.

We successfully completed all milestones this year, three related to stress analysis and mechanical design. We developed a finite-element model (FEM) of the substrate for the substrate and support structure to meet design needs. The results defined a substrate design with sufficiently low stress levels in the die attach layer for a prototype application. We developed processes for the photo-mask production of a wick

structure on metal substrates. We defined laser-weld schedules for the assembly and sealing of the substrate. We used a simple developmental fill-and-seal process to complete the first prototype. Finally, we developed an infrared (IR) thermal test system and measured the first results for heat transfer properties of the prototype design. The initial heat-pipe substrate prototype showed a twofold improvement of effective conductivity over that in a similar geometry with only Kovar. Extensive discussions on Defense Programs and industry-based applications indicate that this effort when completed should have direct impact on cooling technology needs. The novel processes and designs from this work are developing into new intellectual property for patent and licensing activity.

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3506.270

Integration of Microsensor Technology into a Miniature Robotic Vehicle

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The goal of this work is to develop a miniature robotic vehicle capable of deploying environmental sensors (like Sandia-invented radFETs, volatile organic compounds [VOCs], hydrogen sensors, etc.) and navigation sensors (like Sandia's three-axis accelerometer). We will fabricate the sensors, signal processing, communications, power, and control electronics using surface-micromachining techniques. We will fabricate the vehicle chassis and drive mechanism using various precision-machining technologies developed at Sandia. We will use electro-magnetic, optical, or other signals to power and communicate with the vehicle. A base station will transmit command signals to the vehicle, which will direct the vehicle to reposition itself, take sensor readings, or transmit sensor readings. We will determine the location of the vehicle in two ways. We will first determine vehicle position by measuring the time of flight (TOF) between multiple base station transmission and reception signals. We will determine secondary position information via navigation sensors. Combining vehicle position and environmental sensor information will make it possible for multiple vehicles to map out the location and characteristics of radioactive, chemical, military, or other entities. While the ultimate goal of this project is to fabricate working prototype units, this project will also focus on developing the integration technologies (including integrating control and sensing electronics with sensors on single dies) necessary to design, build, and test future intelligent miniature systems for DOE and DoD applications. This project will access current internal and external capabilities, specify the design and analysis tools, develop a prototype manufacturing and testing environment, and design and fabricate prototype vehicles and sensors.

During this first year, we developed a prototype miniature robotic vehicle

with a microelectromechanical systems (MEMS) sensor. This first vehicle is slightly larger than a magic marker and detects and moves toward vibration sources. At this point, we use it for tabletop demonstrations, but it could be modified to detect vibrations from tanks, marching soldiers, etc. The vibration is detected using a commercial MEMS accelerometer by analog devices. A 12.7 x 50.8-mm printed circuit board contains surface-mount electronics to read the accelerometer and drive two DC Micro-Mo motors, a microprocessor to provide the control logic, a radio frequency (RF) transmitter that sends status information to a PC base station, and a voltage regulator to step up the battery's 1.2 volts to the required 5 volts. The whole unit draws 250 mW of power when both motors are running, but only 50 mW when the motors are off. With a motor-on duty cycle of 10%, the battery will last approximately 2 hours. The transmitter is capable of transmitting up to 40 meters. The vehicle is reprogrammable and rechargeable without disassembly.

We plan to replace the analog device accelerometer with a three-axis accelerometer. We fabricated an initial version of the three-axis accelerometer this year and characterized its performance. We designed the accelerometer to operate over a range of ± 25 Gs, and the mechanical proof mass and spring structures are fully integrated with on-chip microelectronics. The sensor demonstrated sensitivity performance of $110 \mu\text{g Hz}^{-1/2}$ in the x axis, $160 \mu\text{g Hz}^{-1/2}$ in the y axis, and $990 \mu\text{g Hz}^{-1/2}$ in the z axis.

We considered several approaches to address the problem of remote powering and charging of the vehicle, including the following:

- (1) Tethered power
- (2) Direct contact power (docking station with charging contact pads)
- (3) RF coupling
- (4) Photovoltaic power coupling
- (5) Focused optical power coupling
- (6) Inductive power coupling.

Tethered power and direct contact power are the most efficient; however, they are also the most difficult to conceal. RF, optical, photovoltaic, and inductive coupling are easier to make covert, but are not as efficient.

Vacuum Encapsulation of MEMS Structures

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Sniegowski

Recent developments in the design and fabrication of surface-micromachined resonant structures using semiconductor batch processing demonstrated the feasibility of a low-cost, low-power family of surface-micromachined inertial sensors built on a single chip. As described in the microsystems roadmap, development of on-chip vacuum encapsulation and microelectromechanical systems (MEMS) release/dicing technology are cited as two key enablers for many new MEMS sensors. Commercial interest in these areas is also high. The market for MEMS-based inertial sensor systems alone is expected to be greater than \$70 billion per year. A reliable, on-chip vacuum encapsulation technology is critical in achieving devices for this enormous market. Vacuum encapsulation of surface-micromachined resonant sensors will result in lowering overall system size, cost, and operating voltages while increasing system sensitivity. We will use a combination of pre-stressed chemical vapor deposition (CVD) films, a novel approach to resonant structure release and innovative use of macroscopic mechanical lid design applied to microscopic vacuum structures. The resulting process will produce the high-quality vacuum necessary for high-Q, surface-micromachined resonators while offering a high degree of protection for these resonators during packaging. Encapsulated MEMS devices can be diced after wafer-scale release and wafer-level electrical testing, greatly simplifying the packaging process. When combined with

the integrated micromachine/complementary metal oxide semiconductor (CMOS) technology, this process will become the generic enabling technology for a new class of high-performance integrated sensors.

We completed modeling of film properties and lid deflection estimates for the lid (under vacuum). We decided to use a low-stress polysilicon film for the cover over the cavity. This cavity will eventually contain the resonant MEMS structure.

We designed the first test lot to demonstrate the feasibility of the polysilicon lid deposition process over the planarized trench typically used in the integrated micromechanics process. The lot used wafers from a partially completed integrated MEMS lot. We embedded and planarized the micromachines in a 6-mm-deep trench. We deposited a polysilicon cover and dry-etched small, 1-mm-wide etch release holes in the lid to allow access to the embedded structures during the release etch.

The spacing between the top of the micromechanical structure in the cavity and the lid is on the order of 0.5 micron. On the final device, we will increase the trench depth to a 2-micron separation distance, which will allow for slight lid deflection due to the atmospheric/vacuum pressure differential. This lot demonstrated the feasibility of depositing *in situ* lids over the micromachines while the devices are in fabrication.

We ran a second short-loop lot without micromechanical devices in the trench in parallel to develop lid planarization and lid-to-substrate attachment techniques. These issues are critical to successful integration of the lids process to the integrated technology. To ensure an unsupported span over the trench that is large enough to accommodate a useful resonant structure, and to prevent deflection in the Z-axis of the lid under pressure, the polysilicon lid must

be greater than 3 microns thick. This requirement would normally prevent integration of the CMOS logic on the same wafer by causing patterning problems with the subsequent photoresist layers. We used a two-level, recessed trench to attach the lid to the substrate. In addition, this enables planarization of the wafer surface without removing the lid, which eliminates topography-related photoresist patterning problems.

Thick-film stress levels across the silicon wafer can lead to stress cracks in the sacrificial oxide films in the silicon cavities. It is necessary to reduce the thick-film stress across the wafer by forming islands of thick oxide in the cavities with the chemical-mechanical-polishing (CMP) planarization process. We achieved stress-crack-free films in the silicon cavities on the order of 9 microns thick. Previously, films of only 6.7 microns showed no degradation due to film-stress cracks.

The sealing process is the next issue. After the final release etch, the small, 1-mm etch release holes must be sealed (under vacuum) with silicon nitride, polysilicon, or metal. All films will impart some stress in the lid, which may cause it to deflect. The amount of deflection for each film can be estimated, but the actual amount of deflection remains to be determined on actual devices.

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Other

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Massively Parallel Sensor Arrays for Volatile Organic Detection

A. J. Ricco, W. G. Yelton, G. C. Osbourn, J. W. Bartholomew

We will develop a flexible chemical sensor "microlab" for detecting volatile organic compounds (VOCs) with high chemical selectivity based on large (~ 50 sensors) arrays of sorption-based resistors (chemiresistors). This microlab will comprise a "massively parallel" (MP) microsensor array using inexpensive, easily fabricated, polymer-coated planar interdigitated resistors; polymers are rendered conductive through admixture of conductive colloidal particles. Using chip-based electronics, we can inexpensively monitor sensor-array resistance changes due to VOC exposure in real time. The response of each sensor is rapid, reversible, and repeatable; hundreds of polymers with distinct sorptive characteristics are commercially available. Limits of detection (LODs) can reach ppb levels; for high-volatility species, this is likely to require adding a preconcentrator as a "front-end" for this microlab. In contrast to separations-based microlab concepts, this approach is analogous to spectroscopy: The rich "spectrum" of resistor responses enables high chemical selectivity through multivariate analyses without separations; sensor redundancy provides improved system robustness.

The detection of VOCs is a key national security concern: detection of the proliferation of weapons of mass destruction (WMD). Particular combinations of chemical precursors, solvents, and by-products signal the production of nuclear, chemical, and biological WMD. We will determine system performance for WMD compounds, including various multicomponent VOC mixtures, and their relevant

LODs. In addition, DOE environmental monitoring and remediation applications, as well as industrial-waste minimization, require the development of effective, inexpensive VOC microlabs; key species, many of which are potential interferants for WMD detection and must therefore be included in any case, will be addressed for these as well.

From a selection of over 80 polymers, we used 50 to construct chemiresistors. (We are still looking for the proper solvent to dissolve the other 30.) We explored in detail the colloidal metal loading, which ranges from 5–60% carbon (by weight) for the thin-film sensors. In addition, we fabricated an array of chemiresistors (18 combinations) using six metal-colloid types and three loading concentrations (15%, 25%, and 40%). The polymer selected for this matrix, neoprene, appears to be exceptionally sensitive to ring and chlorinated compounds. Moreover, we investigated the use of high-energy ultrasonics as well as the addition of surfactants, including Cabosil (fumed silica) and ionic surfactants, in an effort to improve metal distribution in the polymer films.

We procured and are examining a range of conducting colloidal particles. These include graphitized carbon, rhodium (5%) on carbon, ruthenium (5%) on carbon, palladium (10%) on carbon, platinum (10%) on carbon, platinum, silver, and ruthenium oxide. The range of conductive colloids offers the potential to tune the selectivity based upon interactions between analytes and the transition-metal particles (to complement selectivity from analyte/polymer solubility interactions). In addition, the carbon-supported transition metals are tens of nanometers in diameter and therefore may be more easily dispersed (no gravitational settling) in the polymer matrices.

The matrix of analytes used to date isotherm analyses include iso-octane, ethanol, water, DIMP (diisopropylmethylphosphonate), and, to a lesser extent, toluene, xylene, and cyclohexane. We have primarily produced single-component isotherms to date, but also generated a small number of binary mixtures also (water with iso-octane and ethanol). We also designed and machined a custom test fixture that will allow us to measure AC impedance from 12 separate chemiresistors at once; we interfaced the inductive capacitance resistance (ICR) meter to the computer system and multiplexer and wrote software to record data from the array of chemiresistors using the multiplexed ICR meter.

We devised a row/column addressing scheme for large arrays of chemiresistors on a single chip. We formed a collaboration with scientists at Pacific Northwest National Laboratory (PNNL), who have a "microdispensing" machine that they demonstrated to be capable of depositing polymer films with 25- μ m resolution on a particular area (in this case, a single chemiresistor structure). Unlike inkjet technology, this commercial instrument uses syringe-pump technology and can therefore handle a wide range of viscosities, solvents, and suspended solids (e.g., the conducting particles).

We began data analyses ahead of schedule. We are examining data on individual VOCs (iso-octane, ethanol, DIMP, cyclohexane, toluene, m-xylene, and water) and will expand this to a much larger set by the end of FY97. We are using our visually empirical region of influence (VERI) pattern-recognition analysis to examine separation of the chemical classes provided by the sensors to determine their effectiveness at distinguishing the chemicals.

Agile Dry Etching of Compound Semiconductors for Science-Based Manufacturing Using In Situ Process Control

C. I. H. Ashby, G. A. Hebner, G. A. Vawter, R. J. Shul, J. R. Woodworth, W. G. Breiland

Sandia extended the ADVISOR (Analysis of Deposition Using Virtual Interfaces and Spectroscopic Optical Reflectance) method to model etching at all incidence angles, installed a reflectance monitor on the inductively coupled plasma (ICP) etch tool, developed a method for extracting etch rate and composition over a moving data window, and developed an alternative endpoint detection scheme that is ready for testing. We collected in situ reflectance data on both patterned and unpatterned substrates.

We extended the ADVISOR method from its original normal-incidence model to include all angles of incidence and both *s* and *p* polarizations. This will allow us to monitor etching behavior in reactors for which no normal incidence access is available. This extension also opens up the opportunity to use polarization-dependent measurement methods such as ellipsometry or *Rp/Rs* ratio techniques. We installed a single-wavelength normal-incidence reflectance monitor on the ICP etch tool. We made comparisons between the reflectance waveforms during etching and waveforms recorded on the EMCORE 3200 during deposition. We observed the expected "unwinding" of the deposition waveform in the etching waveform. We also recorded reflectance from patterned wafers. Although somewhat distorted, distinct transitions at the layer interfaces are still observable, indicating that endpoint schemes can be developed. We built a full spectroscopic reflectance

system that is scheduled for installation after the ICP reactor is brought back up from preventive maintenance.

We developed two methods that we can use as endpoint schemes. The first uses the known optical constants of the deposited material to extract the etch rate and chemical composition of the film from a moving data window that can be as short as 5 seconds. It should be possible to detect a change in composition at an interface between two compositionally similar materials for which no selective etch scheme is available. The second endpoint method calculates the residual from an ADVISOR extrapolation into lower parts of the film. When a new material is encountered, the residual will exceed some threshold value to signal the endpoint.

3506.320

Precision-Formed Micromagnets

T. R. Christenson, E. L. Venturini, T. J. Garino

A limitation currently exists in magnetic microactuator development that does not allow for the inclusion of precision high-quality permanent magnets. The availability of such magnetic components, however, would allow an improvement in magnetic microactuator efficiency as well as the consideration of an additional large class of magnetic devices. The property of the permanent magnet that makes the above possible is its ability to produce a magnetic field without resistive coil losses that become a much greater concern as device size decreases. The proposed work makes use of precision plastic molds fabricated by deep x-ray lithography, or LIGA (a German acronym representing x-ray lithography, electroplating, and injection molding) techniques, which have

critical dimensions down to 5 microns with tolerances of 0.5 micron. The mold is nearly perfectly prismatic with a lateral runout of less than 0.1 micron per 100-micron structure height with structure heights ranging from 50 microns to 1 mm. To replicate this mold, we use a bonded magnet powder. The magnetic materials of interest are SmCo and NdFeB and, in a bonded form, result in energy densities of 9 MGOe (mega Gauss-Oersted), which is as large as any non-rare-earth (non-RE) fully dense permanent magnet.

We fabricated a variety of permanent magnet geometries using a fully integrated process with deep x-ray lithography-defined molds. We implemented permanent magnet powders of SmCo and NdFeB with several different binder materials. Typical powder sizes used range from 10 to 20 microns and depend on the molded magnet dimensions. A larger powder size consistent with the minimum mold aperture is optimal since packing density is increased and magnetic properties degrade for smaller particles. We incorporated the binder material at 10 to 30 vol%. We used a test mask containing magnet dimensions ranging from 250 microns up to several millimeters. Optical microscopy reveals exceptional replication of the precision molds. We achieved energy products in the range of 8–10 MGOe, which is typical of RE-bonded magnets. Empirical investigation into locally magnetizing individual permanent micromagnets revealed higher-than-predicted field requirements for the epoxy-based binder materials. Thus, we used fixturing to batch-orient micromagnets with an electromagnet that encompasses the entire substrate. The result imposes restrictions on magnet orientation via demagnetization effects that must therefore be anticipated in the mask layout. We received commercial interest from private industry. We are planning to file a technical advance.

Time-Resolved Ion-Beam-Induced Charge-Collection (TRIBICC) Imaging

F. W. Sexton, D. S. Walsh, P. E. Dodd, R. S. Flores, J. F. Aurand

Single-event upset (SEU) has traditionally been a reliability concern for space-based electronics due to naturally occurring energetic heavy ions in the space environment. However, with the continuing shrinkage of microelectronic device dimensions, SEU is becoming a reliability concern for avionics and ground-based systems as well, due to terrestrial cosmic rays. A technique called time-resolved ion-beam-induced charge collection (TRIBICC) has been developed to measure charge transients resulting from heavy-ion strikes to integrated circuits (ICs). The transient response is fundamental to developing a clear understanding of SEU mechanisms. This technique measures the transient response as a function of position using a 1.0-(mm)m focused beam of heavy ions that is raster-scanned across a device. Here we describe the TRIBICC measurement system. TRIBICC measurements of test transistors fabricated in Sandia's complementary metal oxide semiconductor 6 (CMOS6) technology showed fast transient pulses consistent with drift charge collection and slowly decaying transient pulses consistent with diffusive charge collection. Transients from the center of the n-channel drain region exhibit both drift and diffusive charge collection, while transients on the edge of the drain show only diffusive charge collection. The fast transients are at the limit of the present 5-GHz system, with 70-ps risetimes. We describe the importance of this technique in developing improved models of SEU in ICs. TRIBICC is a companion technique to two other microbeam techniques developed at Sandia: SEU-imaging, which provides in situ observation of upset location, and ion-beam-induced charge collection (IBICC), which measures the amount of charge

arising from heavy-ion strikes as a function of position across a device.

The TRIBICC system comprises three major elements: (1) a source of energetic heavy ions, (2) a means of focusing the heavy-ion beam to submicron dimensions, and (3) the measurement system used to capture and analyze charge transients resulting from heavy-ion strikes on an IC. For this work, the source of heavy ions was provided by a 6-MV EN tandem van de Graaff accelerator, while we accomplished beam focusing using a magnetically focused double-doublet microbeam system. The TRIBICC measurement system is composed of a specially designed high-frequency assembly mounted in a vacuum chamber, which holds the device under test (DUT) and passes electrical signals to external electronics. A 5-GHz amplification and triggering system amplifies and captures transient signals. The front-edge triggered digitized waveform along with the corresponding ion beam position is stored by a PC-based system, resulting in 4-D spatial charge distribution maps, 2D-Q(t). This system differs from prior transient analysis systems in that a transient signal is measured from each ion strike. Earlier systems required multiple ion strikes to measure a single transient signal. However, damage from the heavy-ion beam accumulates in the semiconductor device and changes the transient response during a measurement. Also, this system measures transients across a region that is defined by the dimensions of the scan, rather than at a single point. Scan dimension can vary from tens to hundreds of microns.

To demonstrate the capability of this technique, we performed initial measurements of test structures from the Sandia CMOS6 technology. We measured an n-channel MOS transistor with 0.5-(μ m)m channel length. We exposed the drain region to a 1.0-(μ m)m beam of 12-MeV C ions, while the gate, substrate, source, and drain were held at zero bias. The drain regions measured 20 x 3

(μ m)m as drawn. Transients differed depending on the location of the heavy-ion strike. The transient in the center of the drain had a risetime of about 70 ps, at the resolution limit of the 5-GHz digitizer, and exhibited two time regimes: (1) a fast transient with a width of about 200 ps, and (2) a slowly decaying tail that extends for 2.5 ns. The fast transient is consistent with an electric field-driven charge-collection process (drift) in the pn-junction formed by the transistor drain region. The slow component is consistent with a diffusive charge collection process associated with charge collected below the n+ diffusion that forms this drain region. Charge transients at the edge of the drain had a considerably smaller pulse height and showed the slow decay characteristic of diffusive charge collection. Total charge collected was ~ 100 fC in the drain center and ~ 80 fC at the drain edge. Although only 20% less charge is collected by the smaller transient, both the amount of charge and, more importantly, the rate at which charge is collected determine whether a circuit will upset when struck by an energetic heavy ion. These data will begin to shed light on the non-abrupt shape of the threshold region seen in error cross-section curves.

TRIBICC measurements are a key to validating 3-D SEU modeling tools. This will lead to a refined understanding of charge-collection processes and an improved estimate of the SEU-sensitive volume. Improved charge-collection models will result in increased simulation accuracy, reducing our reliance on empirical studies of the design space for hardening devices to SEU. Empirical studies require variations in processing and design that are both expensive and time-consuming. Model-based design trade-off studies can easily be one to two orders of magnitude cheaper, with months to years shorter development times. Also, SEU-hardened devices can be made more manufacturable by clearly understanding the trade-offs between SEU sensitivity, performance, and process complexity.

Composite-Resonator Surface-Emitting Lasers

K. D. Choquette, W. W. Chow

Applications of vertical-cavity surface-emitting lasers (VCSELs) have requirements ranging from amplitude modulation, frequency tunability, amplitude or frequency stability to high output power. The present single-resonator VCSEL lacks the agility to readily perform many of the above functions. Sandia proposes the use of composite resonators to control spectral and temporal properties; this structure in effect is a coupled-resonator vertical-cavity laser (CRVCL). The composite resonator will consist of a primary resonator containing the gain section and an active or passive secondary resonator. Separate contacts provide independent current injection into the resonators. The coupling between the resonators is controlled by the transmission of the shared distributed Bragg reflector (DBR). We will use different configurations of a monolithic composite-resonator surface-emitting laser structure to demonstrate (1) amplitude modulation, (2) gain switching, and (3) frequency tuning. The latter will allow fine-tuning of the mode/gain alignment after growth to compensate for temperature and injection current fluctuations. Successful

demonstration of the above functions will be a major step toward making VCSEL technology viable for many defense and commercial applications. Moreover, the advances made will also keep Sandia in the forefront of VCSEL research and development.

We established a viable device structure and began to examine the VCSEL characteristics, as described below.

(1) We modeled the resulting cavity resonances of coupled-resonator vertical-cavity structure; the resonances shift opposite in frequency with changing middle mirror reflectivity.

(2) We developed an optical model of coupled cavity resonator; obtaining the cavity wave functions provided insight into the expected CRVCL properties.

(3) Using stringent growth control and uniformity, we designed and grew epitaxial wafers consisting of CRVCLs.

(4) Using selective oxidation, we designed and fabricated CRVCLs containing multiple contacts to enable independent biasing of the two cavities.

(5) We demonstrated live CRVCL devices and began to examine their novel output characteristics, such as amplitude modulation.

(6) We modeled modulation of CRVCL output under square-wave excitation, which suggests that extremely short-pulse operation may be possible.

Role of Defects in III-Nitride-Based Electronics

J. C. Zolper, D. M. Follstaedt, S. R. Lee, J. Han, A. F. Wright, R. J. Shul, C. H. Seager, S. M. Myers, Jr., M. H. Crawford, T. J. Drummond

Wide-bandgap III-nitride semiconductors are extremely promising materials for the compact, high-power, high-frequency amplifiers required for future satellite cross-, up-, and downlinks, and for the robust microelectronics required for future severe-environment national security applications. In addition, they will enable a new generation of optoelectronic devices in the ultraviolet (UV) region of the visible spectrum. This proposal aims to place Sandia at the forefront of the material development and electronic device applications of these wide-bandgap semiconductors. We propose to accomplish this by leveraging Sandia's broad semiconductor expertise in first-principles defect calculations, fundamental material analysis, and advanced device processing capabilities. Our initial focus will be to use advanced analytical capabilities (some available only at Sandia) to understand and control unintentional intrinsic and extrinsic defects in GaN, and thereby achieve the semi-insulating GaN required for virtually all electronic and optical devices. We will then correlate this understanding with Sandia's unique in situ reflectometry diagnostics during growth to achieve real-time feedback on the

quality of the semiconductor crystal. With the demonstration of semi-insulating GaN, the emphasis will turn to understanding p- and n-type doping required for electronic and optical devices.

The accomplishments of this project are broken up into five areas:

(1) *GaN MOCVD growth.* The key enabler for this proposal is the demonstration of high-quality GaN epitaxial layers on sapphire substrates by metalorganic chemical vapor deposition (MOCVD). In this first year, we used Sandia's unique rotating disk reactor with *in situ* reflectometry to rapidly converge on the growth conditions that result in background free electron concentration as low as $7 \times 10^{16} \text{ cm}^{-3}$ and room-temperature mobilities as high as $520 \text{ cm}^2/\text{Vs}$ ($1100 \text{ cm}^2/\text{Vs}$ at 100°K). These values are comparable to the best reported for GaN. These results were expedited by the *in situ* reflectometry pioneered by Sandia that allows real-time feedback on the growth process. Key understanding and real-time feedback with the reflectometry technique of the role of the buffer layer and subsequent etchback enabled the rapid convergence on optimum growth conditions.

(2) *AlGaIn growth.* AlGaIn/GaN heterostructures are also required for high-performance transistors since this allows modulation doping and the formation of a high-mobility 2-D electron gas (2DEG). We achieved growth of the first AlGaIn layers by introducing trimethylaluminum (TMA) as an aluminum source and reducing the growth pressure to suppress undesirable prereactions in the gas phase. Photoluminescence (PL) of a 15% AlGaIn-film at 4°K exhibited a peak at 323 nm. We also used

the growth procedure to grow a heterostructure field-effect transistor (HFET) structure with a 30-nm Si-doped AlGaIn layer on undoped GaN. We are presently processing this structure into transistors.

(3) *N-type Si-implantation of GaN.*

The ability to high-dope selective areas of GaN by ion-implantation will greatly reduce the access resistance of GaN-based transistors. We improved the implant activation of Si-implanted GaN to achieve $\sim 100\%$ activation of high-dose ($5 \times 10^{15} \text{ cm}^{-2}$) implants. Previously we achieved $< 50\%$. The improvement was based on the incorporation of an AlN encapsulation layer on AlN to reduce decomposition of the GaN and to allow the annealing temperature to increase from the $\sim 1100^\circ \text{C}$ previously employed to 1400°C . At a temperature of 1300°C the implant is 100% activated, and we achieve an electron mobility of $60 \text{ cm}^2/\text{Vs}$. The electron sheet carrier concentration corresponds to an electron peak-volume concentration of $\sim 3.5 \times 10^{20} \text{ cm}^{-3}$. The mobility is comparable to what can be achieved for GaN epitaxially doped with Si at a similar level.

(4) *Low-resistance, thermally stable ohmic contact.* For high-power or high-temperature operation, we required thermally stable, robust, low-resistance ohmic contacts. We accomplished this by combining high-dose Si-implantation and refractory tungsten (W) ohmic metallization.

(5) *Plasma etch development.*

Controlled etching of GaN and AlGaIn is required for transistor fabrication for forming isolation mesas and recessed gate structures. We used high-density plasmas, both electron cyclotron reso-

nance (ECR) and inductively coupled plasmas (ICP), to achieve well-controlled etching of both these materials.

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Ultra-Low-Power Sensors for Microtelemetry Systems

R. C. Hughes, J. R. Wendt, S. A. Casalnuovo, D. D. Chu

Sandia proposes to design, fabricate, and test ultra-low-power sensors that are capable of being powered and read out by analog circuits that are in turn capable of coupling the sensor information to radio frequency (RF) telemetry. The micro-electrochemical cell (MEC) is a key enabling technology for a wide variety of chemical sensors in the sensor/tag combination and opens the door to new applications in sensing for counter-proliferation, weapon monitoring, and many other areas. The current state of electronic "tagging" circuits is effective for grain-of-rice- to jelly bean-sized chips that can be remotely powered, programmed, and read out. The first new sensors proposed for this project would be ultra-small-gap electrochemical cells with 100-300-nm gaps formed by electron-beam (e-beam) lithography. We would grow chemically sensing electroactive polymers between the fingers. We have two patent disclosures that describe how photolithographic microelectrodes can be used as MECs to provide information about the chemical environment. A considerable literature on electroactive chemically sensitive films has developed over the last few years, and Sandia has the technology to combine the tagging electronics with these low-power electrochemical sensors. A challenging aspect of this project would be the means of using the RF interrogation pulses to initiate power-up of the tag and get the sensor data into memory. Issues to be resolved include the quality and type of data to be transmitted, how to handle analog data from the sensor as well as ultra-low-power management, and the range of operation. Other technical issues would involve the levels of voltage and charge required to obtain a reliable readout. We can also envisage ultra-small versions of the radioactive field-effect transistor (radFET) and hydrogen sensor that require only a small number of coulombs.

We fabricated a large number of planar interdigitated electrodes (IDEs) on small quartz plates and placed

chemical sensor coatings between the electrodes. The sensors are about 1 mm², not including the bonding pads, with 8-micron lines and spaces. The bonding pads allow us to use spring-loaded pogo pins to make electrical contact to the IDEs inside a fixture that is in an oven inside a hood so that several sensors can be exposed simultaneously to a wide range of analytes. The sensor fixture and oven are in a walk-in hood that also contains the flow controllers and bubblers for the various analytes. The coatings all display changes in electrical impedance, either DC or low frequency, to a variety of analytes. We used several sensing mechanisms. One takes advantage of solid-state ionic conductivity in thin films composed of ionic polymers or intercalated clays. Another type involves metal particles loaded into polymer films of different hydrophilic or hydrophobic nature, called *metal-loaded polymers*. The model for the resistance of these films involves current flowing through strings and branches of the metal particles embedded in the polymer. Any analyte that allows the polymer to swell will pull apart some of the conducting chains and cause the resistance to increase.

The following is a summary of the types of conductive coatings that we have investigated so far:

- *Ionic conductors:* (1) polyhexane viologen with PF₆ as the anion, (2) thin-film hectorite (clay) with ion-exchanged cations (iron, copper) and gold, and (3) polyvinylalcohol (PVA) with liquid crystal inclusions
- *Metal-loaded polymers:* polyisobutylene (PIB), polybutadiene (PBS), PVA, and poly-neoprene (PCP)
- *Conducting polymers:* (1) polyoctylthiophene and (2) polyphenylene-vinylene.

These polymers represent a cross-section of types that have varying solubilities for polar and nonpolar analytes. For example, the ionic conducting clays have a much stronger response to water vapor than xylene, with the opposite true for PIB. We can test up to six sensors at once in our fixture, and we were able to use pattern-recognition techniques to classify a variety of analytes from water vapor to nerve-gas simulant (diisopropylmethylphosphonate [DIMP] and dimethylmethylphosphonate [DMMP]) to aromatic solvents like

xylene. This means that we can identify individual analytes independent of their concentration, then use individual sensor data to extrapolate to the actual concentration. The ability to recognize solvent molecules, and the fact that very high concentrations of solvent can cause the resistance to become very large (several decades larger), led to the invention of a "chemical fuse" that can alert the user to solvent spills. This concept has already led to a spin-off to a Defense Program weapons application and generated a new budget to develop sensors especially for that use.

This type of sensor is particularly well adapted to ultra-small size and low-power readout. For example, the PIB sensor with a base resistance of 7000 ohms can be read out easily with millisecond-voltage pulses and a personal computer memory card interface adapter audio/digital (PCMCIA A/D) card with 16-bit resolution. The signal-to-noise is so high that vapor pressures as low as 1 ppm of xylene can be read if changes of resistance of one part in 10⁴ can be read (as with the 16-bit A/D). We constructed a breadboard circuit for this type of readout; it consists simply of a constant current chip driven by a voltage reference chip so that we can use batteries with variable and unpredictable voltages as the power supply. The circuits used in these chips could be fabricated in an application-specific integrated circuit (ASIC) chip with dimensions of less than 2 mm². Thus we feel that our premise of a very small footprint for both the sensor and read-out circuitry is quite feasible.

3506.370

Double Quantum-Well Long-Wavelength Optoelectronic Devices

J. A. Simmons, J. L. Reno, J. R. Wendt, S. Lin, S. R. Kurtz, S. K. Lyo

This project seeks to research and develop practical long-wavelength emitters and detectors based on intrasubband transitions in semiconductor-coupled quantum wells (QWs). Present work on long-wavelength optoelectronics is largely based on optical transitions across the intrinsic bandgap in the more exotic

semiconductors. In contrast, the unipolar quantum structures on which Sandia proposes to work can be fabricated in the mature AlGaAs system. Transition energies, and thus wavelength and other properties, can be tailored across a wide range by appropriately engineering the composition and thickness of the QWs and intervening barriers. The structures can also be electronically tuned.

Our approach will leverage Sandia's innovative processing technology, initially developed for fundamental quantum transport experiments in nanostructures, to realize interband tunneling light emitters but with certain features that should enable superior performance. In addition, we will explore alternative intrasubband transitions that could reduce the primary constraints in the devices that have been reported thus far.

Because the nature of light emission and detection is substantially different from that in conventional lasers and detectors, this research provides rich opportunities for investigating the fundamental phenomena involved, including tunneling, photon- and phonon-mediated relaxation processes, and electronic states in artificially structured materials.

The primary goal of this project is to develop room-temperature, long-wavelength semiconductor lasers that will be directly relevant to requirements for sensing and other applications. Semiconductor lasers should offer a variety of benefits for systems in terms of functionality. Mid-infrared lasers and detectors can be used for chemical analysis and thermal detection. Electronic tunability and narrowband operation are particularly attractive for spectroscopic systems.

(1) We obtained, installed, and developed a highly sophisticated modeling platform, NEMO (Nano-electronic Modeling), which enables the modeling of current-voltage curves and was developed by Texas Instruments and a three-letter agency. In addition, we modified our own self-consistent Schrodinger-Poisson finite-element (FE) solver so that the mesh spacing automatically increases with each iteration, resulting in roughly an order-of-magnitude decrease in simulation time.

(2) Using the above platforms, we modeled several different structures for both far infrared (FIR) detection and intersubband light emitters. A triple QW structure appears most promising for light emission, consisting of a fairly wide central well in which the light emission occurs via an electron, making a transition from the second subband to the ground subband. We chose the well width so that the energy of the transition would yield a photon of ~ 100 meV energy. Thinner source and drain QWs on either side of the emitting QW serve to laterally inject and remove, respectively, the carriers. When bias of order 100 mV is applied, the ground subband of the source QW should align with the second subband of the emitting QW, and the ground subband of the drain QW should align with the ground subband of the emitting QW.

(3) We grew three triple well emitter structures using molecular beam epitaxy (MBE). We then fabricated several laterally fed emitters. We used our recently developed epoxy bond-and-stop-etch (EBASE) technique to place gates on both sides of the 0.7-micron-thick structure. The finished samples had both front and back gates, enabling independent contacts to the source and drain QWs and enabling fine-tuning of the subband line-ups.

(4) We characterized Hall bars from the triple QW emitter wafers at 0.3°K and determined them to be similar to the simulation results. We then completed light emitter devices at 77°K. This included evaluation of contact integrity and resistances of the active regions. In addition, we swept all gates to determine whether the three different QWs could be depleted before the onset of significant gate leakage current. We found this to be the case. Some devices showed negative transconductance, indicative of the device current being determined by the strong tunneling resonances.

(5) We set up a photoemission measurement system consisting of an FIR spectrometer attached to a 4°K closed-cycle refrigerator. We wired the refrigerator for low-temperature measurements and designed and machined sample holders.

(6) For energies from 1 meV to 50 meV, Princeton University set up a special system in a collaboration with Sandia. The system consists of a 4°K helium dewar containing two independent superconducting magnets and a bolometer at the base of the dewar. The first magnet sweeps the field around a cyclotron resonance FIR notch filter, which removes photons at energies proportional to the field. The second magnet sweeps the field at the sample.

(7) In a double QW detector device, we clearly demonstrated the narrowband detection of FIR radiation in the photoresponse. The measurements were performed at 4°K using an organic gas FIR laser in cooperation with Princeton University and the University of Maryland. The difference in QW densities corresponded to a difference in Fermi energy of approximately 2 meV. We clearly demonstrated the narrowband nature of the detector by observing a sharp peak in emission at ~ 2 meV. In addition, we showed that the photon energy to which the detector is sensitive can be electrically tuned. These very significant results represent one of the major milestones of this project.

(8) We developed a theory of FIR photon-assisted tunneling in double QW detector structures. We then extended this theory to cover the case of both in-plane and perpendicular magnetic fields. It should be highly useful in analyzing the performance of actual double QW detector structures.

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The Development of Integrated Chemical Microsensors in GaAs

S. A. Casalnuovo, E. J. Heller, K. O. Wessendorf, G. C. Frye, J. L. Reno, V. M. Hietala

By taking advantage of both the piezoelectric and semiconducting properties of gallium arsenide (GaAs), Sandia proposes to fabricate arrays of acoustic-resonator chemical microsensors integrated with microelectronic resonator circuitry on a single GaAs substrate, resulting in a compact, extremely low-power, highly sensitive chemical detection system capable of discrimination among large numbers of liquid and gaseous chemicals. GaAs has several advantages in this application. Its piezoelectric coefficient is comparable to that of quartz, the standard material for acoustic-resonator chemical sensors. High-frequency (nominally 1 GHz) resonator microelectronics are easily fabricated in GaAs using existing GaAs microfabrication technology and are process-compatible with GaAs acoustic devices. Selective etching of GaAs and aluminum gallium arsenide (AlGaAs) epitaxial films makes possible the fabrication of thin (typically 1 to 10 microns) piezoelectric membranes, nominally 100 microns in diameter, capable of high-sensitivity (10–15 grams) detection. No other piezoelectric material can support the integrated microelectronics nor produce the thin-film resonators. No other semiconductor, particularly silicon (Si), is piezoelectric, and fabrication process incompatibilities make the integration of Si and piezoelectrics difficult.

We produced 100-MHz GaAs surface acoustic-wave (SAW) chemical microsensors with detectivities identical to

conventional quartz SAW microsensors. We demonstrated that chemically selective coatings, developed for quartz sensors, function equally well with GaAs devices. We fabricated higher-frequency (up to 500 MHz) GaAs SAW devices that should have proportionally higher detectivities. We are currently testing these devices.

We produced the first integrated GaAs SAW chemical microsensor that incorporates a SAW device and the oscillator circuit required to drive it. We demonstrated functional amplifiers in this circuit.

We developed the bulk and surface-micromachining technology necessary to fabricate large-area (approximately 1 square millimeter) GaAs membranes. We are now developing piezoelectric microsensors based on these membranes that are potentially 100 to 1000 times more sensitive than conventional SAW sensors. We concluded that temperature-compensated coatings are not feasible as a means of reducing the temperature dependence of GaAs SAW devices and other methods of temperature compensation; for example, we will have to evaluate signal-processing techniques, active temperature control, and on-chip temperature reference.

Publications

Other

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Systems Studies in Compound Semiconductor Processing (U)

J. P. Anthes, S. R. Smith, C. Reber, S. H. Kravitz, M. G. Armendariz, E. I. Cole, Jr.

The work performed in this project is classified.

Sandia performed four tasks:

- (1) Analysis of relevant systems information,*
- (2) Planning and execution of required experiments,*
- (3) Formulation of physical models, and*
- (4) Laboratory demonstration/validation of the models using previously untested configurations.*

PHENOMENOLOGICAL

MODELING & ENGINEERING SIMULATION

This area supports development of computer models that predict if and why a component will fail; projects that describe how a product will perform across the spectrum of operating conditions; and projects that enhance or expand use of the Sandia teraflop computer. The driving force for this area

is to engineer all aspects of the product life cycle and use engineering based on a valid computer-simulated environment. Success will require unprecedented levels of confidence in computer simulation.

Three key research areas support this effort: (1) increased model fidelity (developing a computer model that will contain sufficient resolution to allow for predictions of product failure); (2) experimental validation (developing experimental methods adequate to achieve the above goal); and (3) uncertainty quantification (developing computational methods rigorous enough to quantify the validity of the simulation).

The evaluation of mechanical stress is an area of vigorous research. Of particular interest is how stress affects the performance and reliability of mechanical hardware. Researchers are developing a noncontact stress-measurement technique based on laser ultrasonics. The technique will allow experimental evaluation of material stresses. Also this technique will aid in evaluating computerized models and structural analyses to enable model-based design.

A technology — called the *optically recording velocity interferometer* — is being developed. It is the first experimental diagnostic technique for real-time probing for microscopic mechanical deformations. It will be used to validate three-dimensional numerical simulations of shocked materials.

A novel ultrasound method, laser ultrasonics is providing stress measurements needed for experimental evaluation and validation for model-based designs. The technique provides at least an order of magnitude advance in measurement path length over conventional systems.

Using Higher-Order Gradients to Modeling Localization Phenomena

D. J. Bammann, D. A. Mosher, N. R. Moody, D. A. Hughes

Prediction of structural failure in components due to void growth and ductile crack propagation requires a constitutive model based upon the physics of these processes. Much research is currently directed toward bridging the micro-to-macro scales in mechanics of materials to bring better descriptions of material response into our finite-element (FE) calculations. Often, an attempt to include micromechanical phenomena into a macroscale model results in mesh dependency when implemented into an FE code. This has been demonstrated in particular for problems such as damage or crack propagation and strain localization. Attempts to describe these by local continuum damage models leads to the unacceptable condition that any refinement of the FE mesh results in a change in the result. This mesh dependency results from the lack of a length scale in the formulation of the local continuum theory. Currently, Sandia's most accurate finite-element model (FEM) constitutive models use a state-variable approach but still do not contain a length scale. In this project Sandia is taking the next step in extending these models by embedding a length scale into the continuum by introducing higher-order spatial gradients into the evolution of the state variables. We can easily identify these state variables with specific underlying micromechanisms and can write accurate balance laws to describe the evolution of the microstructure. By introducing a higher-order gradient in the evolution of the state variable representing dislocation density, we can accurately model both void coalescence and ductile failure while eliminating the mesh dependency of the solution. This will also allow a more accurate description of shear bands and an understanding of when shear bands lead to failure and when they are acceptable for a particular design. We plan

an experimental program to help guide the appropriate choice of a length scale as well as provide insight into appropriate boundary conditions (BCs).

We developed a nonlocal thermodynamic theory of internal state variables that requires state variables to satisfy complete balance laws instead of the usual temporal evolution equations. This naturally results in the occurrence of spatial gradients in the evolution equations for the state variables, thereby introducing a length scale into the continuum model and eliminating mesh dependency in FE solutions of strain localization and ductile failure. We implemented this model into the FE code HICKORY and utilized it in the solution of several illustrative problems that exhibit anomalous predictions when solved with current local material models. In particular, we utilized the model in the simulation of the prediction of ductile failure in the extension of a uniaxial notched tension specimen. The inclusion of the spatial gradient results in a macroscopic simulation of failure dominated by the coalescence of voids. We also used the model to help explain the apparent "anomalous" experimental results in the torsion of thin wires in which the shear stress appears to depend upon the diameter of the wires. We can explain the apparent anomaly by the introduction of a length scale into the model. We also developed an experimental program to both identify the physical mechanism associated with the numerical length scale and ascertain an approximate magnitude. In these experiments we drilled an array of small holes ranging from diameters of 12 to 170 microns into thin sheets of copper. We reduced the corresponding physical dimensions of the sheet as we decreased the hole diameter to keep the dimensions self-similar. We loaded the sheets in tension and recorded the macroscopic stress response. In addition, we are currently using microscopy and nanoindentation to investigate the spatial dependence of the microstructural features through the width of the shear bands that formed. We will compare these results with model

predictions. Finally, we are using the model to describe dislocation substructures that formed during frictional loading in an effort to gain a better understanding of friction models.

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Unexplored Penetrator Regime Against Super-Hard Underground Facilities

J. D. Rogers, N. R. Hansen, A. V.
Farnsworth, Jr., S. W. Hatch

A major national security concern for the U.S. is how to put at risk the increasing number of hardened underground facilities that are being constructed.

The primary option against underground facilities is the earth-penetrator weapon (EPW). Sandia has substantial experience with penetrator design and testing for impact velocities in the range of 200 to 2500 fps.

The technology problem is that the target depth of these proliferating facilities is increasing, requiring higher-velocity penetrator impacts to put them at risk. Only three full-scale penetrator tests have been run from 3000 to 3500 fps, and there is no credible capability or knowledge base above 3500 fps. This project addresses the unexplored regime from 3000 fps (where strength behavior dominates) up to 10,000 fps (where the penetration process transitions to a hydrodynamic phenomenon). The research assembles a computational data base on system design, survivability, and weapons effects against a set of representative underground facilities. New computational techniques must be developed to address this unexplored regime between strength-dominated response and hydrodynamic behavior.

We considered a variety of hardened targets, which we characterized by depth and hardness, based on the latest intelligence information. We performed weapon effects and target response calculations for conventional and nuclear weapons options against a large set of targets. We included these calculations in the target characterization methodology, producing a single measure that provides

a useful starting point for weapon concept trade-off studies. We completed mission planning studies that evaluate the potential merits of delivery concepts and their impact on penetrating weapon design.

We developed and implemented an abrasion model in the CTH code. We coupled Lagrangian and Eulerian codes, demonstrating increased capability for computational accuracy, and assessed these capabilities with test data. The test data span the region from rigid-body penetrator behavior to eroding-rod, hydrodynamic behavior. We identified and analyzed areas of concern for penetrator design.

We investigated experimentally and analytically concepts for selective, tailored material properties for the penetrator.

3508.030

Optimization of Computationally Challenging Problems in Engineering Sciences

M. S. Eldred, T. L. Paez, W. J. Bohnhoff,
R. Lee, C. D. Moen

Computational simulation methods in the Engineering Science disciplines are important tools in understanding complex systems and reducing design-cycle costs through the use of virtual prototypes. Sandia proposes to leverage these capabilities by integrating complex simulations with advanced optimization algorithms and strategies. We will greatly increase the utility of computational methods by providing a systematic means of design optimization. Simulations in Engineering Science disciplines are typically complex, requiring significant amounts of time on powerful machines. Moreover, the response of the simulations

to variations of the parameters describing the physical configuration tends to be highly nonlinear, discontinuous, noisy, and multimodal. These traits and others make it difficult to apply conventional optimization techniques to such problems. The thrusts of this research are to extend capabilities in fundamental optimization algorithms, to develop hybrid methods having global optimal identification capabilities and rapid local convergence, and to develop effective function approximation strategies that minimize the number of full simulation runs. In addition, we are investigating the techniques of automatic differentiation and adjoint augmentation for obtaining analytic gradients from simulation codes, and parallel processing by developing algorithms and strategies for massively parallel (MP) and distributed architectures.

The DAKOTA software architecture proved to be much more broadly applicable than the originally targeted capability of design optimization. We broadened the architecture to include uncertainty quantification with mean value and sampling methods, parameter estimation with nonlinear least squares solution methods, and sensitivity analysis with general-purpose parameter study capabilities. By employing object-oriented design to implement abstractions of the key concepts involved in these iterative systems analyses, the DAKOTA toolkit became flexible and extensible problem-solving environment for current and future problems of interest. Using DAKOTA, we can now use point solutions from simulation codes for answering more fundamental engineering questions, such as "what is the best design?," "how safe is it?," or "how much confidence do I have in my answer?" Some specific highlights of the FY97 extensions to DAKOTA's architecture components include (1) completion of the

new strategy architecture for management of multiple models and iterators with switch/refine adaptive control, (2) installation of the Input Deck Reader parser with new input syntax and related database development, (3) new methods: Gauss-Newton, bound-constrained/barrier function variants, ellipsoid, parallel direct search (PDS), Latin hypercube sampling (LHS) Monte Carlo, parameter study additions, (4) new features: addition of uncertain and state variables, new function types for least squares and uncertainty quantification applications, new gradient and Hessian settings, file_save and file_tag support, additional method controls, and (5) a new suite of test functions. These software development efforts resulted in the granting of copyright by DOE for Version 1.0.

Hybridization studies from FY96 highlighted the need for variable fidelity modeling within the multilevel optimization algorithm. In FY97, we developed the capabilities for model switching (multiple model objects) and model adapting (through state variables) so that much more efficient hybrids can be deployed. We leveraged this development to meet the need for multiple models in the sequential approximate optimization and optimization under uncertainty strategies, in addition to the multilevel strategy. Strategy development work is continuing in follow-on projects and focuses on extending the adaptive logic for switching/refining models and iterators and on attaining a finer grain of iterator control (from process control to evaluation/cycle control).

Research in artificial neural networks focused on evaluating the direct training approach against more standard training approaches. Comparisons show favorable results for the direct training approach, which validates its inclusion in the DAKOTA software.

We investigated adjoint augmentation of analysis codes for obtaining analytical sensitivities with COYOTE for a thermal design problem in electronics

packaging. Results showed convergence to the optimal solution in less than half the time required for numerical gradient approaches. This approach, as well as the automatic differentiation approach investigated in FY96, provides highly effective alternatives to finite differencing for gradient data.

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Investigation of Nonequilibrium Microscopic Hydrodynamic Phenomena

C. C. Wong, M. L. Hudson, J. K. Cole, A. R. Lopez, M. J. Stevens, D. R. Noble, N. D. Shinn, S. J. Plimpton, K. S. Chen

Recent advances in microscience and technology have generated a group of unique fluid-flow problems that question the traditional continuum and equilibrium approaches used to analyze these transport phenomena. Such problems are fluid flows in microscopic geometries or under high stress. This research is to develop microscale and mesoscale flow simulation capability so that it will provide "hard-to-obtain" quantitative physical information and to develop constitutive relationships and models to complement existing continuum methodologies.

Sandia developed an innovative approach that couples molecular dynamics (MD) simulation with a two-dimensional (2-D) continuum flow solver and demonstrated it by simulating flow between solid walls. We studied microscale Couette and Poiseuille flow problems. Simulation at the molecular level is crucial in determining the boundary condition (BC) (e.g., stick or slip) at the fluid-solid interface. This BC is undetermined in continuum theory, but is an important input into continuum calculations. For the microscale Couette flow problems, MD results show that stick BC, i.e., fluid layers being locked with the solid wall, will occur if there is a strong wall-fluid interaction. If the wall-fluid interaction is weak, slip BC will occur at the interface. Shear direction with respect to the wall lattice orientation is also important. MD results also show that stick-and-slip phenomena may become less influential as the channel width increases. For the microscale Poiseuille flow problems with appropriate parameters, the MD

simulations produce a parabolic velocity profile that agrees with the analytical predictions by solving the Navier-Stokes (N-S) equations with no-slip BCs. As the fluid density decreases, our MD simulations indicate that a transition to slip flow will occur at the wall.

We developed and demonstrated a hybrid scheme that couples MD simulation with 2-D continuum flow solver. The continuum flow solver can be either a Lattice Boltzmann simulator or an analytical formulation of the N-S solutions. Our approach incorporates an overlapping region to which continuum flow solver is applicable but the fluid molecule motion is constrained to satisfy continuity of density, temperature, and stress. With these newly developed capabilities, scientists and engineers for the first time can address fluid-flow problems that involve multiple-length scales, spanning from atomistic scale to macroscopic scale.

With the new capabilities, we studied microscale Couette and Poiseuille flow problems. Simulation at the molecular level is crucial in determining the BC (e.g., stick or slip) at the fluid-solid interface. This BC is undetermined in continuum theory, but is an important input into continuum calculations. For the microscale Couette flow problems, MD results show that stick BC, i.e., fluid layers being locked with the solid wall, will occur if there is a strong wall-fluid interaction. If the wall-fluid interaction is weak, slip BC will occur at the interface. Shear direction with respect to the wall lattice orientation is also important. For the microscale Poiseuille flow problems with appropriate parameters, the MD simulations produce a parabolic velocity profile that agrees with the analytical predictions by solving the N-S equations with no-slip BCs. As the fluid density decreases, our MD simulations indicate that a transition to slip flow will occur at the wall.

We performed several large-scale simulations to further investigate the physical mechanisms that govern the microtransport phenomena. Our interest of performing large-scale simulations is to identify at what length scale the continuum and equilibrium assumptions may break down. Simulation results indicate that stick-and-slip phenomena always exist at the fluid-solid interface; however, this interaction becomes less influential as the channel width increases.

We also collaborated with the Massachusetts Institute of Technology to improve a physical model to simulate inflow and outflow BCs for pressure-driven flows. This model simplifies the molecule interaction process and permits a fewer number of molecules required for a simulation.

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Enhanced Vapor-Phase Diffusion in Porous Media

S. W. Webb, C. K. Ho

Vapor-phase diffusion in porous media may significantly impact many important applications. Examples include the drying of sol-gel coatings and textiles, agricultural processes, and the transport of chemicals such as TNT from buried landmines. Vapor-phase diffusion may also be important in gas transport at high-level nuclear-waste repositories. In addition, in many environmental remediation and waste isolation applications, such as the removal of nonaqueous phase liquid (NAPL) contaminants from low-permeability layers in the subsurface, vapor-phase diffusion is the limiting transport mechanism. Enhancement of vapor-phase diffusion by up to several orders of magnitude has been postulated, but not directly measured, in the presence of its liquid through local pore-scale condensation and evaporation at vapor-liquid interfaces.

The objective of the present work is to resolve critical processes and questions associated with postulated enhanced vapor-phase diffusion mechanisms. The approach taken in the present research is to perform modeling and experimental investigations of enhanced vapor-phase diffusion in porous media at various length scales, including the pore-scale and the laboratory-scale. Results to date include calculation of significant enhancement of vapor-phase diffusion at the pore-scale.

Experiments. Enhanced vapor-phase diffusion in porous media has never been directly measured; it has been inferred from other information such as total liquid water movement. We are conducting a series of experiments at three different length scales—the pore-scale, a pore network, and a porous medium. These data will be the first known direct measurements of enhanced vapor diffusion in porous media.

To obtain data on the pore-scale, a series of innovative experiments is currently being conducted at New Mexico Tech. These experiments are made out of glass and plexiglas to allow for visualization of the pore-scale processes. A single pore throat connects

two small chambers. We impose a concentration gradient across the pore throat by the presence of pure water in one chamber and brine in the other. Water vapor will diffuse from the chamber with water to the chamber with brine through the pore throat. We directly measure the vapor diffusion rate with and without a liquid island in the pore and can calculate any enhancement caused by the liquid island.

Pore network experiments being performed at Sandia will evaluate enhanced vapor diffusion in a 2-D network. We designed these tests also to allow visualization of the flow. We are using a "sandwich" consisting of two glass plates with roughened surfaces facing each other. The glass sandwich contains liquid islands, and we impose a concentration gradient across the test section similar to the pore-scale tests. We measure vapor mass transfer rates in and out of the test section and will use them to quantify enhanced vapor-phase diffusion at the pore network scale.

Finally, porous media experiments are being conducted at Washington State University. These experiments are 3-D with limited viewing capability. We subject a bed of glass beads to different boundary conditions (BCs) and measure the vapor diffusion rate in and out of the test section. We impose various BCs, including concentration and temperature gradients, to study the effects on porous media vapor diffusion rates. The acquisition of data at three different scales will allow for an evaluation of scaling effects.

Modeling. To understand the processes involved in enhanced vapor diffusion, and to be able to interpret the pore-scale experimental data, we performed pore-scale modeling. The pore-scale model is a detailed representation of advection, Fickian diffusion, and Knudsen diffusion in the gas phase on the pore-scale with control volumes 5 microns on a side. Liquid is present as individual islands in pore throats. We calculated capillary pressure and vapor pressure lowering due to the local curvature at the gas-liquid interfaces. Liquid may flow within the liquid island in response to capillary pressure gradients. We calculated heat transfer in the solid particles, including particle-to-particle heat transfer. When we imposed a concentration gradient on the pore-scale

model, the presence of the liquid island significantly enhanced the vapor diffusion rate across the model as vapor diffused "through" the liquid island. This enhancement was a strong function of the length of the liquid island and may be up to an order of magnitude. This model represents the first completely mechanistic calculation of enhanced vapor diffusion in porous media.

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Numerical and Experimental Investigation of Vortical Flow-Flame Interaction

H. N. Najm, K. D. Devine, S. N. Kempka,
R. W. Schefer

Sandia developed a two-dimensional (2-D) coupled Lagrangian-Eulerian adaptive mesh refinement (AMR) code and used it to study lifted reacting diffusion jet flame flow. We also conducted an experimental investigation on the same flow, a rectangular methane-air diffusion jet flame, which we acoustically forced to enhance the organization of large-scale structures. We used experimental laser diagnostic techniques, planar laser-induced fluorescence (PLIF) imaging, and particle imaging velocimetry (PIV) to image the scalar and velocity fields and to provide data for validation of the computed jet flow. The numerical model included the use of the 2-D Lagrangian vortex method for solving the momentum equations, and a Eulerian finite-difference (FD) method for solving the scalar transport equations on the adaptive mesh. We included coupling terms to model the expansion field due to combustion heat release and for generating baroclinic vorticity.

We used the code to study a reacting jet flow and compared it to experimental data. Results demonstrate similar flame dynamics in the vicinity of the stabilization point. We observed a triple-flame structure at the flame stabilization point in the numerical results, a structure that has been postulated but not yet observed experimentally in this flow.

Our project accomplishments fit into numerical and experimental sections.

Numerical. The starting point was an existing parallel AMR code for propagating a single scalar field with a known velocity field. We developed this code in this project to solve the energy and species conservation equations for a multispecies reacting mixture with

detailed chemical kinetics and variable transport properties. We wrote a massively parallel (MP) Lagrangian vortex-method code to solve the momentum equations in 2-D low-Mach-number flow. We used a fast multipole method for the evaluation of n -body interactions. We used a potential panel method to enforce domain boundary conditions (BCs) on the vortex-method model. We coupled the two codes together by importing velocity field information from the Lagrangian code to the AMR code, and baroclinic, viscous, and expansion source field information in the reverse direction. We implemented a second-order predictor-corrector time integration procedure, allowing large Lagrangian timesteps, while local mesh cell size per numerical stability constraints governed Eulerian timesteps. We demonstrated the overall code to run on the Intel Paragon MP architecture. Dynamic load-balancing is in progress.

We used the code to study both nonreacting and reacting jet flow. In the latter case we used a single-step irreversible global reaction mechanism. We chose inflow profiles and forcing frequencies to replicate those in the experimental jet. We observed shedding of large-scale vortex structures similar to the experimentally observed shedding in amplitude and frequency. The reacting jet simulations revealed the expected weakening of vortex structures due to the expansion field of the flame. We found the flame stabilization point at the base of the jet to exhibit dynamics similar to those observed in the experiment, including the intermittent entrainment and curvature of the flame by strong vortices shed from the jet, and the detachment of flame segments by the jet vortices.

We observed a triple-flame structure at the jet stabilization point, including a premixed flame front at the stoichiometric mixture fraction contour, a rich flame branch into the jet fuel stream, and a lean flame branch into the coflow air stream.

This structure has been postulated but not yet observed experimentally or numerically in this unsteady jet flow. The main reason for its observation here is the fine resolution allowed by the AMR and Lagrangian codes in the vicinity of the jet stabilization point.

Work continues on code optimization and validation.

Experimental. We completed the design and assembly of the planar forced jet. We achieved excellent control over vortex size and amplitude. We selected operating conditions for detailed study and comparisons with the computational model predictions. We implemented both PIV and PLIF diagnostic capabilities in the planar jet apparatus. In the non-reacting flows, we finished complete data sets using PIV for the instantaneous velocity field and PLIF for the acetone distribution (used as a scalar marker for the fuel) to characterize turbulent mixing and provide model validation data. In the reacting flows, we completed PIV and PLIF measurements of the instantaneous velocity, acetone, and OH fields to study the effects of vortex interactions on mixing, flame structure, and chemistry.

PLIF measurements of the CH distribution and comparisons with model calculations are in progress.

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Temporal & Spatial Resolution of Fluid Flows

S. R. Tieszen, L. D. Perea, R. W. Schefer,
T. J. O'Hern

The purpose of this project is to develop the technology to temporally and spatially resolve fluid flows for the purpose of developing and validating the emerging generation of fluid solvers. The key difference between the emerging solvers, such as large-eddy-simulation (LES) and vortex dynamics, is the temporal resolution that permits simulation of transient, large-scale, coherent, vortical structures. These structures dominate scalar transport (heat transfer, entrainment, etc.) in virtually all buoyant flows. The development and validation of these numerical tools require data with simultaneous temporal and spatial resolution.

Sandia based the approach on particle image velocimetry (PIV). The goal is to temporally and spatially resolve at least two orders of magnitude in both time and length scales in flows of practical importance to Sandia's missions. Prior to this project, we applied PIV technology only to laboratory-scale flows of limited practical interest and relevance to development and validation of numerical tools for fully developed turbulent flows.

PIV works by slicing a seeded flow with a laser light sheet. The particles scatter the light, which is collected by a camera. By collecting multiple pictures, we determined quantitative information on particle velocity versus time. We used a 0.3 J/pulse, 308-nm, 200-Hz, XeCl excimer laser and 35-mm pin-registered movie cameras. We conducted the experiments on nonreacting and reacting plumes in the Smoke Emission Reduction Facility (SMERF) at the Lurance Canyon Burn Site using a 1-m-base-diameter source with helium, hydrogen, and methane.

Development was required to scale up PIV techniques to meter-size scales relevant to fully turbulent flows and attempts at conducting simultaneous planar laser-induced fluorescence (PLIF)

to mark an important scalar simultaneously with the velocity field.

Our accomplishments include the following:

(1) Demonstrated that we could successfully use the SMERF, which was designed for container certification tests, as a research enclosure for studying buoyant flows with repeatable and characterizable boundary conditions.

(2) Demonstrated that images suitable for PIV analysis can be acquired in helium flows and methane fires with seeding in both the ambient and plume fluids. Even at the one-meter scale, the laser light passed through the soot field and flame zones with enough intensity to image appropriately. In hydrogen fires, particle images were distorted, making PIV difficult in the interior of these fires. In both methane and hydrogen fires, the combustion products thermally destroyed the glass microballoons employed as particles, so PIV in this zone is not possible.

(3) Obtained PLIF images for all flows with varying levels of success. In helium, we imaged an acetone tracer concentration, but only at the expense of decreasing the laser sheet height by a factor of five to get the required intensity. In hydrogen, we recorded interesting images of the products of combustion of the glass microballoons. The images are a good marker for the product zones in the fire. In methane, we obtained images that are visually similar to poly-aromatic-hydrocarbon (PAH) images obtained in smaller methane flames. These images are good markers for the flame zone.

3508.090

Characterization of Fluid Transport in Microscale Structures

P. H. Paul, J. H. Smith

Liquid flow in microchannels (a few to 100-micron cross-section) is strongly dependent on the details of liquid-liquid and liquid-solid interactions. This project seeks to develop new flow diagnostic tools

to be able to image scalar and velocity fields in microchannels and to apply these tools to both fundamental research on such flows and as a means of validating engineering device performance. Studies concentrated on pressure and electrokinetically driven flows in electrolytes, specifically water and acetonitrile mixtures, as flowing in glass or silica and silicon-based plastic channels.

The primary goals of this project were (1) to develop *in situ* laser-based imaging techniques to measure scalar and velocity fields in liquid flows in microchannels, (2) to apply these tools to characterize pressure and electrokinetic (EK) flow phenomena in capillaries (round microchannels), and (3) to develop and fabricate planar microchannels with suitable optical access to investigate flow in rectangular cross-section microchannels. We developed a microflow-imaging microscope with the demonstrated capability to provide scalar images with a resolution of better than 2 microns and velocity field images with a resolution of better than 5 microns. We obtained velocity images from scalar-image time sequences by inverting the conserved scalar convection-advection equation. We undertook studies in capillaries of both pressure- and EK-driven flows. These demonstrated the ability to measure and provide quantitative data on scalar transport properties, flow friction factor, and zeta potential for both neutral and charged species for a range of liquids. The planar microchannel development and manufacturing portion of the project did not yield any structures suitable for flow testing. We obtained planar microchannels with suitable optical access from other sources, and flow studies in these structures are in progress.

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Refereed

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Stress Evaluation and Model Validation Using Laser Ultrasonics

W. Y. Lu, L. W. Peng, J. J. Dike

The evaluation of mechanical stress has been, and continues to be, an area of vigorous research due to its effect on the performance and reliability of mechanical hardware. Of particular interest to Sandia is the ability to predict and experimentally verify stress fields in engineering components resulting from both their intended operation (external loading) and fabrication process (residual stress). The purpose of this project is to develop a noncontact stress measurement technique that is needed for experimental evaluation of stresses for validation of constitutive models and structural analyses to enable model-based design.

Laser ultrasonics (LU), a novel method for the optical generation and detection of ultrasound, can make ultrasonic velocity measurements over a path length of a few millimeters, an improvement in spatial resolution of at least an order of magnitude over conventional methods. The technique allows us to experimentally validate the acoustoelastic behavior of candidate materials, thus qualifying this stress measurement technique.

We improved the accuracy of time-of-flight (TOF) measurement by developing a two-point detection method and replaced the 200-MHz digitizer by a faster unit, RTD720 (1 GHz). We developed a LabView virtual instrument (VI) to

acquire, average, and store waveforms. We obtained the acoustoelastic constants of Al6061-T6 and determined the sensitivity and resolution of LU stress and stress-gradient measurement, which were the focuses of FY97 experiments. We developed and validated finite-element (FE) models for simulating thermal and mechanical responses due to heating by a laser pulse. We obtained good agreement with theoretical and experimental data for the thermal and mechanical analyses. We also made a comparison of calculated waveform and frequency content for focused and unfocused laser sources with our experimental data.

The focus of this year's experimental work is to determine the sensitivity and resolution of LU stress and stress-gradient measurements. To improve the accuracy of TOF measurement, we developed a simple two-point detection method to eliminate the error due to the triggering jitter. The method has the advantage of two detectors but uses only one interferometer. We further improved the resolution of time measurement by replacing the 200-MHz digitizer, RTD710, with a faster sampling unit, RTD720 (1 GHz).

Using the technique described above, we obtained the acoustoelastic properties of Al6061-T6 by measuring the transit times of Rayleigh waves propagated on uniformly stressed tensile specimens that were loaded uniaxially. LU-measured acoustoelastic constant K_1 is $-0.22E-6$, which is in accord with theoretical predictions. Experiments include various distances between receivers; the shortest distance considered was 0.8 mm. Current spatial

resolution is less than 1 cm (between detectors). The stress resolution is about 40 Mpa.

Rayleigh waves are dispersive when the stress gradient is not zero. We designed a four-point bending experiment to study the dispersion of Rayleigh waves. At the middle section of the beam, the stress gradient is uniform. Experimental results show that we can evaluate the stress gradient from the dispersion of Rayleigh wave. Current stress gradient resolution is about 40 Mpa/mm.

We developed and validated FE models for simulating thermal and mechanical responses due to heating by a laser pulse. The overall approach in developing a technique to predict waveforms caused by a laser pulse is sequential thermal and mechanical analyses. Because the region heated by the laser pulse is very localized, the mesh used in the thermal analyses is much smaller in physical extent and has much smaller elements than those used in the mechanical analyses of wave propagation. Element sizes on the order of $2E-4$ mm are used in the thermal analysis, while elements on the order of $5E-1$ mm are adequate to capture waves with wavelengths of interest to our work. We used the thermal code COYOTE to perform the thermal analysis. We used the utility code MERLIN to map the temperature histories to a subregion of the mechanical mesh. We wrote several small software routines to manipulate the temperature histories to extend the temperature histories to the remainder of the mechanical mesh. We used both PRONTO and ABAQUS mechanical codes to perform the wave propagation simula-

tions. ABAQUS has features not present in PRONTO (such as material damping, shell elements, etc.) that allow various techniques for determining what aspects of the simulations are most important to be evaluated. The majority of analyses to date have been 2-D axisymmetric.

We obtained very good agreement with analytical and experimental data from the literature for the thermal analyses. Validation of the expected waveforms focused on comparisons with analytical waveforms calculated by transform techniques at Johns Hopkins. The waveforms used for comparison had previously been compared with experimental data with good agreement. Waveforms currently predicted using the ABAQUS and PRONTO codes agree well with and show most of the important features exhibited by the analytical waveforms. We demonstrated that the addition of a small amount of material damping significantly improves the response in a sample mechanical analysis. We modified PRONTO2D's elastic material subroutine to include material stiffness proportional damping.

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Refereed

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3508.120

Altered Simulation Properties for Tetrahedral Finite Elements for Use in Engineering Simulation

S. W. Key, C. M. Stone, M. L. Blanford, M. W. Heinstein, F. J. Mello

The finite-element method (FEM) is a numerical technique for generating a finite dimensional approximation space in which to seek solutions to partial differential equations (PDEs). The physical applications are many and varied. Here Sandia is concerned with PDEs that characterize the large-deformation, inelastic response of solids. Discussions of FEM technology focus on the elementary volumes and the placement of nodal points (points at which displacement degrees of freedom [DOFs] are defined). The following remarks concern existing practices and proceed to the tetrahedron as the elementary volume of interest here.

We expended considerable effort in perfecting the algorithmic properties of eight-node hexahedral FEs. Today the element is well understood and performs well when used in modeling 3-D explicit transient dynamic events. However, the automatic generation of all-hexahedral meshes remains an elusive achievement. The alternative of automatic generation for all-tetrahedral meshes is a reality. Unfortunately, in solid mechanics the four-node linear tetrahedral FE is a notoriously poor performer (its widespread use notwithstanding), and the ten-node quadratic tetrahedral FE, while a better performer numerically, is computationally expensive. To use the all-tetrahedral mesh generation extant today, we explored the creation of a quality eight-node tetrahedral FE (a four-node tetrahedral FE enriched with four mid-face nodal points). We present the derivation of the element's gradient operator, studies in obtaining a suitable mass lumping, and the element's performance in applications.

After derivation of the element's gradient operator, obtaining the correct mass lumping at the nodal points, and trial implementation in software, we obtained good results in a number of simulations. In particular, we examined the eight-node tetrahedral FE's behavior in longitudinal plane-wave propagation, in

transverse cylindrical-wave propagation, and in simulating Taylor bar impacts. The element samples only constant strain states and therefore has twelve hourglass nodes. In this regard, it bears similarities to the eight-node, mean-quadrature hexahedral FE. Given automatic all-tetrahedral meshing, the eight-node, constant-strain tetrahedral FE is a suitable replacement for the eight-node hexahedral FE and "hand-built" meshes. It remains to perfect the hourglass control and to test the formulation for compatibility with contact algorithms, which account for the interaction between independently meshed domains to allow wider application of the new tetrahedral FE.

Publications

Refereed

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Development, Implementation, and Experimental Validation of the Lattice Boltzmann Method for Modeling Three-Dimensional Complex Flows

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O'Connor, S. N. Kempka, H. W. Stockman

This project is (1) developing codes based on the Lattice Boltzmann (LB) method for modeling nonreactive and reactive transport in complex geometries, including implementation of scalable, distributed algorithms, (2) developing methods and computational algorithms to extract quantitative statistical descriptions of the microgeometry of porous media, and (3) validating the numerical codes by comparison with both laboratory transport and flow experiments, as well as by comparison with both calculations based on other numerical methods and problems for which there are analytic solutions. The LB method shows exceptional promise for modeling both phenomena at intermediate scales where neither continuum models nor molecular dynamics (MD) methods are practical, and also for modeling very large-scale continuum flows where conventional computational fluid dynamics (CFD) methods suffer severe difficulties. This project couples innovative experimental approaches, physical and chemical theory, novel algorithms, and advanced computing techniques and capabilities, and is developing an advanced computational framework in which to investigate fundamental phenomena characterizing micro- and macroscale complex flows.

Work focused on development of an elementary capability to model complex flows using the LB method and on initial development of advanced computational algorithms to statistically characterize and numerically simulate complex 3-D microscale flows.

We developed a 2-D LB code with the capability to simulate multicomponent flow with buoyancy, anisotropic diffusion, and precipitation and dissolution. We investigated an alternative boundary condition (BC) specification at the solid/fluid interface. Sensitivity studies based on numerical simulation of classic 2-D

Taylor-Aris dispersion reveal that the new no-flux BC is an order of magnitude more accurate than the standard "bounce-back" condition. Comparison reveals maximum error of ~1% at channel widths ranging from five to twenty sites, whereas the maximum error for the bounce-back BC is ~10%. Optimization of the fundamental translation/collision algorithm led to major speed improvements.

We developed distributed, single-component 2-D and 3-D LB codes using message passing interface (MPI) protocol. MPI provides portability to a variety of platforms, including massively parallel (MP), UNIX, and WinNT. We demonstrated optimal scaling in simulations performed on the Paragon, SP2, SGI Power Challenge, network of workstations, and single-processor SGI. We incorporated a visualization layer using OpenGL.

We quantified accuracy of the LB method by comparison with analytical solutions and results obtained using conventional CFD methods. As noted, 2-D simulation of Taylor-Aris dispersion indicates accuracy of ~1% when compared with the analytic solution. Flow over a backward facing step is another classical 2-D flow that involves recirculation. We compared the lengths of the primary and secondary recirculation regions to previous numerical results for a Reynolds number between 200 and 800, and the LB results agree well with previous results in the literature. Comparison of 2-D simulations for dispersion in an alveolated channel and for mixing at a fracture junction showed good agreement with previous numerical solutions, approximate analytic solutions, and experimental results. We obtained assessment of the 3-D code by simulation of flow through a duct with square cross-section. Comparison with an analytical solution shows that for this flow, the LB method incurs < 1% error with eight grid points spanning the duct in each direction, and error decreases with the square of the grid size and exhibits second-order accuracy.

We identified three classes of random complex porous media of interest, including geomaterials, fibrous ceramic insulations, and sintered glass beads. We imaged samples via laser scanning confocal microscopy (LSCM)

and collected representative data sets. Experimental measurements of transport properties exist through previous or ongoing work. We performed detailed investigation of alternative approaches for image processing and binarization. We extended the 3dma code (SUNY-SB) to import and manipulate the LSCM volumetric image data format. We motivated new statistical metrics and incorporated them into the code. Additional functionality includes two-point correlation functions in 1-D, 2-D, and 3-D, and geometric measurements of coordination and connectivity based on medial axis analysis. We analyzed representative data sets, and extracted and validated statistical descriptions of first-order geometric parameters such as porosity and specific surface area by comparison with measurements obtained previously. We also derived higher-order microgeometric parameters. As a prelude for 3-D LB simulations through random, complex porous media as determined from LSCM and analyzed with 3dma, we created a numerical pipeline between the 3dma and LB codes.

Design of experiments with simple model systems (glass bead packs) using magnetic resonance imaging (MRI) to reveal flow fields for validation of LB simulations is in progress.

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3508.150

Nondeterministic Modeling in Engineering Science

J. R. Red-Horse, D. G. Robinson, K. S. Chen, L. Swiler, V. J. Romero, T. L. Paez

Physical processes that are the subject of engineering analyses invariably contain parametric entities that can, at most, be specified to within some level of uncertainty. The ability to evaluate the nature of the predicted system response in the face of this inevitability is a vital risk-reducing capability made necessary by the new model-based weapons design initiative. The subject approach is to use approximate analytical methods to estimate response uncertainty using probabilistic measures. These approximation schemes will require only that point analysis results be available through which analytically complete probabilistic descriptions will result. Thus, not only can the methodologies be easily wrapped around existing analysis codes, but significant reductions in computational requirements, relative to Monte Carlo methods, are often realized as well without a reduction in probabilistic information. The objectives of this research effort are to develop a suite of viable, computationally feasible, analytical approaches that can characterize (1) certain classes of input uncertainty, (2) the propagation of statistical uncertainty through analytical models to response quantities of interest, and (3) the proportion that particular physical model primitives contribute to that propagation process; that is, we will develop a means for performing probabilistic sensitivity analyses.

(1) We simplified coding and exercising of a number of fast probability integration schemes, again to investigate their feasibility for our applications.

(2) We coded a more general formulation of advanced mean value (AMV) and exercised it in the full probability regions on both an analytical example possessing a closed-form solution and a realistically sized structural dynamics application whose results were verified through Monte Carlo simulation.

(3) We investigated the implications of design spaces with dimension greater than one. Based on preliminary studies, such analyses appear tractable using AMV.

(4) We developed a Gauss point integration scheme based on AMV/AMV+ to reduce the number of thresholds necessary in evaluating response statistics.

(5) We devised formulation of an approximation approach to response surface modeling in which the response surface is progressively constructed via levels of structured sampling. We successfully analyzed analytical and application-based test problems using the approach.

(6) We developed an algorithm to compute confidence bounds on computed probabilities given a particular class of uncertainty in input parameter specification.

(7) We initiated experimental data collection. We will then use these data in subsequent program years as the basis for developing methods for input characterization and for establishing vital metrics necessary for addressing response uncertainty quantification.

Joint Task: Capturing Recrystallization of Metals with a Multiscale Material Model

D. A. Hughes, A. W. Godfrey, E. A. Holm, S. M. Foiles, D. J. Bammann

The goal of this research is to develop a predictive continuum model that incorporates essential mechanisms from the atomic dislocation substructure and grain-size length scales. Sandia will accomplish this goal by developing a nonlinear nonequilibrium thermodynamic gradient theory that provides the mathematical framework for these microstructural processes. We will predict the physics at each length scale from experimental discovery and theoretical calculations, and will establish the bridges between each length scale and the continuum level by their contribution to the thermodynamic process. Although the framework we are developing is more general, the test application we chose is the prediction of recrystallization in metals. Recrystallization occurs when deformed metals are heated and new strain-free grains nucleate and grow to consume the deformed grains. This ubiquitous process drastically changes the material's mechanical properties, including hardness, ductility, grain size, grain orientation, and dislocation density, as well as its electrical and magnetic properties. Recrystallization often occurs during manufacturing, during high-rate deformation, and in high-temperature environments, e.g., gas transfer systems and earth penetrators. The continuum-level model will evolve the macroscale material response based on models at lower length scales. A mesoscale recrystallization model based on a Monte Carlo Potts model will embody the local dislocation structure,

grain orientation, and strain energy that will be correlated with the variables in the continuum model. At the microscale, we will combine quantitative statistical measurements of dislocation structure, strain energy, boundary properties, and nucleation with results of atomic-scale simulations and scaling theory to provide relevant parameters for the mesoscale. Bridging these three length scales and the required experimental discovery has never before been attempted.

We developed a thermodynamic formulation within the continuum framework that will enable the incorporation of dislocation structure evolution, nucleation, and recrystallization. We modified the mesoscale recrystallization model to include variable grain boundary energies and mobilities and variable grain orientations, including a crystal orientation distribution function scheme to model the effects of orientation pinning during growth. We modeled subgrain growth to explore this process as a nucleation model. For the experiments, we designed a bicrystal compression sample with a special boundary to enable us to use various atomistic models to look at recovery and nucleation events in the deformed and annealed bicrystals. Bicrystal fabrication is 50% complete. We modeled the special bicrystal boundary structure atomistically with the embedded atom method (EAM). We installed a new field-emission transmission electron microscope (FEGTEM) and laboratory that we will use to experimentally acquire statistical data regarding dislocation structure evolution and to study nucleation in the bicrystal samples. We measured the distributions of dislocation boundary spacings in the FEGTEM as a function of strain in compressed single-crystal samples. We found these distributions to follow a scaling law like the dislocation boundary misorientation

angle. We are developing a kinetic Monte Carlo model that will take into account these observed scaling laws for dislocation structure evolution and strain energy distributions. We created an initial kinetic Monte Carlo model for dislocation tangle point defect interaction and used it to model dislocation motion.

Publications

Refereed

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Lagrangian Modeling of Radiative Transport

L. A. Gritz, J. H. Strickland

Many complex multiphysics, multiscaled, time-dependent processes include radiative heat transfer in turbulent flow. Conventional grid-based models are not well suited for such problems due to the complexity of gridding domains, which are large compared to the scale of the important transport phenomena. Gridless, Lagrangian-based approaches employed in vortex methods to model fluid flow, and used in the transport element method to solve the species transport and energy equations, are a logical alternative.

In FY97, Sandia developed a gridless technique (compatible with vortex and transport element methods) for the solution of the integral form of the radiative transfer equation in an emitting and absorbing media with uniform properties. The medium is represented by Lagrangian elements whose "strength" is dependent on the gradients of local temperature. Results to date show significantly better accuracy than other techniques when compared to established and newly developed closed-form solutions for a planar medium. We investigated axisymmetric forms of the radiative transfer equation. We developed a 3-D direct solver and verified the results using closed-form solutions for planar media. We also developed a fast-solver algorithm, based on the expansion of the Green's function in terms of a convergent separable series, for a planar medium. We achieved computations with an accuracy of better than 0.1% for 20,000 source and target points in 1% of the time required for a direct solution. A 3-D fast solver is presently under development. We performed analyses of highly resolved temperature fields representative of flame sheets, as appropriate for fire and combustion calculations. We performed and are reviewing coupling of the axisymmetric transport element method with solutions of the radiative transfer equation.

We developed a gridless technique for the solution of the integral form of the

radiative transfer equation for an emitting and absorbing medium with uniform properties. We obtained the solution by representing the medium with emitting and absorbing elements whose "strength" is dependent on the gradients of local temperature as given by $s_i(x) = \partial(T_4(x))/\partial x$. The solution for the net radiative heat flux, q_r , the volumetric energy deposition, $\text{div}(q_r)$, and its gradient, $\text{grad}(\text{div}(q_r))$ (as required for the transport element method) at a location x_r , are accordingly given by $F_i(x_r) = S s_i(x_s) E_n(|x_r - x_s|)$ for exponential integrals $E_n(x)$ of the order $n = 1, 2$, and 3 , respectively. By expressing the source strength in terms of gradients, and by determining the effect of the field of sources by adding their individual contributions at any specified location in the field, the technique is compatible with numerical simulation of the flow and temperature field by gridless vortex and transport element methods, respectively. We compared results obtained using this approach to established and newly developed closed-form solutions for transport in a planar medium. We illustrated significant errors in other techniques that solve simplified governing equations by direct comparison with the solution of the exact form of the integral equations yielded by the present study. Investigation of forms of the radiative transfer equation for axisymmetric geometries did not yield a compact form of the integral equations, but we obtained a series solution suitable for generating tabular results. We also developed a 3-D direct solver. We performed verification by comparing results from 3-D, effectively planar geometries with closed-form solutions for planar media.

We also developed a fast algorithm, based on the expansion of the exponential integrals $E_n(x)$ for $n = 1, 2$, and 3 in terms of a convergent separable series, for the solution of q_r , $\text{div}(q_r)$, and $\text{grad}(\text{div}(q_r))$, in a planar medium. This algorithm provides fast simulations of radiation problems in planar media with emission and absorption when there are many temperature fronts within a few optical paths. We decomposed the source

domain into a binary tree structure consisting of boxes containing equal numbers of sources at each level. We then used multipole expansions to compute values of the sum over source points x_s at discrete evaluation points x_r . We can make computations with an accuracy of better than 0.1% for 20,000 source and target points in about 1% of the time required for a direct solution. Additional improvements in computational tractability occur since numerical representation is required only for the portion of the domain with significant temperature gradients. The framework for similar fast solvers for 3-D temperature fields is complete.

We applied the technique to a temperature field representative of single and multiple (150) flame sheets, as appropriate for fire and combustion calculations. We noted additional utility for subgrid analyses, in conjunction with direct numerical simulation or reduced dimensional mixing and turbulence models.

We installed a complete review of the axisymmetric formulation of the transport element method for Sandia's record. We also completed an axisymmetric simulation of a reacting plume (such as a fire) without radiative transport. The inclusion of a radiative source term in the transport element method results in a form of the energy equation that can no longer be solved subject to the simplifications of a Shvab-Zeldovich transformation, which eliminates the heat release source term. Identification of the necessary terms in the transport element method, the enhancement of the numerical model to accept such source terms, and their preliminary implementation are complete.

Publications

Refereed

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The Manufacturing Science and Technology investment area emphasizes advanced manufacturing and production technologies, especially those related to Defense Programs as well as to energy and environmental concerns. Projects that reduce cost, shorten the design and manufacturing cycle, and improve

product predictability are encouraged.

Areas focus on three main thrusts: (1) making information flow efficiently through the stages of manufacturing; that is, from designer to planner to producer to inspector and across customer and supplier networks; (2) developing faster, more affordable processes that are more versatile than those now used in the nuclear weapons complex, including projects that study rapid prototyping as well as how to eliminate the need for prototyping; hardware that can be reconfigured according to manufacturing needs; processes to predict whether a design can be manufactured; and efficient, affordable production of small lots; and (3) minimizing the impact manufacturing has on the environment and on energy resources without reducing performance or reliability.

Manufacturing weapons components directly from a computer model has the potential to revolutionize both weapons production and the industrial production of a spectrum of other structural components. Researchers are pursuing this goal by refining the laser-spray fabrication process (LENS™) developed at Sandia. Computer models of weapons components are sliced to provide detailed geometric information. Sensors are being developed and refined to control the LENS™ manufacturing process.

Modern manufacturing often uses automated robots to assemble manufactured components. Engineers are applying human-like motions to the fabrication of Sandia components. Current production processes are limited to procedures based on orthogonal motion. Applying more complex motions will reduce manufacturing time and cost while increasing product quality. This process will be scaled to both micro and macro environments.

The ROTOPOD, a mechanism that demonstrates high dexterity in six-degrees-of-freedom (DOF) work space, belongs to the class of parallel linked robots. Parallel robots, unlike commonly known robots that are serially linked, promise higher stiffness, speed, accuracy, and payload handling.

MANUFACTURING SCIENCE & TECHNOLOGY

VIEWS—Virtual Interactive Environment Work Space

A. Breckenridge

Virtual environments (VE), alternately known as virtual reality (VR), synthetic environments, and other names, are a collection of technologies that offer the opportunity to integrate the human into a computing system. Sandia has made steady improvements in the human-computer interface for VEs. During the third year, we propose to apply this technology to an actual Sandia manufacturing process-enhanced surety system. We will concentrate on one case study that exemplifies the application of VEs in several aspects of manufacturing.

(1) *Built the basic VE.* We will base the initial graphical representation on the Pro/E modeling that is currently available for the surety system. If possible, we will obtain additional information to utilize tools developed under this project, such as the ACIS (Alan, Charles, Ian System—part of the CAD system) application programming interface (API), the command line interface for Exodus II finite-element (FE) data, linkage to data acquisition and display system (DADS) for reading dynamic analysis, and incorporating predefined movement of mechanical parts using liaisons.

(2) *Incorporated multiple sources of sensor-based process control data.* Currently, the surety system collects data based on sensors placed on strategic functions in the process. We will apply data fusion into one VE to study all the information. We will provide tools to give the analysis the ability to collate the information. If possible, we will add some automatic detection of normal or abnormal states to focus immediately on important indicators. We need to purchase minor equipment to add additional sensors.

(3) *Mapped one or more of the data sources into other human senses such as auditory and haptic interfaces.* Currently, the surety system collects eight or more sources of information. To cross-collate this information to be presented efficiently, we will map one or more of the data sources to a nonvisual interface, e.g., mapping revolutions per minute (RPM) to sonification or force to haptic device. We need to purchase equipment to add the necessary interfaces for haptics.

(4) *Simulated one or more of the physical properties.* We need to understand the characteristics of the system such as the validation of the initial start-up or the cutting process. Several of the components are based on force, torque, etc.; information can not be lost between the physical model and the VE. We will simulate the physical properties where appropriate. We should capture data to verify that the physical model is simulated correctly.

(5) *Parameterized one or more of the data sources to determine the cause/effect or optimization of the total process.* We will divide the visualization into a hierarchical model with increasing details for individual components. However, we will also need to examine the system as a whole. If possible, we will change and optimize numerous parameters to see the overall effect. We will calculate fault tolerance and will attempt to calculate assurance in the simulated environment.

(6) *Modified the simulated model.* We will prototype the physical model; however, the exact configuration may need variations to be deployed. The VE will provide a mechanism to scale the model or make minor modifications.

(7) *Improved the human computer interface.* Computers promise to revolutionize the manufacturing process. VR promises to revolutionize how we interact with these computers. However, the computer needs to add benefit without focusing the attention away from the real

problem. The VE provides a unique way of examining the information that is more natural to the operator. Instead of using a simple mouse and keyboard, we will use head tracking, sonification, and force-feedback devices. We need to purchase minor equipment to add the necessary interfaces.

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Distributed Object and Intelligent Agents in a Wide-Area Network Test-Bed

C. M. Pancerella

To meet changing DOE needs it is necessary to recognize that a heterogeneous distributed information system is critical and that distributed software components (those combining distributed objects, intelligent agents, and distributed knowledge-based systems) must be integrated in a wide-area distributed system. Sandia proposed to integrate these technologies in support of concurrent engineering, team collaboration, and manufacturing across organizational and geographic boundaries.

A standard for the deployment of wide-area distributed object systems is CORBA (Common Object Request Broker Architecture). CORBA addresses issues of interoperability in a distributed, heterogeneous system; however, it does not define a protocol for knowledge exchange. We have some results on the integration of the Advanced Research Projects Agency (ARPA) Knowledge Sharing Effort's agent communication language with CORBA objects to produce robust, intelligent software agents.

We proposed to create a test-bed for the development, application, and testing of a wide-area network (WAN) of cooperating agents to support the future Sandia and DOE business needs.

Deviation from Plan. The original intent of this project was to use the AMTnet (Advanced Manufacturing Technologies) and the IMTL as a wide-area test-bed for testing agent and object technologies, but the project took on a more research-focused (and less experimental) theme.

Our key accomplishments included the following:

- (1) Developed JAT (Java Agent Template) Center for Design Research (CDR) as a template for building Knowledge Query and Manipulation Language (KQML)-speaking agents on the Internet.
- (2) Designed an agent architecture using Java, CORBA, and KQML, allowing a design agent to integrate with both inspection agents and manufacturing agents.
- (3) Evaluated agent and object technologies as methods for integrating engineering and manufacturing enterprises.
- (4) Developed guidelines and methodology for integrating engineering applications within Sandia and DOE.

Publications

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Solid Variant Geometry Modeling

P. A. Watterberg

The concept of a "maximum material part" remains a useful theoretical tool. However, attempts in this project to tie American National Standards Institute (ANSI) tolerancing specifications to this theory have been unsuccessful. Emphasis shifted to producing a software system that will take a toleranced part in ACIS (Alan, Charles, Ian System—part of the CAD system) format as input and produce a random variation of the nominal part. This part could then be used by various assembly and function analysis systems. Ey

analyzing enough of these random (but within tolerance) parts, these systems could find statistical problems with the design of the part and potentially fatal flaws. The software system is at a prototype level.

The practice and standards of tolerancing mechanical parts have been developed over decades from shop floor practice. As a consequence, they are frequently inconsistent and vague. The concept of a maximum material part as put forth in this work could go a long way toward mathematizing the tolerancing problem. This would, in turn, allow for rigorous automatic analysis of whether assemblies would assemble and function when composed of parts within tolerances. Unfortunately, deriving maximum material parts from ANSI tolerance specifications proved to be too difficult for this project, and we abandoned the effort. Consequently, we can create the maximum material part for only a few special cases.

Since the software system would not now be able to produce maximum material parts, it had to move in a different direction. We redirected the effort to produce randomly varying parts from a nominal toleranced model. We achieved some success here, but the results of this approach (working with ACIS as the geometric modeler) seem to indicate that the approach of varying the Pro/E model directly, based on the given tolerances, would be more productive. Follow-on projects will proceed in this direction.

3510.440

Rapid Prototyping/Rapid Manufacturing via Freeform Fabrication of Polymer-Matrix Composites

S. G. Kaufman, T. R. Guess, B. L. Spletzer

This year, Sandia developed the curing system control to the point that we can cure nylon/graphite thermoplastic pieces up to 0.125 inch thick. Micrographic analysis of the samples indicates good consolidation of the samples through the entire thickness. We also developed methods for making structures with multiple directions of fiber.

We obtained follow-on funding for the technology from Lockheed-Martin Tactical Aircraft Systems (LMTAS) and filed a patent application in March 1997.

This year's technical effort concentrated on the curing process that takes place on the reconfigurable forming surface. The engineering of the control of the application of heat and pressure was the most time-consuming, but we found the proper process parameters to cure pieces of nylon/graphite thermoplastic composite up to 0.125 inch thick. Micrographic analysis of the test articles cured under these conditions showed good consolidation through the entire thickness of the test articles. The process

also produces a very smooth surface finish.

We also developed two methods of feeding composite material in multiple directions. These will allow fabrication of structures having up to four directions of fiber. Our original method allowed only a single fiber direction. Without the ability to incorporate multiple fiber directions, the utility of this system would be very limited.

Publications

Refereed

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Solid Model Design Simplification

A. L. Ames, J. J. Rivera, A. J. Webb

In developing automatic analysis and manufacturing applications based on solid model descriptions of part geometry, we are confronted with a curious dilemma:

Designers are rewarded for including as much geometric detail as possible, yet that detail causes great difficulty for automated analysis and manufacturing applications. Extra detail at best causes the algorithms to require far more time and space to execute; at worst, the application completely fails.

This project is an effort to develop a capability to simplify Pro/Engineer design data in an easy, efficient manner. Sandia is developing the capability to automatically search through design data to find features (of parts) and parts (of assemblies) that are unnecessary for analysis, and the ability to automatically suppress the unnecessary data (where possible) or suggest simplification approaches (when automatic suppression fails). We are implementing extensions to Pro/Engineer and using these design simplification tools in a production setting.

With the ability to rapidly simplify models and focus on just the geometry that is important, we can dramatically improve our ability to really use the design information we create. The increasingly small lot sizes and varied product mix we address will demand that we make sharing data among all disciplines more tightly coupled and commonplace, with each discipline viewing only the data they wish to see. This project is developing a fundamental manufacturing technology that is in demand for Defense Program agile strategies for future weapon development and that can be shared with agencies throughout government and industry.

(1) *Tested simplification algorithms in a production setting.* We tested the Pro/Develop algorithms developed last year to search for and suppress unnecessary detail in two settings: in preparing models for radar cross-section analysis and in preparing a neutron-generator model for hexahedral finite-element (FE)

analysis by CUBIT. The algorithms performed well at locating small details and degeneracies that should be eliminated and reported a number of details (surface degeneracies) that historically have been show-stoppers in moving design data to downstream applications.

Production testing suggested a variety of enhancements to the geometric search algorithms developed last year. These include searching for visible surfaces and detecting small gaps and overlaps between parts. These algorithms proved difficult to develop in Pro/Develop due to the complexity of the assembly structure and lack of provision for geometry creation. These algorithms exist outside of the Pro/Engineer context, so they are being addressed through technology developed as part of "application-driven simplification." The FE meshing application would benefit from completion of algorithms that measure influence of faces through the interior of the part.

(2) *Enabled application-driven simplification.* We developed algorithms to permit any applications external to Pro/Engineer to automatically drive the simplification process. As a test case for this approach, we chose an application (called Decomp) that decomposes piecewise 2-1/2-dimensional (2-1/2-D) geometry for hexahedral meshing. The algorithm proceeds as follows: We mark faces in Pro/Engineer in a persistent manner. We export geometry to Decomp, which determines whether the model is 2-1/2-D in any direction. We collect faces that fail the criteria and return the references to the simplification algorithm, which constructs a list of the features required to remove the faces. Simplification happens automatically if the model is constructed properly. The algorithm is easy to implement, robust, and works with any application outside of Pro/Engineer.

(3) *Investigated simplification outside of Pro/Engineer.* We investigated simplification in a number of non-Pro/Engineer-based modelers, including Catia and SolidWorks.

The difficulty of simplification in non-Pro/Engineer feature-based systems varies with the modeler. Search for small features is essentially identical,

as is removal by suppressing features. Newly emerging modelers tend to be less difficult than Pro/Engineer with respect to degeneracy detection and parent/child conflicts, but require the same recognition technology in cases where models are imported from external sources (such as Pro/Engineer). In a separate related (special-purpose) project, we determined that meshable geometry would be most easily produced by developing a special-purpose feature evaluator.

We can address simplification in non-feature-based boundary representation in limited cases. We can directly modify boundary representation if adequate construction geometry exists; or can be created by extrapolation of surfaces present in the model. We can automatically make decisions about how to remove details in certain simple cases; otherwise, they must be human-guided.

Publications

Other

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3510.460

Laser-Spray Fabrication for Net-Shape Rapid Product Realization

E. M. Schlienger, C. L. Atwood, J. E. Smugeresky, M. L. Griffith

The primary purpose of this project is to characterize the laser-deposition process and determine the feasibility of fabricating complex near net shapes directly from a computer-aided design (CAD) solid model. Although Sandia has demonstrated that the laser-engineered net-shaping (LENSTM) process is compatible with metal deposition for simple geometries, using this process to produce net-shape high-performance metal, ceramic, and composite components in a controllable fashion is not yet feasible. Process characterization results from the feasibility study will provide direction in developing a system to fabricate complex shapes directly from a CAD solid model. Our goal is to develop a system that is

robust and provides a significant advancement in existing technology. Sensors will need to be identified, developed (where necessary), and implemented to provide closed-loop process control. It will also be necessary to develop methodologies to slice CAD solid models to directly drive the motion control. We must develop the interfaces to be interactive with sensor inputs from the process. Development of this process will allow design engineers to produce functional models of their designs directly from CAD files. The turnaround time for complex geometrical shaped parts will be hours instead of days, and days instead of months. With the reduced turnaround time, we can spend more time on the product design phase to ensure that we achieve the best component design. Maturation of this technology will revolutionize the way the world produces structural components.

We used the LENS™ process to produce injection molding dies, trial forming dies for neutron-generator tubes, and extrusion dies. We are exploring LENS™ as a means of producing *in situ* magnets as well. We made good progress in the areas of CAD solid model slicing, the production of fully dense parts, and the improvement of surface quality. Over the course of this project, the time to produce a cubic inch of material decreased from 8 hours to under 3 hours with no loss of quality. Nozzle design improved such that the development and drop-in of metal deposits on the nozzle were largely eliminated. We accomplished planned parameter characterization studies and achieved additional process insights with regard to deposition stability. Sensor development efforts shifted from sensing the thermal environment to more fully characterizing the process for enhanced repeatability. As a result of these efforts, we implemented coriolis flow meter technologies for powder mass flow determination. This new sensing capability allowed a fuller characterization of the powder feed and resulted in new insights into control methodologies for controlling powder feed.

We demonstrated a charge-coupled device (CCD) Z-height sensor that images the deposition spot and measures

its location relative to the powder nozzle on the bench and are currently constructing it for installation on the LENS™ machine. With the installation of this device, we can make a real-time measurement of the deposition thickness. Once this measurement is in hand, it will be possible to close the loop in the Z-dimension, thus providing control in an axis that is presently operated as open-looped. Experiments showed that the first-order impact on deposition thickness occurs as a function power density, which is a product of travel speed and laser power. As such, we may adjust either feed speed or laser power to maintain the desired Z-height. We are connecting the CCD sensor to the laser power as a first step at controlling the deposition thickness in a closed-loop fashion.

Process characterization efforts determined that the major issue impacting surface quality of the deposited material is powder size. During operation, surface irregularities associated with the successive laser deposition of layers are quite small when full fusion between layers is being accomplished. Analysis of the deposited surface indicates that the primary surface features may be attributed to discrete powders that have adhered to the surface, but have not fully melted. This observation leads to the conceptualization of several schemes for improving the surface quality. Among such schemes are changing powder size or changing powder morphology of powderless circumferential laser passes.

We also made progress in the production of graded materials. We produced samples that demonstrate a continuously graded structure that transitions from an austenitic to ferritic stainless steel.

In a similar effort, we infiltrated an alumina part fabricated via the direct-write ceramic process with TiCuSi, a titanium-copper-silver alloy, and placed a stainless-steel deposit on top of it. The resulting part is a direct fabrication sample that demonstrates an alumina-to-stainless steel transition.

Publications

Refereed

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Carbon Coatings for Improved Sprytron-Tube Performance and Reliability

T. A. Friedmann, D. R. Tallant, M. E. Smith, M. P. Siegal

Sandia is developing enhanced carbon coatings for new sprytron-tube designs that have simplified the construction, improved the reliability, and reduced the cost of these devices. The sprytron tube relies on a carbon-based coating to fire the device. The coating technology now used, chemical vapor deposition (CVD), produces a form of carbon that is nondirectional in its application and difficult to mask, thus coating the entire piece. This is undesirable in some cases because further processing (laser etching of the coated piece) is required to make a functioning sprytron tube, and this limits the design of sprytron tubes to certain specific geometries. This project studies the use of pulsed-laser deposition (PLD) of carbon coatings for simplified design fabrication.

We combined two Sandia capabilities in a synergistic manner, namely, understanding of carbon film deposition developed in part under research foundation support, with sprytron tube manufacturing expertise. This unique combination has allowed for improved Sprytron tube understanding leading to enhanced reliability, enhanced performance, and lower cost.

We developed several new sprytron designs with enhanced properties. For example, several designs show increased lifetime (some have been fired over 5000 times without failure), and one operates at a trigger voltage reduced by a factor of ten. The simplified new designs require fewer process steps, leading to reduced production costs. In addition, we developed more compact packages. Combined, these improvements not only help ensure that future DP demands can be met at a much reduced cost, but also open the

possibility of new applications and customers.

We coated optically polished sapphire plates and the ends of optical fibers with carbon coatings. These coatings are for testing of strategies for optical triggering using sprytron-type switches. We would use a laser pulse guided by a fiber optic in place of the electrical trigger circuit.

Surprisingly, the carbon coatings did not adhere well to the polished sapphire (versus the ceramic Al_2O_3 where adhesion is not a problem). We found after extensive testing that it was necessary to deposit the carbon coatings at high temperature (800°C) to achieve the necessary thickness range (0.1–0.5 μm). We then annealed these coatings in an inert environment in a rapid-thermal-annealing oven to 1000°C to simulate the effect of brazing. The resistivity and raman spectra of these coatings were similar to the carbon coatings used for poco sprytron designs tested earlier.

In addition, we compared raman spectra of carbon coatings on the walls of fired sprytron tubes to those of annealed graphite. We did a study of annealed graphite coatings to further refine our estimates of the temperatures inside a sprytron tube during firing.

We performed optical testing of these coatings and found that the carbon required a factor of ten less power density for ablation than the equivalent thickness of metal film, making them interesting candidates for optical ignition strategies. We are pursuing feasibility testing of this strategy and expect to provide carbon coatings on sprytron parts for this testing.

Publications

Refereed

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Low-Cost Pd-Catalyzed Metallization Technology for Rapid Prototyping of Electronic Substrates and Devices

K. S. Chen, J. L. Zich, W. P. Morgan

Metallization of polymeric substrates has widespread applications, e.g., in fabrication of electronic interconnects such as flex circuits and printed wiring boards, radar and communication reflectors/horns, and pulsed-power accelerator parts. The objective of this project was to develop a low-cost metallization technology, via palladium-catalyzing with thermal activation, and electroless/electrolytic plating for rapid prototyping of electronic substrates and devices. Conventional metallization technologies are either capital-intensive or involve adhesives or too many wet-processing steps (and often with poor adhesion). Metallic patterns such as electronic interconnects are conventionally fabricated by the subtraction process in which metallized patterns are produced by chemical etching (a process known to be time-consuming, costly, and environmentally unfriendly).

For full-coverage metallization, Sandia developed a process for fabricating adhesiveless copper/polyimide laminates with high peel strengths and thick copper coating. The process involves coating and drying of catalyst solution, thermal activation of catalytic palladium clusters and curing of polyamic-acid polymer carrier, electroless plating of the seed-layer

copper, and electrolytic plating to build copper coating to the desired thickness. We modified this metallization process and successfully applied it in metallizing 3-D microporous carbon foams.

For patterned metallization, we developed an additive process using catalyst-solution printing/plotting. In this process we selectively deposited catalyst solution in areas where metallization is desired. Lastly, we demonstrated feasibility of fine-line metallization using selective ultraviolet (UV) activation.

(1) Developed a thermally activated palladium-catalyzed process for fabricating adhesiveless copper/polyimide laminates with high peel strengths (> 6 lbs/in.) and thick copper coating (> 25 microns). We achieved peel strength as high as 9 lbs/in. as measured by the IPC-TM-650 technique (a 90-degree peel test) and successfully plated copper coating as high as 60 microns. The process involves coating and drying of catalyst solution, thermal activation of catalytic palladium clusters and curing of polyamic-acid polymer carrier, electroless plating of the seed copper layer, and electrolytic plating to build copper coating to desired thickness.

(2) Successfully metallized 3-D microporous open-cell vitreous carbon foams with an average pore size of 80 pores per inch using the thermally activated palladium-catalyzed process. In this application we employed a catalyst formulation based on polyvinylchloride latex resin.

(3) Developed an additive patterned-metallization process using selective catalyst printing/plotting.

(4) Demonstrated feasibility of selective activation using UV radiation for fine-line patterned metallization.

(5) Conducted an experimental and theoretical study of equilibrium characteristics of electroless copper plating (both Cu-tartrate and Cu-EDTA systems).

(6) Filed a U.S. patent application titled "Process for Metallization of a Substrate."

Publications

Refereed

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Smart Cutting Tools for Precision Manufacturing

J. M. Redmond, P. S. Barney

Recent advances in smart materials have renewed interest in the development of improved manufacturing processes featuring sensing, processing, and active control. In particular, vibration suppression in metal cutting has received much attention because of its potential for enhancing part quality while reducing the time and cost of production. Although active tool clamps have been widely demonstrated, they are often accompanied by interfacing issues that limit their applicability to specific machines. In this project, Sandia will develop an alternative approach in which a commercially available boring bar is modified to incorporate lead zirconate titanate (PZT) stack actuators to suppress bending vibrations. Since the modified tool requires no specialized mounting hardware, it can be mounted readily on many machines. Cutting tests conducted on a horizontal lathe fitted with a hardened steel workpiece verify that the active tool yields significant vibration reduction and improved surface finish as compared to an unmodified tool.

In this project, we validated the concept of improving machining capabilities through the development of smart cutting tools. Two primary accomplishments include the development of a computer simulation to assess the performance of a cutting tool and experimental validation of a prototype smart cutting tool.

In the first year of this two-year project, we developed a computer simulation of the boring process to analytically evaluate the performance of a boring bar without conducting extensive cutting tests. We used simple measurements of the boring bar's vibrational characteristics to form a dynamic model of the cutting tool. We determined cutting forces that drive the tool vibra-

tions by the instantaneous chip area, which depends on user-selected machining parameters such as workpiece speed, tool feed rate, and depth of cut. Past tool vibration history leaves a waviness on the workpiece surface that also influences chip area, potentially leading to unstable regenerative chatter vibration. Tool vibration histories normal and tangential to the workpiece surface are provided as output, along with predicted cutting forces and an estimate of workpiece surface finish. We evaluated a number of potential tool designs, leading to the development and testing of a prototype cutting tool.

Second-year efforts focused on developing and testing prototype cutting tools with length-to-diameter (L/D) ratios of 6, 8, and 10. We mounted piezoelectric stack actuators in cutouts in the bar root to control bending vibrations induced by cutting forces. Closed-loop benchtop tests showed dramatic improvement in the dynamic characteristics of each bar, indicating the potential for significant enhancements to cutting performance. A series of cutting tests conducted at Sandia on a "Binns and Barry" horizontal lathe validated the project hypothesis. Active vibration control (AVC) yielded a dramatic enlargement of the stable machining envelope for a bar with L/D of 6. For stable cuts, AVC produced a 2-3-time reduction in workpiece surface roughness as compared to an unmodified bar. Unfortunately, unanticipated project delays limited the time available for evaluation of the bars with L/D of 8 and 10, and only minimal data are available.

Publications

Refereed

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3510.510

Solution Synthesis and Processing of PZT Materials for Neutron-Generator Applications

J. A. Voigt, R. H. Moore, S. J. Lockwood, B. A. Tuttle, T. W. Scofield, J. D. Keck

Neutron-generator power supplies require two unique ferroelectric materials, specifically, lead zirconate titanate with a Zr-to-Ti ratio of 95:5 (PZT 95/5) and PZT 95/5 with a partial substitution of tin for zirconia (PSZT). These PZT formulations are unique to neutron generators, and there are no current U.S. suppliers of the material. Sandia has a limited supply of the materials that we prepared commercially using a traditional multistep mixed-oxide processing route. There are several concerns about acquisition of qualified PZT and PSZT when the current supply

runs out: (1) Will U.S. industry be willing to produce these difficult-to-process materials in the limited quantities required, and, if so, can they produce qualified material? (2) Past experience shows that the success of the current mixed-oxide process is highly dependent on the source of raw materials used. Will the required raw materials be available? (3) The current preparation process has many powder-handling and processing steps that are of an environmental, safety, and health (ES&H) concern because of the PbO used in their synthesis. (4) The current process is extremely labor-intensive and requires extensive in-process testing and "tweaking" to produce qualified material. (5) Finally, the lack of scientific understanding of the mixed-oxide process makes it difficult to address problems when they occur. Based on Sandia's past experience in which we successfully developed and transferred to industry chemical preparation processes, we propose to develop an alternate process based on solution chemistry to prepare the PZT powders. We will develop the process such that we will satisfactorily address the concerns listed above. We will emphasize the underlying fundamentals of system solution chemistry and how these fundamentals relate to the ceramic material properties that are critical to neutron-generator applications.

The goal of this project is to develop an improved method for preparing the PZT materials based on the use of the chemical processing approach. In chemical processing, powder components are intimately mixed as solutions or vapors. Because of the high degree of mixing, precursor powders prepared by chemical methods have short component diffusion distances; as a result, the precursors often can be converted to final form at significantly lower temperatures than mixed-oxide processed powders. Chemical synthesis methods are also well suited for controlled, homogeneous

incorporation of dopants due to the mixing approach used. In addition to the improved mixing and better control of starting materials relative to the mixed-oxide method, the fact that this approach is based on well-established solution chemistry concepts provides a strong scientific base for process development.

This year we continued to work on two chemical routes to the PZT 95/5 voltage bar material. We based one of the processes on aqueous coprecipitation and carried out in-house modifications to improve the process. We devoted the majority of the project to further developing and understanding the nonaqueous process (referred to as the Sandia Process [SP]) that we developed last year as part of this project. This process has the advantage that its solution chemistry is more readily modified to incorporate additional cations than the aqueous process.

We studied the SP using the Plackett-Burman experimental design approach. We investigated twelve processing variables at the 100-g batch size. Based on the results of this study, we established a more robust processing baseline. Using these baseline conditions, we successfully scaled the process to the 1.5-kg size. We showed the scaled process to be highly reproducible with respect to the required stoichiometry control. We produced and processed several batches of this size. Results of processing studies showed that we can produce PZT 95/5 ceramics to which we added the necessary pore former with physical and ferroelectric properties that meet power supply requirements. Also, hydrostatic depoling results indicate that we can meet depoling pressure and charge release specifications.

Because we have two processes that look encouraging, i.e., the British process and the newly developed

process, we continued to investigate the fundamental aspects of both in parallel.

We met the following milestones in FY97:

(1) Studied in detail the PZT 95/5 synthesis process developed in Year 1 and the British process.

(2) Developed the process for incorporation of the amount and type of porosity required for the PZT 95/5 neutron-generator application.

(3) Prepared sufficient powder for slug preparation.

(4) Established reproducibility of the PZT 95/5 synthesis process of choice.

(5) Analyzed results of slug machining, electroding hydrostatic poling, and hysteresis loop testing with respect to neutron-generator performance requirements.

Publications

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Development of an Immersive Environment to Aid in Automatic Mesh Generation

C. J. Pavlakos, S. A. Mitchell, J. S. Jones

This work explores the use of immersive technologies, such as those used in synthetic virtual environments (commonly referred to as virtual reality [VR]), in enhancing the mesh-generation process for complex three-dimensional (3-D) models. The idea is to demonstrate the ability to interact with the mesh-generation process in a highly visual and intuitive manner, allowing a much greater understanding of the mesh as it is being constructed, as well as allowing powerful interactive feedback to the creation process. This work is based on Sandia's CUBIT mesh-generation research and explores use of capabilities developed for Sandia's Multi-Dimensional User-Oriented Synthetic Environment (MuSE) as well as a more recently developed system called FLIGHT that incorporates a haptic input device. The preliminary work focused on assisting the CUBIT developer, with longer-term focus on assisting the end user.

We implemented a prototype MuSE application for viewing and understanding CUBIT meshes. Features of the application include the ability to import CUBIT meshes, both via file and on the fly via a socket connection; the ability to visually differentiate between nodes in the mesh that belong to various numbers of elements, indicating various degrees of complexity in the mesh; the ability to display node identifiers; the ability to highlight specific elements in the mesh

for visual scrutiny; the ability to "tether" to (i.e., visually focus attention to) a specific node, which also highlights the edges of all of the elements that contain the node for further scrutiny; the ability to grab and move nodes in the mesh; and the ability to interact with all of these features in a fully stereoscopic environment, supported by advanced human-computer interface capabilities provided by MuSE. We believe that the prototype offers a capability that on the desktop would increase our productivity by a factor of four or five for looking at meshes.

We completed a migration of the prototype application to a relatively "low-end" desktop platform. We completed an OpenGL port of the application for increased portability and for use with the OpenGL version of MuSE.

We implemented a recent enhancement to the MuSE application to demonstrate the use of such a system in support of "whisker-weaving" algorithm development. The prototype capability allows inspection of 2-D "sheet diagrams" in combination with the associated 3-D mesh. When a specific entity is selected in a sheet diagram, its associated entity is highlighted in the mesh, enabling the algorithm developer to interactively inspect relationships between the sheet diagrams and the mesh.

An important emphasis this year is to work on approaches that would enable use of such a system with large meshes, which is of particular importance to end-users of a meshing system. We modified the prototype MuSE application to allow a range of options for how meshes are viewed. Options include the ability to view the mesh as a set of simple bound-

ing boxes enveloping mesh element blocks, as well as an option that allows viewing only the exterior faces of elements and element blocks—these alternatives allow larger meshes to be rendered at high frame rates while still providing a global context for the mesh. Together with these options, we implemented a mechanism for selecting a local area in the mesh that can be displayed in complete detail.

During the course of this project, the opportunity arose to experiment with a new data exploration system called FLIGHT that incorporates a haptic input device for navigation about 3-D data, as well as for force feedback. We implemented a capability for exploring meshes within FLIGHT and enabled stereoscopic viewing. One feature of FLIGHT is that its user-interface components are implemented in three dimensions within the normal viewing space so they can still be viewed properly when stereo is in effect. FLIGHT also allows the use of a SpaceBall for 3-D input as an alternative to the haptic device, which we wanted to experiment with, particularly for the desktop.

Publications

Refereed

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Effect of Composition and Processing Conditions on the Reliability of Cermet/Alumina Components

J. J. Stephens, Jr., M. E. Miskiel, K. G. Ewsuk, J. S. Glass, R. H. Moore, S. L. Monroe, E. L. Hoffman, J. E. Smugeresky

High residual stresses and cracking of cermet/alumina parts used for neutron tube subassemblies have raised questions regarding the design, processing, and reliability of cermet components for war reserve (WR) applications. The goal of this project is to develop cermets and cermet fabrication processes to produce high-reliability subassemblies that are free from significant residual stresses and the associated potential for crack formation. Sandia is developing molybdenum-based alloys that closely match the coefficient of thermal expansion (CTE) of the alumina-ceramic phase of the subassembly and that retain good hydrogen compatibility for fabrication. We made coarse powders using the plasma rotating electrode process (PREP) for both the Mo-27V and Mo-22V-3Fe alloys.

Initial sintering studies suggested that the Mo-V alloys suffer from excessive reaction with the alumina-ceramic phase at 1625°C; lower sintering temperatures are probably required to avoid these reactions. Alternative metal/alumina cermets based on the use of pure iridium as the metallic phase were also sintered and do not have a reaction problem with alumina ceramic at 1625°C.

Additionally, we are evaluating residual stresses and warping arising from differences in sintering kinetics and sintering shrinkage between the cermet and alumina phases to develop more reliable processes that yield improved reliability components. We are also developing fabrication methods to produce composite

cermet/alumina test samples for determination of interfacial strength between the cermet and 94% alumina.

(1) We fabricated ingots (approximately 50 lbs each) with nominal compositions of Mo-27V and Mo-22V-3Fe using the plasma arc remelt processes. Electrodes from both ingots were ground at Sandia and sent to Nuclear Metals, Inc., who used the PREP to make relatively coarse powders for both alloys. In the case of Mo-27V alloy, we successfully obtained 5 pounds from the PREP, while we obtained 10 pounds for Mo-22V-3Fe alloy. In the case of the Mo-27V alloy, we found that dry planetary milling for approximately 10 hours served to generate fine powders suitable for cermet compatibility studies, with a minimum amount of tungsten contamination from the grinding media.

Separate efforts to fabricate Mo-22V-3Fe powder using the mechanical alloying process yielded small lots (~ 100 gm) of fine powder with sizes that were suitable for cermet sintering evaluations.

(2) We performed a limited amount of cermet fabrication using the alloy powders—the time required to produce fine powders from the PREP impacted the FY97 time available to pursue this activity. The sintering conditions used included temperatures close to the present CND50 (pure Mo as metallic phase, ~ 27 vol% Mo, 73 vol% alumina ceramic) cermet process (1625°C), using either wet or dry hydrogen atmospheres. It is important to emphasize that we have not optimized the sintering conditions for these alternative cermet materials. However, we obtained important results from the experiments run: (a) both Nb and Mo-27V appear to have extensive reaction with the alumina ceramic—either of these materials will undoubtedly need lower sintering temperatures to produce useful cermets, and (b) Ir appears to have no detrimental reaction

with the alumina-ceramic phase using the standard CND50 processing conditions.

The results in (a) suggest that we will want to evaluate the effect of lower sintering temperatures on the Nb- or V-reaction with the alumina ceramic.

We made progress in developing a process to make composite four-point bend specimens to permit evaluation of the interfacial bond strength between cermet and alumina ceramic. These samples have a center span of CND50 cermet, with the outer portions composed of 94ND2 ceramic. We fabricated and tested samples; however, in all samples, fracture initiated within the cermet rather than at the interface or in the alumina. Finite-element analysis of this geometry suggested that large tensile residual stresses developed in the cermet center portion, which reduced the load required to cause fracture.

Publications

Refereed

Glass, S. J., E. K. Beauchamp, S. L. Monroe, J. J. Stephens, R. H. Moore, J. P. Brainard, K. G. Ewsuk, E. L. Hoffman, R. E. Loehman, G. A. Pressly, and J. E. Smugeresky. 1997. "Mo-Al₂O₃ Cermet Research and Development." Sandia Technical Report SAND97-1894, 1 August. Sandia National Laboratories, Albuquerque, NM.

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3510.540

Ultra-Precise Assembly of Microelectromechanical Systems (MEMS)

J. T. Feddema, W. D. Bonivert, T. R. Christenson, M. A. Polosky, R. W. Simon

Sandia is currently developing processes to make surface-machined silicon and LIGA (Lithographie Galvanoformung Abformung) parts with 100-micron outside dimensions (OD) and submicron tolerances for use in weapons surety devices. LIGA parts are of special interest because they are thicker than typical surface machined parts, they can be made of metals that make them stronger (in tension) than surface-machined silicon, and when assembled the components are not restricted to the plane. This last advantage (assembly required) is also a disadvantage. Today, most micro-components are assembled manually using microscopes and teleoperated precision mechanisms. The task is time-consuming and tedious. An automated assembly system is needed.

The goal of this project is to develop a visual feedback and robotic control system that improves positioning accuracy and eliminates the manual assembly of LIGA components. One possibility is to develop fixtures for the LIGA parts and teach points to a robotic system to perform a repetitive motion. Unfortunately, it is difficult to build fixtures with submicron tolerances, and it is not effective to teach points in an agile environment with a variety of parts. Therefore, this project uses vision and force sensing in the feedback loop to pick up and assemble randomly placed LIGA parts. Both the vision and force sensing allow for the assembly operations to be performed using relative position information rather than absolute. We use computer-aided design (CAD) information about the parts to generate an augmented assembly plan that accounts for uncertainties and microscale effects such as electrostatics, surface tension, and van der Waals forces.

During this second year, we redesigned and built improved LIGA microtweezers with more precise motion. We used these tweezers to put 100-micron OD, 50-micron ID LIGA gears on a set of LIGA shafts ranging from 35 to 44 microns. We tested nickel, copper, and permalloy versions of the tweezers. We found the nickel and permalloy to have a permanent magnetic field that caused uncontrollable repulsive and attractive forces between the permalloy gears and the tweezers. The copper version does not have this problem.

Earlier this year, we instrumented the older version of the LIGA tweezers with strain gages and measured contact forces successfully.

We also designed a tool holder that allows the tweezers to be automatically changed. In this way, we can design the shape of the tweezers' tip for specific tasks.

We developed software that automates the visual servoing of the gears to their desired position. The software reads a CAD drawing ("dxf" file) of a LIGA part and generates synthetic images of the part using Fourier optics methods. We then use these synthetic images to test image processing routines and to generate reference image features that we use to servo the actual part to the desired position.

Publications

Other

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3510.550

Self-Tuning Process-Monitoring System for Process-Based Product Validation

R. G. Hillaire, C. S. Loucks

The hidden qualities of a product are often revealed in the process. Subsurface material damage, surface cracks, and unusual burr formation can occur during a poorly controlled machining process. Standard post-process inspections are costly and may not reveal these conditions. However, monitoring the proper process parameters makes these conditions readily detectable without incurring the cost of post-process inspection. In addition, many unforeseen process anomalies may be detected using an advanced process-monitoring system.

This work created a process-monitoring system for milling machines that mapped the forces, power, vibration, and acoustic emissions generated during a cutting cycle onto a 3-D model of the part being machined. We can analyze and visualize the "hyperpoint overlay" with extendible VRML (Virtual Reality Modeling Language). By using these technologies for "in-process" signature analysis of a machining operation process stability, we can detect and fully visualize product-to-product uniformity, material characteristics, and tool condition.

Once we deploy the process-monitoring system, we may significantly reduce or eliminate detailed inspection. The project developed a Pro/Engineer-to-VRML-model

conversion routine, and advanced visualization interface, hyperpoint overlay routine, stable sensor array, sensor calibration routine, and machine calibration methodology.

The technology created in this project can help validate production of war reserve (WR) components by generating a process signature for a product, process, and lot run. We can compare the signatures of all products across all products made within and across lot runs to determine if the processes that produced the products are consistently providing superior quality.

As a result of this work, we expect to ensure online quality and eliminate potential errors before they occur. In addition, this system can work over a wide range of manufacturing conditions for a spectrum of Defense Program products. Process drift, material consistency, part uniformity, and tool condition may be readily detectable. It will enhance process and product improvement due to advanced visualization of manufacturing processes.

The work created several utilities, each of which is useful in and of itself. A Web-enabled utility translates from Pro/Engineer to VRML.

The advanced visualization interface provides a graphical user interface (GUI) and a data-acquisition utility to allow real-time collection and display of sensor data and calibration of sensors. We developed the GUI using Lab Windows and cross-compiled it in Visual C++ for its multi-threaded capability and timing. We used WinRT libraries for interrupt handling.

A hyperpoint overlay utility attaches the force, torque, vibration, and acoustic hyperpoints to the VRML model of the part.

We modified an industrial tool-monitoring system with sensors for spindle power, vibration, and acoustic emissions and used it for the process-monitoring system. In addition, a Kistler dynamometer measures three axes of force. We monitor the machine position using a four-axis encoder interface card. An IBM PC with a National Instruments Data Acquisition Card reads all sensor signals.

Calibrating the sensors is critical to ensure that sensor information is consistent and meaningful. Power is measured directly through current and voltage (no calibration is needed). We calibrate the force sensors by applying forces through a precalibrated portable dynamometer to the process-monitoring dynamometer. The calibration of vibration and acoustics sensors is not economically feasible. Instead, maintaining the factory calibration data and deployment of a fitness-for-use test is the most reasonable alternative.

Machine calibration is critical to ensure that process monitoring will provide consistent indication of product quality across different machining platforms. The machine calibration is a derivative of the ASME B5.5-1992 "Methods for Performance Evaluation of Computer Numerically Controlled Machining Centers": rotating error motion, linear displacement accuracy test, contouring performance test, and machine compliance test.

We evaluated the system on three different part productions. We created the first part design with "Design of Experiments" to evaluate the sensor sensitivity. The machine feeds and speeds; we varied wall thicknesses for several slots in aluminum to determine the effect of these parameters on the quality of the part.

The next design was an ASME B5.54/NAS part: "Circle Diamond Square." This design was useful for the process-monitoring system.

Finally, using a cooling chuck design, we produced more parts so that we may purposely manufacture bad parts to verify that the system would catch them.

The result of this research shows that this system can easily detect differences in production of parts. Changes in sensor signatures can be significant before degradation of product quality, indicating that the system is adept in catching production changes even if product quality appears unaffected.

This system does not detect all problems. Parts were produced poorly, yet no indication of change in the process was apparent from the data.

The results of these evaluation runs show that the most significant indicator of part quality is acoustic emissions. Force and power vary according to the size of cut being made, not the quality of the cut. However, force and power may be a good indicator of consistency.

Process Optimization for Electron-Beam Joining of Ceramic and Glass Components

B. N. Turman, B. B. McKenzie, P. Yang, T. E. Voth, J. A. Halbleib, Sr., L. F. Bieg, J. S. Glass

The purpose of this project is to develop and extend the electron-beam joining process to applications related to Mo/Al₂O₃ cermet for neutron-tube fabrication, glass seals for flat-panel displays, and structural ceramics. The key issue is the identification of the allowable operating ranges that produce thermal conditions favorable to robust joining and sealing. Sandia produced high-strength, hermetic braze joints between ceramic components using high-energy electron beams. With a penetration depth into a typical ceramic of ~ 1 cm for a 10-MeV electron beam, this method provides the capability for rapid, transient brazing operations where temperature control of critical components is essential. Because of transient heating, higher thermal conductivity, lower heat capacity, and lower melting temperature of braze metals relative to the ceramic materials, a pulsed high-power beam can melt a braze metal without producing excessive ceramic temperatures. We demonstrated the feasibility of this process related to ceramic coupons as well as ceramic and glass tubes. We predicted the transient thermal response, using as input the energy absorption predicted from the coupled electron-photon transport analysis. We conducted the joining experiments with an RF linac accelerator at 10–13 MV and power up to 1.5 kW. The duration of the joining runs varied from 5 to 600 sec. Joining experiments provided high strength between alumina-alumina and alumina-cermet joints in cylindrical geometry. These joints provided good hermetic seals. We conducted a series of tests to determine the minimum beam power and exposure time for producing a hermetic seal. We developed an empirical scaling relation, showing linear scaling of strength with exposure time, while the strength is related to beam power raised to the 1.5 exponent.

We examined and tested approximately fifty representative samples from several ceramic and braze materials

combinations and sets of joining conditions. We used optical and scanning electron microscopy (SEM) to evaluate melting and wetting of the bonding materials and to evaluate the degree of reaction between the braze metals and the ceramic substrates. Using shear strength tests, we evaluated the mechanical integrity of coupon and cylinder joints. Prior to shear testing or sectioning for microstructural examination, we examined some samples nondestructively using ultrasound to evaluate the degree of bonding in the joint area. We made a total of thirty sample tensile strength measurements, with a range of beam power from 280 to 840 watts and a range of process times from 80 to 555 seconds. We also observed the melt time for these experiments with video camera monitoring. We fit these data with an empirical formula that gives a good fit to the measured strength data, showing a linear relation with exposure time, and scaling with beam power raised to the 1.5 exponent. We measured hermeticity using a helium-leak detector at 10⁻⁹ torr vacuum. These seal data define the operating range for alumina cylinders, limited by thermal stress cracking at high power, and braze melt and flow at low power.

Publications

Other

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3510.570

Finite-Element Meshing Approached as a Global Minimization Process

J. Jung, S. A. Mitchell, D. J. Segalman, W. R. Witkowski, C. R. Dohrmann

The ability to generate a suitable finite-element (FE) mesh in an automatic fashion is becoming the key to being able to

automate the entire engineering analysis process. However, placing an all-hexahedron mesh in a general three-dimensional (3-D) body continues to be an elusive goal. Current practices, such as "plastering," build a mesh from the outside of the body working in using local decisions to construct the mesh. This usually leaves voids in the interior of the body that cannot be meshed with hexahedral elements. The approach proposed in this project is fundamentally different from any other that we know of. We start from the premise that the problem of placing an all-hex mesh in an arbitrary 3-D geometry needs to be addressed from a global optimization perspective. Sandia proposes to employ a physical analogy for the actual meshing problem that will allow us to construct a global mathematical description of the problem. The analogy is that of minimizing the electrical potential of the system of charged particles within a charged domain (the particles can represent either nodes or elements). The mathematical description of this problem is easily extendible from 2-D to 3-D problems.

The first year of this project was one of immense discovery, with the project team generating several new approaches to the problem and sifting through these approaches to determine the most promising before proceeding. Among the many good ideas generated were node-based methods that placed the nodes first through an optimization procedure and then connected the nodes to form the connectivity. Also, we developed two element-based procedures. One of these methods represents elements as particles with spatial coordinates and angular orientations (three degrees of freedom). We developed a mathematical functional that distributes the particles in an equipotential manner and also describes how the particles should orient themselves relative to each other, creating the mesh connectivity. The basic functional was adequate to create very simple meshes; however, it was not adequate for closing more complex meshes. Recently, we developed a new algorithm that recursively applies the alignment portion of the functional to realign the particles to successfully close several meshes.

Application of Parallel Mechanism Technology to Manufacturing

L. F. Bieg, D. J. Schmitt

The purpose of this project is to apply human-like motion to the fabrication of Sandia components. Currently, Defense Program (DP) products are realized by processes and tools based on orthogonal motion. However, the constraints of orthogonal systems have become more apparent as component designs have increased in complexity. In an orthogonal world, the fabrication of complex parts requires multiple manufacturing processes and setups, resulting in numerous fixture transitions. Aside from cost, time, and quality disadvantages, orthogonal manufacturing processes also lead to orthogonal designs. Freeing designers from this bias will allow new and innovative designs to be developed based purely on component and assembly functionality.

The overall challenge is to develop, control, and apply human-like motion to manufacturing. Non-orthogonal parallel motion (NOPM) devices need to be developed and evaluated. Sandia has evaluated the scalability and accessibility of NOPM devices for fabrication, microassembly, and micropackaging applications. The power of this paradigm cuts across the spectrum of Sandia's design and fabrication requirements and applies equally well to the micro and macro environments.

Our goals and accomplishments include the following:

(1) *Evaluated known systems and concepts based on a developed metric.* We evaluated seven individual mechanism designs, both for micro and macro applications, based on 20 metrics. We defined micro as systems having a workspace of 3 inches cube maximum and suitable for applications such as microassembly and microsurgery. Macro systems, on the other hand, have a larger workspace, including, for example, machines used in the metal-cutting (i.e., five-axes milling, grinding, turning), component assembly, and quality assurance industries. The seven mecha-

nisms evaluated include commercially available mechanisms, the leading kinematic concepts from the research literature, and the Sandia Rotopod design. The metrics included categories for kinematic, dynamic, reliability, and application-related properties. We developed a grid that rated each mechanism in each of the 20 categories and provided a basis for comparison to determine which mechanisms we would study in further detail.

(2) *Selected at least one system based on the metric.* Based on the system comparison from task 1, we chose the Rotopod as a candidate mechanism for continued study and prototyping.

(3) *Defined sensor and feedback control for parallel actuated systems.* To develop complete servo control for a precise mechanism, feedback devices are necessary that will yield approximately 10 times the positional accuracy required. This is because to control the system smoothly without a true velocity feedback sensor, a smooth velocity estimate is necessary. We evaluated several encoders with accuracies anywhere from the 0.02-micron radians on up. Once we identify required forces and torques for the actuators, we can acquire appropriately sized and geared motors.

(4) *Designed and fabricated one NOPM prototype device.* We designed and fabricated a hand-actuated functional prototype. We constructed the main knee joint by utilizing an electromechanical clutch assembly, allowing for the joint to be unlocked for free movement or locked at specific spatial locations of the moving platform. We recognized the limitations inherent in commercially available joints and bearings during the fabrication of the prototype device. As a result, we designed and fabricated new joints. We procured angle-drive actuators and are currently modifying and fitting them with dual-feedback devices. These drives will have both a velocity and a position feedback, one controlling speeds and feeds, the other controlling accuracy. We are still on schedule to produce a computer-controlled prototype NOPM device by the end of FY97.

(5) *Developed control systems kinematics for NOPM prototype device.* We developed the closed-form inverse kinematic solution for the Rotopod design and tested the accuracy of the developed solution by comparing it to numerically obtained results using the data acquisition and display system (DADS) mechanism dynamic analysis software. The inverse kinematic solution is a key element in the software structure of the mechanism control system. We also developed a set of Matlab programs based on this inverse kinematic solution for evaluating and comparing the workspace of various Rotopod designs. Accessible workspace is one of the distinguishing features of the Rotopod from other NOPM designs, and these programs are being used to study Rotopod designs that maximize that workspace. In addition, a 16th-order polynomial is required to solve the forward kinematics. We identified a method to solve the forward kinematics utilizing three additional passive joint sensors, which reduces the polynomial to a third-order function.

(6) *Demonstrated and characterized NOPM device.* Our current prototype (see task 4) was useful in demonstrating the basic concept of an NOPM device, visualizing the kinematics and its constraints, and showing specific shortcomings that need improvement, modeling, and/or redesign. We also used this prototype for presentations given to selected U.S. private industry visiting Sandia.

Publications

Other

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Investigation of the Impact of Cleaning on the Adhesive Bond and the Process Implications

J. A. Emerson, E. Reedy, Jr., E. P. Lopez, J. G. Curro

Surface cleaning is the most common process step in DOE manufacturing operations—approximately 75% of AlliedSignal/Federal Manufacturing & Technologies' (AS/FM&T's) critical process steps for weapons manufacture involve surface cleaning or preparation. We do not understand the link between a successful adhesive bond and the surface clean performed prior to adhesion. When qualifying a new solvent for weapons manufacture, the cleaning engineer must rely on cumbersome laboratory tests, which are expensive, repetitious, and time-consuming. For many years, the cleaning community has called for an understanding of "how clean is clean?" Very little work has been done in this area since it requires a fundamental understanding of the process following the clean. This project, applying Sandia's computer modeling expertise, fracture mechanics understanding, and cleaning experience, is truly innovative. Modeling has not been used to deal with cleaning processes. Understanding the link between surface preparation and adhesion would result in reduced cleaning development time and testing, improved bonds, and improved manufacturability, and may also result in an understanding that leads to improved aging. This capability can ultimately be applied to agile manufacturing tools. Developing a validated model for cleaning and surface preparation in adhesive bonding, coating, encapsulation, or painting processes would complete Sandia's capability for a process that ensures efficient, low-cost production of small lots.

Sandia is developing tools, involving the convergence of several expert areas across the labs, that allow for the robust manufacture of bonded structures. These tools will include models and test techniques that can be applied to adhesively bonded components (structural joints, weapon subassemblies) and to encapsulated

components (neutron generators, electronic packaging). Moreover, we will establish a more fundamental understanding of the effect of known contaminants on the bond interface for both adhesives and encapsulants. The final customer is the manufacturing complex, whether internal or external, which can use this technology to make the work of a cleaning engineer in the weapons complex, as well as in private industry, easier and more efficient.

The first year of this project had specific requirements: to (1) develop fracture test methodology, (2) characterize contamination, and (3) develop modeling techniques. We conducted a series of fracture tests and calculated the average fracture stress and standard deviation. We repeated the process until the variation in fracture stress came into an acceptable range. We verified the hypothesis using computer simulation. An example of this was the difficulty with the butt joint test. Large variation in test results led us to use a finite-element stress analysis of the test sample. Analysis confirmed strain gage test results indicating that the loading of the test joint was not uniform due to the way the sample was mounted in the tensile tester. Further simulation revealed a better design that, when tested with strain gages, showed a more uniform loading that produced a narrower variation in butt joint test results. A figure of merit in evaluating stability of a process is coefficient of variation (CV), defined as process standard deviation divided by the mean.

3510.610

Standard Cells for Microelectromechanical Systems (MEMS)

B. R. Davies, M. S. Rodgers, J. J. Sniegowski, J. J. Allen

Microelectromechanical systems (MEMS) design tends to take place by a trial-and-error approach resulting in the necessity for several iterated fabrication runs before working MEMS devices are achieved. This precludes the devices from

being integrated together in a single fabrication run or, even more importantly, into a single monolithically integrated system design (micromachines with microelectronics). Typically, each design starts from scratch since no standard part definitions exist. This lack of standardization and compatibility in both manufacturing processes and device designs is a major factor preventing MEMS from attaining the same level of success as that is achieved by microelectronics. The focus of this project is to amass a set of verified, useful, diverse, standardized MEMS parts that can all be fabricated in the same process technology: Sandia's multilevel polysilicon surface-micromachining process. These parts will provide an appropriate range of actuation, sensing, energy storage, etc., functionality. By creating a set of diverse modules that can be fabricated together on the same chip, we will be creating a library of standard cells similar to those common in the highly successful integrated circuit (IC) manufacturing industry. In the final year of the project we plan to expand the library to include mechanical parts with monolithically integrated signal-conditioning circuitry, creating a set of integrated sensor and actuator functional blocks.

We designed and fabricated a rotary actuator that was scheduled for next year; instead, the second design iteration will occur next year. We also designed a number of other standard components and completed the layout, including an accelerometer and rotary rate sensor, rotary and linear actuators, mechanical energy-storage devices, mechanical pendulum generators, modulated corner cube reflector, gears and gear trains, and various other linkages and standard devices.

We implemented a standard components database that contains design and operational information relevant to a variety of both standard components and reticle sets previously fabricated. This database allows designers to import standard component device geometries into AutoCAD designs and provides design rule checking and information referencing via the World Wide Web (WWW) and AutoCAD. This database will enhance the ability of both internal and external designers to design MEMS

devices for the standard component library and/or their specific applications.

Work proposed for the next two years includes both improving designs developed during this fiscal year and increasing the scope of components. We implemented a database structure that will make available design rule checking and standard component operational and design information to internal and external customers through the WWW and/or AutoCAD. We introduced analysis tools, including finite-element analysis and 3-D visualization.

Publications

Other

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3510.620

Laser Wire Deposition for Fully Dense Net Shapes

L. D. Harwell, J. A. Romero, T. B. Crenshaw, T. E. Buchheit, M. L. Griffith, V. Tikare

The primary purpose of this project is to characterize the laser wire deposition (3DWire) process and determine the feasibility of fabricating complex near-net shapes directly from a computer-aided design (CAD) solid model. This additive process builds a solid metal part directly from a CAD model, saving numerous steps and time compared to current methods and technologies. The initial goals of this work are to understand the processing conditions (laser power, wire feed rate, traverse velocity) and the materials properties, and to model the solidification behavior of the weld pool. By understanding the experimental and theoretical aspects for the laser wire deposition process, it will be possible to produce a solid, functional metal part directly from a CAD solid model.

Sandia's goal is to develop a system that rapidly fabricates accurate, dense parts with good material properties. We must identify, develop (where necessary), and implement sensors to provide closed-loop process control. It will be necessary to develop methodologies to directly drive the motion control from the sliced CAD file. We must develop interfaces to interact with sensor inputs from the process control. Development of this process will allow engineers to produce functional parts of their designs directly from CAD files. The turnaround time will be hours instead of days, and days instead of months. With reduced turnaround time, more time can be spent on the product design phase to ensure that the best component design is achieved.

We developed six major areas over the past year:

(1) *Process understanding.* Initially, we developed and implemented test matrices to identify the key factors controlling the 3DWire process for selected materials (308L SS, Aermet 100). The key processing variables include laser power, wire feed rate, wire feed direction and angle, and traverse velocity. From previous work with laser-engineered net shaping (LENSTM), we found laser power, wire feed rate, and traverse velocity are interrelated and reasonably controllable in the 3DWire process. We required extra experimental studies to understand the relationship between the wire and the weld pool. This study included varying the wire feed direction, wire feed height (w.r.t. the substrate), and insertion angle. The wire must intersect the weld pool in a manner that maintains stability along the solidification front.

(2) *Shape fabrication.* From the process variable experiments, we optimized the laser wire deposition parameters to demonstrate the feasibility of part fabrication. We added new test matrices to understand how layer thickness and hatch (fill) spacing affected the fabrication of parts. With this understanding, we were able to increase the geometric complexity of 3DWire fabrication. We can fabricate three types of geometries: (a) unidirectional fabrication using a rotary stage to build hollow

cylinders, (b) bidirectional patterns to fabricate walls, and (c) with an understanding of hatch spacing and layer thickness, fabrication of 2-D dense, rectangular shapes. All shapes possess 100% utilization of the wire, where the material inserted into the weld pool is directly used to produce a block. 3DWire parts can be fabricated in short times, approximately 1–2 hours per inch³.

(3) *System controls.* Initial setup consisted of overhauling the laser system, attaching and modifying the wire feeder, and integrating the computer controls with these systems.

(4) *Process monitoring and sensing.* We are implementing process diagnostics to provide further information for analysis of the process. We attached a camera, 300x magnification, to the z axis to monitor the weld bead and wire interaction during fabrication. This enabled us to determine the optimal direction and angle to place the wire in the weld pool to maintain contact. We identified sensors to monitor the process, which include Z-height, laser power, and wire feed rate.

(5) *Material characterization.* Metallographic analysis reveals dense, fine-grain microstructures (< 4 microns) produced by the 3DWire process. Densities were always greater than 98%. In some samples, we found porosity due to the hatch spacing or laser-power build parameters. However, this porosity did not result in a reduction of the mechanical properties. The 3DWire parts had superior strengths without a loss of ductility compared to wrought material.

(6) *Predictive model.* We modified the Potts Monte Carlo model to simulate microstructural evolution during the 3DWire process. We added two major components to the model: the addition of materials in the 2-D plane of a layer and the evolution of microstructure in a dynamic temperature profile. The resulting simulation was capable of predicting the elongation of the grain structure as a function of the temperature profile and raster speed of the laser. It was also able to show misalignment of the laser beam with the raster direction leading to asymmetry in the elongated grain structures.

High-Throughput Dry Processes for Large-Area Devices

D. S. Ruby, C. I. H. Ashby, S. R. Vosen, E. Meeks, P. Yang, G. A. Hebner, D. J. Rieger

The goal of this work is to develop guidelines for high-throughput dry processes that can effectively replace wet processes used in manufacturing large-area devices and/or batches of moderate-area devices. Wet processes generally increase worker exposure to toxic and hazardous chemicals and tend to generate a large volume of liquid hazardous waste. Successful development of high-throughput dry processing could eliminate much of the waste stream while minimizing worker exposure. This interdisciplinary project utilizes Sandia's expertise in photovoltaics, plasma processing, sensor-based controls, and process modeling to develop environmentally benign processes that can reduce costs and product realization times. We will use large-area commercial silicon solar cells as the test vehicle in this program. We will develop a sequence of dry processes for selective etching of the emitter, defect passivation, and deposition of the antireflection coating. Successful completion of this project will provide validated process models that can be used in a variety of applications for surface cleaning, selective etching, and thin-film deposition. The models will provide guidance for development of the next generation of plasma reactors and the development of new applications.

The team performed an initial survey of available equipment at Sandia to do the

processing for this project, including downstream etchers, batch plasma reactors, diode plasma reactors, and inductively coupled high-density plasma reactors, and selected our target reactors based on reactor availability, compatibility with process chemistries, perceived process robustness, accessibility for diagnostics, degree of modeling complexity required, and reactor cost. These considerations led to the selection of the Vacutec reactive ion etch (RIE) and chemical vapor deposition (CVD) tools. Empirical characterization of plasma etch and plasma CVD in these tools showed adequate performance.

We conducted empirical characterization of etching performance in SF_6 , CF_4 , and Cl_2 . A literature survey of polymer-deposition issues that arise in CF_4 -silicon etching systems led to the elimination of CF_4 as a candidate reagent in the etching process. The enhanced etching of silicon by Cl_2 in the vicinity of silver-masked regions was unacceptable and resulted in its elimination. Through experimentation with SF_6 etching, we succeeded in finding a set of parameters that resulted in negligible metal gridline damage, adequate emitter uniformity, and acceptably low levels of silicon surface damage. To reduce the cost and improve the solar cell performance, we introduced a low-temperature, plasma-enhanced CVD nitride deposition process for surface passivation. The process also provides a good antireflection coating and can be combined with plasma-hydrogenation treatments for bulk defect passivation.

As a preliminary to the Langmuir probe measurements, we performed

measurements of the spatially resolved ion saturation current (proportional to the electron density) and a survey of the plasma optical emission to provide an indication of the species present in the plasma. We used ion saturation of current measurements of the spatial uniformity of plasma to verify trends in the model predictions of electron density, improve the uniformity of the discharge, and identify regions of plasma instability that can lead to nonuniform processing. We observed significant nonuniformities in the plasma in certain regions of the parameter space that need to be avoided to ensure uniform silicon etching.

We assembled gas-phase and surface-etch chemistry mechanisms for medium-pressure (~ 1 torr) plasma etching of silicon in SF_6 plasma and used these mechanisms in well-stirred plasma-reactor model to predict plasma composition and etch rates. These initial model results indicated that the plasma operating conditions chosen for the experimental study corresponded to a weakly dissociated, highly electronegative plasma regime. This information has helped determine the appropriate diagnostics measurements that we will make to test and validate the chemistry model.

Publications

Refereed

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3510.640

Assuring High Reliability and Production Readiness in Low-Volume Manufacturing

S. V. Crowder, A. J. Johnson, C. J. Decarli, J. T. Spooner

The first year of the project focused on the development of mathematical and statistical tools, including data requirements, that can be used to address the problem of ensuring high reliability and production readiness in low-volume manufacturing. The goal was to develop a mathematical and statistical framework for this problem. We believe the mathematical and statistical methods should focus on process characterization to determine optimal operating conditions and process sensitivities, and on process control to maintain stability in the process once it has been achieved. The challenge in low-volume manufacturing is to perform characterization and control with limited data. The results below describe our efforts to develop methods for low-volume characterization and control. The mathematical and statistical techniques used in our research include adaptive filtering for statistical process control (SPC), neural networks for process characterization and control, and statistical design of experiments (DOEx) for process characterization, all with possibly limited data.

A second goal for this year was to establish a partnership with a Sandia product design and manufacturing organization. We established a working relationship with Sandia organizations involved in the design and production of neutron tubes and will collect baseline data

from specific processes. We will use the processes as data sources in the future to validate and refine any new methods developed.

(1) *Low-volume statistical process control.* None of the methods for low-volume SPC proposed to date appear to be effective at quickly detecting small- to moderate-sized shifts in a process. We developed an approach to estimating an unknown process mean and variance in low-volume manufacturing that we believe is better than existing methods. We also developed software to implement the algorithm that we developed and will evaluate its usefulness on a low-volume manufacturing process at Sandia, the neutron-tube production process. We will then make any necessary modifications to improve the technique.

Our research to date has produced an algorithm for implementation of an adaptive filtering model. The two-stage procedure first uses maximum likelihood estimation to obtain estimates of the unknown variance components. Once these estimates are made, they are then substituted into the filtering equations to estimate the unknown process means. We developed Matlab, Fortran, and C code to implement this two-stage procedure and performed simulations to study the small sample properties of the estimators. From this analysis we determined how effective the procedure is as a function of the amount of available data.

(2) *Neural-network applications.* We investigated two relevant applications of neural networks for low-volume manufacturing. The first is to use various neural-network architectures to model the relationship between process inputs and part quality. In this phase of the study,

proper neural-network architectures and data requirements were the primary point of concern. We showed through simulation that neural networks may provide some benefit to the process engineer in terms of selecting appropriate process operating conditions. We also obtained some empirical results regarding required amounts of data that may provide guidelines for the applicability of the neural-network techniques.

(3) *Design of experiments techniques.* We performed a literature search to obtain any available information concerning process characterization and control for low-volume manufacturing. We identified and investigated various types of statistical experimental designs for their applicability to statistical process characterization and optimization in a low-volume production environment. In the investigation, the focus was on statistical experimental design techniques that require only a small number of runs. We chose a 12-run limit as appropriate for low-volume experiments. We identified many experimental design arrays that can tolerate the 12-run limit. All of these experimental designs, while appropriate for small numbers of runs, can also accommodate more than 12 runs if required. We recommended several experimental design techniques that are useful for low-volume applications and identified statistical software packages that can generate these designs. To be useful for low-volume work, not only must DOEx software generate experiments with small numbers of runs, but it must also be user-friendly to nonstatisticians, have data analysis capability including good graphics, and prevent users from catastrophic errors when selecting designs. With these requirements in mind, we performed a search and evaluation of DOEx software.

Advanced Control Methods for Improved Grinding Processes

J. E. Hurtado, E. D. Apodaca

Previous work at Sandia developed a magnetic bearing-grinding machine test-bed aimed at improving the grinding process. The test-bed has a hybrid permanent and electromagnetic (EM) bearing spindle. This hybrid magnetic bearing system is well suited for vibration suppression, damping control, and balancing.

The purpose of this project was to investigate traditional and advanced active control methods for the grinding process using the magnetic bearing test-bed. A first step in any active control study, however, is to obtain a robust model of the structure. This proved to be a challenging aspect of our study.

We obtained experimental frequency response functions of the spindle

displacement probe outputs to the magnet voltage control inputs. We then used many system identification techniques to obtain a mathematical representation of the system. The system identification methods that we used included the following:

(1) *Eigensystem realization algorithm (ERA)*. This is a time-domain method that takes as inputs to the algorithm the impulse response functions of the system outputs. The algorithm then attempts to find the best linear system representation in the form of state-space matrices.

(2) *Canonical variance analysis (CVA)*. This method operates on the time histories of the system inputs and outputs and attempts to find the best linear system representation in the form of state-space matrices.

(3) *Structural dynamics toolbox*. This software package takes as inputs the measured frequency response functions of the system and uses a nonlinear

optimization routine to obtain the best linear system representation.

Unfortunately, the magnetic bearing test-bed proved to be a highly damped, coupled, nonlinear system. Thus, our linear system identification methods did not perform well. The problem is twofold: The system is nonlinear *and* highly damped. Our system identification and modal efforts in the past have always assumed a lightly damped, linear system response. This assumption is clearly not valid with regard to the magnetic bearing test-bed. Perhaps weapons system response to high-level inputs may also violate this assumption. It seems that the valuable lesson learned here is that additional tools need to be developed that enable experimentalists to obtain accurate mathematical representations of highly damped, nonlinear systems.

Because of the mentioned difficulties, we did not perform our active control studies.

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ife-Cycle Systems Engineering studies trace the entire life cycle of a product. Studies consider affordability, performance, design, testing, production, field operation and maintenance, and product retirement. Studies may involve collaboration with other LDRD-funded areas and with programs associated with

national security such as life-cycle studies of nuclear weapons.

Development of modeling and simulation prototypes that support life-cycle studies are encouraged.

Projects are concentrated in five areas: (1) developing single systems that engineers at all stages of product development can use; (2) deepening the understanding of how production technology affects product performance, cost, and usefulness; (3) adding knowledge and capabilities to continuously and affordably improve product development; (4) creating technologies that allow workers to focus on innovation by relieving them of activities that can be automated; and (5) creating innovative collaborative arrangements that create long-distance work environments as productive as those where all workers share the same site.

Documentation is an essential component in producing high-quality products at an affordable cost. Engineers are developing a system that can accept computer models and then generate effective multimedia documentation that can be incorporated into a production system.

Modern weapons production expends more effort on upgrade and dismantlement projects than on new designs. Research is under way to adapt Sandia's automated assembly process to include service, field repair, upgrade, and dismantlement. This will allow use of existing tools to perform critical functions in the weapons life cycle.

The automatic planning of life-cycle assembly processes allows disassembly plans with the fewest possible removed parts. This, in turn, allows easy access to parts that require regular servicing or replacement. The parachute, shown here in the B-61 tail assembly, is an example.

LIFE-CYCLE SYSTEMS ENGINEERING

3511.010

Automatic Generation of Multimedia Documentation for Assembly Operations

R. E. Jones, G. A. Laguna, M. J. McDonald

Realistic, easy-to-understand, and complete documentation is an essential component of any system that is expected to produce consistent, high-quality product at affordable cost. This is especially true when production occurs in low volume at irregular intervals. This is precisely the scenario being faced by Sandia's production organizations. High-quality documentation is rarely produced, largely because the manpower costs and skills required in its production serve as a considerable barrier to widespread use. Sandia proposes to develop automatic tools that can accept computer-aided design (CAD) models as input and generate effective multimedia tools with a minimum of skilled human intervention.

Sandia is recognized worldwide for the significant advances we have made in recent years in automatically generating assembly sequences from CAD data. Potential users of this technology at Sandia and elsewhere have expressed considerable interest in the system's potential to automatically generate assembly training

materials in a variety of forms: text, graphic illustrations, audio instructions, and computer animations. Immediate and continuing long-term requirements for training materials to support the block-upgrade program make assembly processes an excellent example to use in developing techniques to automatically produce multimedia documentation and training materials.

We grouped into two areas key questions we expect to address during this research program: (1) identification of the appropriate components of a multimedia training system (e.g., text, audio, hypertext documents, etc.), and (2) tools for the automatic generation of training materials directly from engineering design data. Anticipated applications include technician training, formal process documentation, archiving of more complete process plans for future reimplementations, etc.

We researched existing multimedia and assembly documentation software tools and concluded that Web-based documentation approaches held the most promise as delivery tools. We established relationships with important potential users of multimedia assembly documentation at Sandia, principally in the neutron-generator fabrication area. We prototyped an example multimedia document starting from existing text documentation and CAD models and socialized the result. This led to a

currently ongoing team effort to produce a second-generation prototype tied into the product data management (PDM) document control system. We also established a relationship with a multimedia effort at Pantex.

We extended the Archimedes system to directly output Web-viewable movie files that can be referenced by Web-enabled documents. We developed a first version of direct output from Archimedes of a Web-viewable basic assembly document including text, still graphics, and movies. We also determined that we needed to update Archimedes to output Virtual Reality Modeling Language 2 (VRML2) format data for viewing 3-D objects on the Web and began work in this direction. We expended significant effort toward converting Archimedes to other platforms and completed a port to SUN workstations (from SGI workstations). We publicized the Archimedes and multimedia efforts significantly.

Publications

Other

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Distributed Life-Cycle Models in Enterprise Simulations to Answer System Questions

M. M. Johnson, A. S. Yoshimura, J. J. Roesch, E. A. Kjeldgaard, T. D. Plantenga

The goal of this project is to develop a distributed computing software framework that can integrate various Sandia planning models into a single discrete event simulation. The framework must address special issues important to potential Sandia customers, including the definition of software interfaces, distributed operation on multiple heterogeneous platforms, enforcement of multilevel access restrictions that derive from differing user classes, and coordination of local planning/scheduling models into a complex-wide life-cycle simulation.

The project will also construct a life-cycle model of the DOE nuclear weapons complex and populate it with enough real information to demonstrate the capabilities of an enterprise simulation. A fully populated enterprise model will provide stockpile managers with an important tool for planning and decision analysis.

Sandia made progress toward a full enterprise simulation. We designed a software infrastructure that unifies disparate stockpile models into a system simulation and tested a prototype in distributed computing environments. We constructed a life-cycle model for nuclear weapons in the stockpile, identified key players in the nuclear weapons complex, and are prepared to integrate three different production models into the simulation. We resolved key design issues, including the interplay between planning/forecasting models and continuous time simulations, codification of decision analysis issues specific to the weapons complex, and appropriate separation of autonomous stockpile models from a centralized simulation.

The project's analysis and design phases are nearly complete, and it is currently turning toward coding and testing of the final software. We created a distributed software framework enabling distributed detailed models to interoperate. To this end, we (1) developed a software infrastructure to interconnect disparate

simulation models associated with the stockpile, and (2) developed a distributed simulation system on top of this infrastructure. Utilizing experience gained from the Sandia Product Realization Environment (PRE), we implemented a framework using the Java language and Common Object Request Broker Architecture (CORBA). The CORBA technology treats disparate system models as independent software objects that can be distributed on distinct computing platforms. Java provides a portable and platform-independent medium in which to cast the system simulation. In FY97 we wrote Java DataBase Connectivity (JDBC) interfaces to both MS Excel and Access, two commercial codes used in certain stockpile models. We also wrote a general-purpose simulation engine in Java and ran it on a network of workstations.

Publications

Other

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Chain Models for Life-Cycle Systems Engineering

J. J. Rivera

Throughout Sandia's history, products have been represented by drawings. Solid modeling systems have recently replaced drawings as the preferred means for representing product geometry. We use these systems for product visualization, engineering analysis, and manufacturing planning.

Unfortunately, solid modeling technology is inadequate for life-cycle system engineering, which requires maintenance of technical history, efficient management of geometric and nongeometric data, and explicit representation of engineering and manufacturing characteristics. Such information is not part of the mathematical

foundation of solid modeling. The current state-of-the-art in life-cycle engineering comprises painstakingly created special-purpose tools that often are incompatible.

New research on "chain modeling" extends classical solid modeling to include physical, manufacturing, and procedural information required for life-cycle engineering. In addition, chain modeling promises to provide the missing theoretical basis for Sandia's parent/child product realization paradigm. In chain modeling, we characterize artifacts and systems in terms of their combinatorial properties: cell complexes, chains, and their operators. This approach is firmly rooted in algebraic topology and is a natural extension of current technology. Indeed, solid models are merely restricted chain models.

This project will provide an opportunity to research chain models. The potential impact of our project would be a framework for applying next-generation modeling technology to life-cycle engineering at Sandia.

We made the following accomplishments in our first year:

(1) *Selected a rolamite.* After careful consideration of several part families at Sandia (radar, batteries, and rolamites), we selected rolamites as the product from which to create a chain model. We did not select radar and batteries because they are electromechanical parts, and current chain model research is geared toward mechanical assemblies. Although rolamites are not a new product, they are currently in production and are being used in nuclear weapons and in the commercial application of air bags.

(2) *Identified relevant life-cycle considerations.* We reviewed design and manufacturing requirements to identify the relevant life-cycle considerations of a rolamite. Life-cycle considerations include lifetime (affects life of storage), acceleration levels, size, environmental conditions, material, changes in available manufacturing processes, and number of actuations. The criteria used to establish the considerations were the requirements likely to be changed, queried, or analyzed throughout the product lifetime and the requirements that could vary with each application.

Immersive CAD

A. L. Ames, J. L. Brazee, P. G. Xavier, D. Hickerson, C. Q. Little

Recent widespread acceptance of solid modeling in product realization is largely due to improved user interfaces. While these interfaces are sufficient for detailed design, they are proving inadequate for conceptual design. The "back-of-the-envelope" is still the concept modeler of choice. Current solid modelers require complete specification of product geometry, which is awkward in early stages of design. Engineers want to see, feel, and manipulate their designs, but are frustrated by overwhelming data complexity (the "hairball effect").

This project is developing a prototype immersive computer-aided design (CAD) environment. The work will involve four fundamental concerns: (1) developing a set of interaction mechanisms that provide easy, natural product model editing, (2) providing means for supporting design constraints, (3) managing the wealth of product information, and (4) dealing with the radical difference in time scales between rendering rates and solid modeler speeds to permit real-time model manipulation. Editing operations that work in multiple, tightly coupled representations (design features, constraints, boundary representation, and facets) on a parallel architecture will address performance requirements, while we will use virtual reality (VR) techniques to address interface concerns. This work steps beyond any current VR CAD system by producing constrained feature-based boundary-representation solid models.

This project has the potential to impact every Sandia program involving the design of mechanical parts and assemblies. The ability to more easily synthesize and visualize design concepts, without complete detailing, will encourage more concepts to be evaluated, yielding better product. Including analyzability and manufacturability constraints in the interface will deliver better products to market faster.

We accomplished the following:

(1) *Acquired VR environment.* To support a variety of potential interface approaches, we acquired copies of the MuSE software from MuSE Technologies, Inc. The software supports a variety of input and output technologies, including head-tracking displays, joysticks, mice, and datagloves. We have become proficient in developing software within the environment defined by these tools.

(2) *Developed connection between solid modeler and faceted representation.* We developed the capability to produce solid models in ACIS (Alan, Charles, Ian System [part of the CAD system]), facet them, and feed an OpenGL pipeline for rendering with MuSE. Flythrough is operational. Given our current-generation SGI computers, we are achieving adequate frame rates to render detailed parts with hundreds of facets (10,000 facets) with an adequate frame rate (15 frames per second).

We investigated approaches for improving the speed of the pipeline to support larger parts/assemblies. We centered on approaches that provide increased graphics speed without sacrificing ability to edit solid models. Two editing modes are interesting: *part editing*, where shape is locally modified, and *position of parts within assemblies*, where part location is modified. Two approaches are feasible: display lists and t-strips. Since creating display lists involves only memory overhead, we will always use it during part editing. During assembly editing, where parts don't change shape but memory is at a premium, we will create display lists and dispose of the original facets used to create the display lists.

Solid-modeling faceting algorithms do not directly produce t-strip representations. Producing t-strips will be an off-line activity, as the search is similar to a spanning tree algorithm. Additionally, solid model editing can produce breaks at arbitrary places in the strips. Thus, t-strips will be most useful for representing portions of geometry that are invariant; during editing, we will not use strip representations in certain localized areas of the model.

(3) *Made parametric editing operations functional; began speed improvement investigations.* In the area of part editing, we showed the ability to achieve a seven-frames-per-second frame rate in performing a simple boolean subtraction of a cylinder from a block. This is fast enough to support local editing operations of solid model if operations are sufficiently localized. The general boolean algorithm compares each facet in one object to all of the facets in the other, with worst-case $O(n^3 \log n)$ performance. Localized boolean operations can be fast enough for sufficiently simple features. This result directs us toward a feature representation that is not sequential (to reduce the number of features requiring regeneration) and approaches that localize the search for intersections.

Faster operations will occur when it can be proven that no new facet/facet intersections occur, as only the shape and location of intersection curves will require recomputation. We are currently implementing collision-detection algorithms to permit recognition of cases in which no new intersections have occurred; we are developing invariance-detection algorithms to note when the shapes of intersection curves are invariant. Both of these techniques will produce algorithms where minor geometry tweaks and some refaceting are all that is necessary to update the model.

In the area of assembly editing, we developed a collection of constraint equations that can be used to permit natural placement and moving of parts in an assembly. The algorithms currently permit rotation and translation of one part with respect to another, while maintaining point-on-surface constraint between the two objects. We developed and demonstrated the algorithms in AVS; migration to MuSE is under way. We are currently extending the algorithms to support higher-order surface interactions so that we can implement exact surface constraints.

Automatic Planning of Life-Cycle Assembly Processes

T. L. Calton, R. G. Brown, R. R. Peters

Sandia today expends more effort on upgrade and dismantlement projects than on clean-slate designs, and many more upgrades are scheduled in the coming years. However, commercial computer-aided design (CAD) tools are better suited to initial product design. Computer-aided analysis, optimization, and visualization of life-cycle assembly processes based on the product CAD data can help ensure accuracy and reduce the effort expended in planning these processes for existing products, as well as provide design-for-lifecycle analysis for new designs.

We propose to adapt and apply Sandia's automated assembly planning and design-for-assembly capabilities to later life-cycle assembly processes of a system—including service, field repair and upgrade, and dismantlement/recycling/disposal. Different goals and constraints (compared to initial assembly) will require significant re-analysis of fundamental assumptions and methods underlying current assembly planning techniques. We will prototype an interactive system to plan, optimize, simulate, visualize, and document the resulting assembly and disassembly processes. The system will support replacing one or several subassemblies, gaining access for inspections, and optimizing dismantlement to minimize disposal costs. We will consider destructive disassembly and nonmonotonic operations where feasible. We will derive the program's quality metric for life-cycle assembly processes from actual Pantex costs for facilities and labor and for long-term storage and/or disposal of radioactive and toxic subassemblies, as well as recovery values from reuse and recycling.

Problems arose in the work with a variety of applications because of a lack of a standardized CAD data format. However, all of the CAD systems can produce stereolithography (STL), or equivalently formatted, data. We developed an STL-to-ACIS (Alan, Charles, Ian System—part of the CAD system) translator that allows us to import a large variety of data into Archimedes by using a more universal, if less direct, data format.

We developed two significant optimization planning algorithms and integrated them into the Archimedes system. The first is the development of an algorithm to minimize the number of parts required to be removed in order to gain access to components of interest. The second algorithm minimizes the number of assembly and subassembly reorientations required during maintenance operations. First, we developed an algorithm to minimize the number of parts required to be removed in order to gain access to components of interest. This is particularly useful in maintenance operations. This algorithm is implemented through a general search optimization data structure (using a hill-climbing strategy on the disassembly tree) and imposes a penalty on any disassembly action that removes an unnecessary part or subassembly (a subassembly that does not contain one of the required parts) or that subdivides a subassembly containing none of the required parts. Second, we developed an algorithm to minimize the number of assembly and subassembly reorientations required during maintenance operations. This makes Archimedes more useful for assessing/comparing the costs of assembly using common flexible automation hardware.

We developed three significant code efficiency algorithms and integrated them into the Archimedes system. First, we wrote an algorithm to automatically generate the CAD-supplied subassemblies. Designers often specify subassemblies in their CAD models. Until recently, the Archimedes system allowed only a manual method to specify these subassembly constraints. For large assemblies this was very time-consuming; mistakes were frequently made and sometimes went unnoticed. We wrote code to utilize the hierarchical structure of the given CAD representation and to automatically generate the subassembly constraints consistent with the designer's intent. This feature provides immediate feedback to the designer regarding the feasibility of operations. Second, we wrote code to preserve the part-to-part contact information. In light of the number of large assemblies to which we have been applying Archimedes, we found it necessary to develop a means to preserve as much information as possible about how parts contact one another to reduce

the amount of time spent recomputing the contacts in an assembly after reload or after the addition of geometric overrides (snapfits, pressfits, etc.). In the application of Archimedes to an Apache helicopter engine and test harness assembly provided by Sikorsky Aircraft, this algorithm reduced an 8-hour process down to a few minutes. The majority of the software applications involve remove-and-replace scenarios of electronic assemblies. In these assemblies, the CAD representation of "like" components is duplicated in memory. Unfortunately, CAD-to-ACIS translators do not eliminate the redundancy. In the past, Archimedes loaded each instantiation of a part in an assembly as a separate ACIS object. We wrote code to eliminate duplication of part instantiation and hence reduce computer memory requirements.

We developed a prototype module that can calculate the cost, in dollars or other units, for remove-and-replace assembly operations. This is an extremely important feature that provides a powerful tool for comparing costs of competing designs, upgrade versus new product, etc.

Publications

Refereed

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Automatic Generation of Foolproof Manufacturing Plans

M. J. McDonald

This project was a study of the application of mistake-proofing and related techniques in low-volume Defense Program (DP) critical environments. The study investigated new manufacturing quality techniques from inside and outside Sandia that could be successfully and economically employed to ensure mistake-free manufacturing of DOE mission-critical devices and components.

Our study found that while low-defect manufacturing approaches, such as mistake-proofing, are currently applied in an *ad hoc*, problem-specific, experiential fashion, there exist underlying manufacturing principals that can significantly aid in appropriate application of the mistake-proofing principals. Of particular interest are Sandia's assembly planning technologies.

While mistake-proofing draws on many techniques, our study found that some techniques can be computationally automated. We extended Sandia's assembly planning tools to support constraints including those needed to optimize assembly order to either minimize part confusion or maximize self-inspection (e.g., poke-yoke) opportunities. In addition, we modified Sandia process planning tools to represent process to inspection links necessary for modeling source inspection.

While neither the mistake-proofing nor Shingo's or Ohno's principals are currently well suited to rigorous engineering, development of the necessary life-cycle system engineering (LCSE) theories appears feasible. In particular, Nam Suh's

axiomatic design theories appear to be extensible to support the critical time-ordering issues needed to model and predict quality prediction.

We performed two literature and state-of-technology reviews. The first review, focusing on mistake-proofing technologies, yielded the conclusion that in addition to mistake-proofing techniques, the driving system principals behind source inspection warranted further study. This was the subject of the second review, during which project staff attended a class at an automobile manufacturer and toured their supplier facilities for further insight, which we used to produce follow-on work proposals.

We performed two feasibility studies. A techniques study investigated automated assembly sequencing for reducing mistakes. In mistake-proofing, it is sometimes important to assemble two similar-looking parts into an assembly at different assembly stations. This reduces the chance of confusing the parts and, for example, putting a slightly shorter screw into the place that the longer screw belongs. Conversely, it is also sometimes important to make sure that parts get assembled as close as possible to one another. This is important when the latter part somehow "inspects" the presence of the earlier part; for example, if the function of a pin is to keep a slide from traveling too far, installing the pin and slide in close sequence allows inspecting the pin's presence by checking the slide's travel.

We extended Sandia assembly planning tools to determine the extent to which these mistake-proofing techniques could be automated. We developed a prototype of a needed constraint system, called MIN_SIMUL-LIAISON, to penalize

any mate that creates a significant number of liaisons in a single action. Additional effort will be required to implement further key mistake-proofing constraints. This will include computing cost functions based on overall plans. We will perform such research in follow-on activities.

We performed a feasibility study investigating the incorporation of poke-yoke and source inspection into formal system design theories by extending Sandia process planning tools to model source inspection steps. Source inspection requires identifying the key features produced in each manufacturing step and then building automatic inspection into that or successive manufacturing steps. (True mistake-proofing is achieved when the process producing the feature of interest "self-inspects" all necessary conditions for successfully producing the feature.) Modeling the linkage between production and inspection is key to quantifying mistake-proofing payoffs.

The second study resulted in a proposal to develop the extended theories and incorporate them into conceptual design support tools. In the assembly example above, assembly plan optimization would require measures or foundations to relate proximity in sequence to expected quality levels. The theoretical work would develop this relationship, and the planning tools would allow modeling the quality results.

Publications

Other

McDonald, M. J. 1997. "Are You Mistake-Proof?" *Organization 9000 Newsletter* (1 September). Sandia National Laboratories, Albuquerque, NM.

Information technology provides crucial support to most Sandia activities. Information Systems ensure that Sandia computers and networks can reduce time and, therefore, costs associated with stockpile stewardship and other, related goals.

Projects include developing secure, high-speed computer networks; networked information access, integration, and preservation; location-insensitive, transparent, distributed computing; information surety; and collaboration tools.

A capability called *mission surety* is being developed to enable engineers who use massive computer-design systems to guarantee the accuracy of results. As computer systems grow more complex and more design is computer-aided, mission surety is critical to detect errors in the datastream.

Security of data transmissions is important to defense and many other applications including the DOE Accelerated Strategic Computing Initiatives requirements. Data encryptors are being designed that will encode data being transmitted at the high rates of speed necessary for use in high-speed computer networks. These encryptors will operate in the 2-gigabit- to 10-gigabit-per-second range.

A 14-layer circuit board is approximately 15 inches square and contains 1.1 million gates of reconfigurable logic. The circuit board is part of a prototype encryptor operating at 10 Gb/s (about 100 times faster than commercially available encryptors).

INFORMATION SYSTEMS

Design of a Highly Secure Smartcard

C. L. Musselman, J. C. Bartberger, J. K. Panitz, P. A. Cahill, D. W. Straub, T. H. Buckle, R. J. Granfield, W. P. Morgan, L. M. Moore, R. L. Hutchinson

The goal of this work is to develop an inherently secure, multiple-application smartcard system. Our approach is to integrate a spectrum of Sandia-unique surety technologies to design, prototype, and test a smartcard system that could be commercially relevant and substantially more secure than any other smartcard systems in production or under development. Our intention is not to replicate commercial research or design efforts, but to leverage them to ensure maximum system surety. The resulting system should be useful in a variety of applications, including electronic banking, personal identification, access control, advanced information management, and secure access to information on the National Information Infrastructure (NII). We expect this project will result in a system that satisfies requirements for both the Department of Energy's Defense Programs (DOE DP) and the NII.

The research effort under this project resulted in the following accomplishments:

(1) *Consideration of security implications of multi-applications on a single smartcard.* Our design proved that a secure system implementation using smartcard systems would necessitate that authentication of the user, the smartcard, and the smartcard reader would occur before any other application was invoked. In addition, the protocol rigor ensured by our design increases confidence in the application secrets stored on a smart card. If application data on the smartcard were encrypted using an application-specific key, protection of the data could be ensured.

(2) *Tamper protection refinement, including assessment of individual system elements capabilities to satisfy tamper resistance, detection, and system response requirements.*

(3) *Conceptual design and prototype of optical smartcard authentication technique.* Our team explored various approaches to distributed verification of biometric and unique card characteristic cryptographic signature schemes. This work resulted in a Sandia technical advance.

(4) *Survey, prototype, and testing of low-cost secure-volume technologies, including capacitive, piezoelectric, guided acoustic wave, titanium/carbon, and conductive foam.* This effort resulted in the design of a low-cost, manufacturable, tamper-resistant capacitive foam material.

(5) *Commission of adversary analysis throughout the project to ensure soundness of design.* The first adversarial analysis effort focused on the concept of operations (CONOPS), which documents system architecture, hardware, and software components. The conclusion of this analysis was that the CONOPS has no obvious flaws; concepts are sound and approach is secure. The second adversary analysis effort focused on system architecture and key system components. The system architecture approach is deemed secure. High-level tests on capacitive foam material samples, which we will use to protect the distributed secrets in our system, are promising. Results proved that the material acts as a sensor and that the sensor is a capacitor.

(6) *Survey and evaluation of smartcard integrated circuit (IC) devices.* (This effort was hampered by the reluctance of smartcard IC manufacturers to allow us to purchase their ICs for analysis.) Public literature, smartcard system design courses and briefings, and lessons learned from smartcard IC analyses (supported under other funding vehicles) contributed to our knowledge and understanding of smartcard ICs. The trust model that our team settled on for design depended less on IC sophistication than on the ability to protect secrets within the reader to ensure the integrity of the system information.

(7) *Consideration of faithful execution of peripheral device issues.* Faithful execution of peripheral devices represents a tough problem. One solution is to integrate the peripherals into the

protected reader enclosure. Another solution is to encrypt data sent between the reader and the peripheral device, which adds cost to the peripherals. Our specific problem dealt with trusting the display device driven by a bad reader to tell the user that the reader is, in fact, not valid. We decided to prevent application access by ensuring that the smartcard kept track of the protocol execution before invoking any application. We then ensured that the smartcard would store information about contact with a bad reader that would be displayed the next time a smartcard was submitted to a valid reader. Procedural intervention would then address the bad reader at the previous location.

Publications

Other

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Object-Oriented Parallel Discrete-Event Simulation System—An Enabling Foundation for Rapid Development of High-Performance, Large-Scale Simulations

M. M. Johnson, A. S. Yoshimura, M. E. Colvin

Traditional discrete-event simulations employ an inherently sequential algorithm and are run on a single computer. However, the demands of many real-world problems exceed the capabilities of sequential simulation systems. Often the capacity of a computer's primary memory limits the size of the models that can be handled, and in some cases parallel execution on multiple processors could significantly reduce the simulation time. Parallel discrete-event simulation is a research topic in academia; no parallel discrete-event system exists that satisfies the software engineering requirements of robustness, portability, and scalability.

Sandia developed IDES (Infrastructure for Distributed Enterprise Simulation), a parallel, distributed, discrete-event simulation system that is robust, portable, and scalable. The system is based on a conservative simulation protocol and maps a message-based model of distributed computing onto an object-oriented (OO) programming model. Utilizing the Java programming language, it is portable across heterogeneous computing architectures, including single-processor systems, networks of workstations, and multiprocessor computers with shared or distributed

memory. IDES provides a simple and sufficient application programming interface (API) that can be used by scientists to quickly model large-scale, complex systems. In the background and without involving the user, the simulation system is capable of making dynamic use of idle processing power available throughout the enterprise network.

IDES is a parallel simulation framework for complex, large-scale enterprise simulations. We developed IDES to support Sandia in the study of issues of importance to national security. Many of these issues involve the analysis of complex systems. IDES is a policy-driven simulation tool capable of performing decision-directed analysis of complex system models. The goal of such analysis is to discover the emergent collective behavior of the system through the interaction of detailed individual submodel simulations—the definition of enterprise simulation.

IDES system research focused on two main goals. To motivate this research, consider an example domain: simulation of a U.S. health maintenance organization (HMO). The first goal deals with the structure of the simulation framework to express the systems to be modeled: Link low-level, complex submodels with high-level, policy-driven resource allocation techniques to perform cost/benefit trade-off analyses. In the HMO example, each patient is modeled with complex disease processes represented by differential equations, including risk for coronary artery disease. Medical treatment policies interact with disease models to affect the health outcome of patients.

The second goal specifies the portability of the system: Development of simulation models using IDES should be

within the reach of systems analysts and support deployment across heterogeneous computing architectures. IDES runs on single-processor systems, networks of workstations, and multiprocessor computers with shared or distributed memory. In addition, IDES incorporates a Web-based interface for distributing simulation subcomponents across the enterprise network.

In support of these design goals, we had to overcome a number of system constraints. First and foremost, IDES had to be capable of hosting massive models with relatively large state. The example HMO model includes ten million patients and one hundred regional hospitals and facilities. Enterprise simulations evolve differently from more traditional parallel simulation models, such as queuing and personal communication system (PCS) networks. For example, simulation entity behavior is not governed by a simple draw on a random number stream, but through the evaluation of complex, coupled-state evolution equations. Hence, the difficulty of extracting look-ahead discourages the use of a purely conservative protocol.

Since the data state of each component is large, we use multiple machines to acquire the memory needed. While a conservative approach to synchronization could use less memory than an optimistic approach, lack of look-ahead limits the effectiveness of conservative synchronization. Consequently, very large state coupled with lack of look-ahead motivated the use of breathing time buckets (BTBs) to constrain optimism. In addition, the state of simulation entities is computationally complex. In the HMO example, evaluation of complex disease models is computationally expensive. Parallelism is evident with a large population.

IDES, currently in production use within two Sandia projects, supports enterprise simulation of large-scale, fine-grained problems. Focusing on the BTB synchronization protocol, we developed a simple model of performance; the purely analytic model is expressed in terms of state transition equations that can be solved efficiently, numerically. In creating IDES, we developed a new algorithm—the preemptive min-reduction, for quickly detecting the end of the BTB synchronization window. In addition, we analyzed and published on alternative strategies for managing communication—to pre-send all messages and have the receiver filter out the risk-free ones once the window edge is known. For the scale of problems and architectures addressed by the IDES framework, we achieved good performance.

Publications

Refereed

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3512.130

Biometric Identity Verification for Remote User Authentication and Access Control Applications

A. M. Bouchard, J. W. Bartholomew, R. F. Martinez, Jr., J. J. Carlson

The goal of this project is to research and develop a new biometric identity verification system that meets the requirements for reliability and user acceptance, and also addresses the needs of remote access applications. Sandia's approach emphasizes three innovative concepts: (1) the use of an entirely new biometric, the acoustic signature of the individual's ear canal, (2) the fusion of multiple coarse biometric features, and (3) remotely extracting, digitizing, and encoding the biometric data to enable remote access capability.

The year's activities focused on two areas: (1) the research and development of the ear biometric, and (2) the use of multiple coarse features from multiple biometrics to verify the identity of an individual.

For the ear biometric problem, we investigated numerous hardware and data acquisition configurations in an attempt to reproducibly extract the acoustic signature from an individual's ear canal. We introduced acoustic waves of a specified frequency or spectral composition into the ear canal via a small speaker. A small microphone acquired the acoustic signal near the ear canal. The recorded, digitized

signal included both the incident wave and the wave reflected from the ear canal. We devised many schemes that theoretically should have enabled the removal of the incident wave from the detected signal, to isolate the reflected signal (the acoustic signature of the ear canal). However, with affordable hardware, and with data acquisition configurations that would be easy and acceptable to users for biometric purposes, signal-to-noise of the computed reflected wave was not good enough to be used reliably as a biometric. We therefore concluded that the proposed technology is not suitable for a user-acceptable, inexpensive, reliable biometric system.

We also investigated the fusion of relatively simple features extracted from digital images of the face and hand and from digitized speech. The results support the conclusion that the identity of individuals can be reliably verified by using a large number of these combined features. The performance of each feature is established in terms of its probability of error. Individually, the coarse features have a relatively high probability of error. However, when fused together in a higher dimensional space, their combined performance is much improved. The basic idea is that a few features can be easily confused, but it is difficult to confuse a large number of features from different sensors simultaneously. This concept is illustrated by using the weighted-nearest-neighbor method to fuse and evaluate the joint performance of the features.

"Robustness-Agile" Asynchronous Transfer Mode (ATM) Encryption and Associated Use Control

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R. J. Granfield, R. L. Hutchinson, L. G.
Pierson

The purpose of this project is to develop technology for "robustness-agile" asynchronous transfer mode (ATM) encryption. Robustness agility is the ability to specify an algorithm and key length so that the strength of encryption for an ATM virtual circuit is commensurate with the sensitivity of the data carried by it. However, robustness-agile encryption has a number of special issues. Since such encryptors can be used to protect data at more than one level of sensitivity, access control features are required to restrict the use of the strongest capabilities of the device. This access control must be secure, yet not place an excessive burden on the end-user. Another issue related to robustness-agile encryption is its impact on the ATM quality of service (QoS) for the virtual circuits that pass through the device. This project explores these issues further and develops techniques for implementing cryptographic algorithms, switching, and access controls for robustness-agile ATM encryption.

This research focused on a number of issues related to robustness-agile and algorithm-agile ATM encryption:

(1) *Access control (or use control)*. A robustness-/algorithm-agile ATM encryptor is typically used to separate information at various levels of sensitivity. Since stronger algorithms are likely used to protect more sensitive information, access to these algorithms must be strictly controlled. This implies the need for strong access control mechanisms based on cryptography. This requires a mechanism for securely storing authentication keys for the end-users. It is desired that this authentication process occur transparently to the user; therefore, it must be practical to implement

this process at the lowest layer possible. In this case, we implemented the authentication function within ATM control signaling using smart cards as a user "token" for key storage. We successfully implemented a prototype access control mechanism, and our findings indicate that this approach meshes well with ATM signaling and presents very little inconvenience to the user.

(2) *QoS effects*. In an encryptor that implements more than one algorithm, ATM cells may follow different paths, with each path having a different delay. The result is that when ATM cells are remultiplexed at the encryptor's output link, cells may incur additional latency and/or jitter. A detailed analysis of this problem shows that cell latency and jitter due to this effect are bounded by the delay of the "longest path" through the encryptor. For secret key algorithms such as the data encryption standard (DES) operating at 155 megabits per second, this delay is on the order of 5 microseconds, which is a small impact for most ATM applications.

(3) *Algorithm implementation issues*. During this project, we developed a "pipelined" implementation of the DES algorithm that allows key-agile encryption at rates up to 1.2 gigabits per second in programmable logic devices (PLDs). This implementation allows for fast context switching between keys because it does not require that the "pipeline" be flushed before the next cryptographic context is "switched-in." Since this algorithm requires four PLDs to implement, we developed a highly configurable circuit board that provides the flexibility required for implementation and experimentation.

(4) *Cell context switching and encryptor architecture*. The key component to the algorithm-agile encryptor architecture is a circuit board that switches cells to the appropriate cryptographic algorithm and multiplexes them back together when they emerge from the algorithm pipelines. To perform experimentation on the QoS effects, we designed this hardware to incorporate

two different output queuing approaches—one where the delays are equalized across the algorithms (resulting in maximum latency), and first-come-first-served queuing (resulting in maximum jitter).

(5) *Key-length agility*. The cryptographic robustness of an encrypted ATM virtual circuit is also affected by the length of the encryption key. This project explored different approaches for obtaining key-length agility for the DES algorithm. As a result, we developed an approach that can take a strong algorithm (such as triple DES) and "dial it down" to arbitrarily reduced levels of cryptographic robustness.

Publications

Refereed

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Tarman, T. D. 1997. "Contents and Structure of the Security Message Exchange (SME) Digital Signature Buffer." Paper presented to the ATM Forum Technical Committee (#AF/97-0545), Montreal, Canada, 21 July. SAND97-1657C.

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Agent-Based Remediation of the Mosaic Classification Problem

E. J. Friedman-Hill

The Nuclear Weapons Complex (NWC) is undergoing many changes. A problem is arising: The sum total of all unclassified information in these systems may be used to reconstruct classified data. This is the "mosaic classification problem (MCP)."

Sandia believes that the best way to attack the MCP is simply by watching what individual users retrieve from databases. The approach involves autonomous software agents programmed only with general knowledge about materials, transportation, and geography. Each agent will understand the job duties of and be assigned to a particular (human) database user. The agents would track each user's access patterns across many distributed information systems and attempt to infer classified information from the aggregate data accessed.

Although we did not perform a specific demonstration of a counterattack on mosaic classification incidents during this project, we made significant progress toward providing the tools and capabilities that would allow such a demonstration to be made. We demonstrated the interaction of intelligent agents based on the Jess system interacting (via Common Object Request Broker Architecture [CORBA]) with a large number of information sources at Sandia. This interaction was made possible by integrating Jess with the product realization environment (PRE) framework, Sandia's new information infrastructure for product realization.

This project led to two noteworthy technical accomplishments, both based on the Java technology, which provides a highly portable virtual machine (VM)

environment with rich network capabilities. By using Java as a portability layer, all software developed under this project can run unchanged on almost every server and desktop computer in the complex. Furthermore, Java provides both security services, which can protect a user's machine from damage from rogue agents, and a serialization and persistence mechanism, which will be used to give the agents motility.

The first accomplishment was the ability to integrate existing CORBA implementations with the Java programming language. The JIDL CORBA IDL (Interface Definition Language) compiler for Java, developed entirely at Sandia under this project, was the first publicly announced Java/CORBA solution. JIDL, written in C++, enables any user with a Netscape World Wide Web (WWW) browser to access CORBA-based services. From the programmer's standpoint, JIDL enables remote C++ objects to be manipulated in Java code as local Java objects. We used JIDL to deploy a number of applications in-house. The product realization backbone used JIDL to deploy platform-independent interactive graphical user interfaces (GUIs) for a number of in-house design codes, and also to demonstrate a prototype machine-shop monitoring system. JIDL's early availability impacted the standards process for the development of an Object Management Group (OMG)-certified Java IDL mapping by providing proof-of-concept and a functional example. Several commercial implementations of the JIDL concept are now available, and further work under this project has used Iona's OrbixWeb product. The Java-to-IDL mapping developed here had an influence on the ultimate standard adopted by the OMG.

The second accomplishment was the completion of a functional implementation of the Rete pattern-matching algorithm in Java. The Rete algorithm is a

method of storing state during multiple successive pattern-matching iterations, and it is perfectly suited to the task of determining the applicability of rules to the current state of a knowledge base. Rete can outperform naive methods by a factor of 100 or more in speed. The Rete implementation is a part of Jess, the Java Expert System Shell. Jess is the reasoning engine for the agents being developed under this project and was written entirely in the Java language. Jess is a clone of the popular CLIPS expert system shell, developed at NASA, and is 100% compatible with it. Besides use within this project, Sandia copyrighted Jess. A book on artificial intelligence programming in Java (Mark Watson's *Intelligent Applications in Java*) includes a chapter about Jess. The principal investigator gave an invited lecture on Jess's architecture.

The combination of Jess and CORBA with the Java platform leads to an exceptional deployment platform for agents: The agents are 100% portable across computer architectures, they are persistent (they can dump their dynamic state to disk or to a network connection), they are mobile (they can reconstitute themselves from either source), and they have the ability to reason using the large body of CLIPS code that the CLIPS user community has written. In addition, they can make use of the already large library of information-service client software being written in Java using PRE at Sandia. This last feature is a great advantage over a more traditional list processing language (LISP), or even CLIPS-based system, because of the dearth of network-access code available for these environments.

Jess-based agents are connected to a number of information sources at Sandia, enabling them to collect information for synthesis. They will play an increasingly important role in the next year as PRE continues to evolve.

Content-Based Search of Geometric Databases

P. G. Xavier, R. A. Lafarge, J. C. Krumm,
A. L. Ames, Y. K. Hwang

Unlike textual or numerical data, geometry currently cannot be indexed or searched. Consequently, users of geometric data, such as designers, are at a considerable disadvantage when attempting to benefit from past experience. The impact of textual search systems such as SMART and Alta Vista hint at the potential if geometric data were to be successfully indexed and made available online.

Sandia is developing algorithms and a prototype system for efficiently searching databases of 3-D geometric data by content. We will form queries by combining images and models, similarly to how keywords are used in text searches. We would use the system's geometric query composer to construct and refine queries, which could incorporate images and models, for input to the search engine. The primary query format of outlines in images and simplified models applies to any renderable geometric data. Other query information consists of features given as codes and accurate local geometry.

We concentrated on searches based on approximate shape, developing and implementing techniques appropriate for 2-D and 3-D queries. We explored methods for indexing based on detailed features and certain high-level features.

The first year of our project focused on researching and implementing basic image/shape indexing techniques suitable for use in an interactive dynamic geometric database system. We concentrated on searches based on approximate shape. In addition to researching and implementing various geometric indexing

algorithms, we also developed software to extract from computer-aided design (CAD) model data the types of information an interactive user would provide in queries. This latter activity continued through the last quarter of the year, in which we also began investigating how to apply geometric hashing techniques in our work.

We began our year by reviewing the literature. Sketching out the system's architecture revealed some problem characteristics that added constraints and other characteristics that reduced requirements, as compared with many problems addressed by techniques from computer vision research. Geometric hashing (to either images or models) approaches appeared to hold some promise for the role of choosing among candidates based on detailed features, and other hashing methods seemed to have potential for search by approximate shape.

Our first major accomplishment was the development of a prototype system that takes faceted boundary representations of 3-D models and produces an index that can be searched given silhouettes, possibly with occluding edges, as queries. Using a preliminary test database of 32 models (essentially randomly chosen), this prototype achieves an accuracy of 97.6% in 500 trials of random single-image queries, with success defined as the highest-ranked object being the correct object. When indistinguishability and near-indistinguishability at viewpoints are accounted for, the accuracy rises to 98%. To construct an index, the system samples views from 1336 points on the sphere (i.e., roughly seven degrees apart) for each model. (Accuracy drops to 93.3% [95%] when only 334 sample viewpoints are used.) For each view, the system normalizes image

size, centering, and roll angle, then computes a key vector (length 13 in the cited experiment) based on the silhouette and the occluding edges. Given a query image, we use the same process to compute a query key vector, and the system searches the index of keys for the closest match.

Our second major accomplishment was to extend this 2-D/3-D indexing method to index 3-D models for use with 3-D queries. The ability to search based on approximate shape is an area of weakness for feature-based classification systems such as Mitro. The primary 3-D-specific extension incorporates the use of 3-D depth information into the keys. For each adjusted viewpoint, we simply divide the image into a grid of cells and record the mean depth, and possibly other statistical depth data, for each cell; we combine these data with the 2-D key. Using 25-element keys, our system achieved an accuracy of 99.4% in 500 trials of single random viewpoint queries. There is potential to reduce the size of the index by restricting views to roughly correspond with 3-D principal axes.

The problem considered in the final quarter of FY97 was how to index and search for similar models that are qualitatively similar in terms of spatial relations among high-level features (e.g., holes, slots, etc.). Our approach is to use geometric hashing. In our planned system, index creation for models in the database must be automated, while the user will be able to identify features on the query object (CAD model, faceted data, or picture/figure). Our efforts this quarter thus have focused on enhancing the present feature-recognition code, investigating how to adapt geometric hashing to qualitative spatial relationships, and implementing code to support feature-based indexing.

Integrated Service Provisioning in an "IPv6 over ATM" Research Network

H. Y. Chen, J. A. Hutchins, T. M. Berg, J. A. Friesen, R. P. Tsang, J. M. Brandt

During the past few years, the world-wide Internet has grown at a phenomenal rate, which has spurred the proposal of innovative network technologies to support the fast, efficient, and low-latency transport of a wide spectrum of multimedia traffic types. Existing network infrastructures have been plagued by their inability to provide for real-time application traffic as well as their general lack of resources and resilience to congestion. This work proposes to address these issues by implementing a prototype high-speed network infrastructure consisting of Internet Protocol Version 6 (IPv6) on top of an asynchronous transfer mode (ATM) transport medium. Since ATM is connection-oriented, whereas IP uses a connectionless paradigm, the efficient integration of IPv6 over ATM is especially challenging and has generated much interest in the research community. Sandia proposed, in collaboration with an industry partner, to implement IPv6 over ATM using a unique approach that integrates IP over

fast ATM hardware while still preserving IP's connectionless paradigm. We achieved this by replacing ATM's control software with IP's routing code and by caching IP's forwarding decisions in ATM's virtual path identifier/virtual circuit identifier (VPI/VCI) translation tables. We will also develop prototype virtual reality (VR) and distributed-parallel-computing applications to exercise the real-time capability of our IPv6 over ATM network.

(1) The background research that we conducted includes the following:

- *IP over ATM*: This work is published in Sandia Report 97-8273, *A Survey of IP-over-ATM Architectures*.
- *Real-time traffic*: This work is published in Sandia Report 97-8274, *Networking Requirement for Various Coded Digital Video Systems*.
- *IPv6*: We installed the public domain IPv6 software, joined the 6BONE test-bed (a global IPv6 test-bed sponsored by the Internet Engineering Task Force [IETF]), and conducted tests that allowed us to share our experiences with other participants via the IETF 6BONE mailing list.

(2) The current status of the IPv6 switch implementation is as follows:

- We installed IPv4 switching test-beds using the prototype components procured in this project. IPv6 switch-

ing implementation is in the debugging phase.

- We procured a Moving Picture Expert Group (MPEG)-2 encoding/decoding system to generate real-time video streams. We will use it to characterize real-time applications traffic and their quality of service (QoS) requirements.

Publications

Refereed

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Virtual Desktop Engineering with Integrated Multimedia Data

J. A. Friesen, J. Schwegel, J. N. Jortner

The growth of the Internet has spurred the development of innovative technologies that support the fusion of a wide spectrum of multimedia data types. Those technologies have made it possible to provide an environment where engineers can design, prototype, and test components in a virtual space while integrating actual data into the process.

This work proposes to insert multimedia streams such as video into a desktop virtual reality (VR) environment. Compressed audio, video, animation, scientific visualization, and text streams will be stored in a distributed database and delivered in real time over the network to desktop computers. Using leading-edge World Wide Web (WWW) technology, such as Java and Virtual Reality Modeling Language (VRML), we will build an integrated VR environment unlike any currently available on high-end visualization servers.

For example, an engineer using ProEngineer to design a mechanical part could call up similar products from a multimedia part database that displays part behavior from a 3-D perspective. In addition, audio/video clips of engineering advisors, test data, and computer simulations could be displayed interactively. After designing the part, the engineer can virtually manufacture the part to predict actual part performance.

Engineers can quickly evaluate the quality of a design in an interactive environment. Using collaboration tools, they will be able to virtually design, manufacture, and test a part before resorting to stereolithography. That will result in significant reduction of cycle time and therefore cost. In addition, the design process can be archived in multimedia form for future use.

(1) Computer and software integration. We are currently integrating VRML, intelligent Common Object Request Broker Architecture (CORBA) agents,

Sandia's Multimedia Server, and ProEngineer in the advanced concurrent engineering (ACE) environment. From within a Web browser, an engineer can now view VRML versions of ProEngineer models, watch audio/video movies from the Multimedia Server, and read textual part information returned from the intelligent agents. Our work focused on developing distributed multimedia databases with automated data input and intelligent data retrieval. We will use intelligent agents to extract VRML model data, audio/video/image data, and textual data from the multimedia databases for display. We are storing all movies in Moving Picture Expert Group (MPEG)-1 and QuickTime formats. We are using TIFF images for high-resolution storage and converting them dynamically to JPEG and GIF for display.

We are using the following software components to implement the above functionality:

- VRML converters (ProEngineer PolyTrans)
- Animation packages (VisLab suite, SoftImage)
- FEA (finite-element analysis) analysis package (EnSight, AVS Express)
- Kinematic and dynamic mechanical analysis package (data acquisition and display system [DADS])
- Video compositing packages (Alias/Wavefront Composer)
- 3-D modeling packages (3-D Studio Pro, SoftImage, VisModel)
- Streaming JPEG video (Graham Technology Solutions)

We have been working on integrating the inputs/outputs of the different software modules for encapsulation into the Product Realization Environment (PRE). This involves identifying the various file formats and generating conversion modules when necessary. PRE is a CORBA-based software architecture that provides the framework for data interchange and the "glue" for linking data files with distributed user interfaces. PRE also provides an information data repository for storing the attributes of the various inputs and outputs.

(2) Pilot project selected. To show the applicability of this project, it was necessary to select an important Sandia project that could effectively utilize the tools we are developing and would benefit that program. We found a match between our proposed work with the needs of the extreme ultraviolet lithography (EUVL) program. Computer modeling and analysis are playing major roles within the EUVL project by helping to shorten the design and development time. By eliminating physical prototype construction, engineers hope to build a working system within 3 years instead of the typical 5. Since we are greatly utilizing visualization and multimedia, it is important that these results are archived and easily accessible.

(3) VRML model defined. We finalized the VRML 2.0 standard in August 1996. Industry accepted it in the months following, and the first implementations became available in the first quarter of calendar year 1997. Because the EUVL design assemblies were in a very early conceptual stage, we chose to test the new animation and video capabilities of VRML 2.0 using a Sandia-designed Collocated Detonator Stronglink (CDSL) assembly.

3512.190

Mission Surety for Large-Scale Real-Time Information Systems

S. J. Bespalko, K. L. Brower, C. J. Hogg

The goal of this project is to provide the scientific basis for extending the state-of-the-art in software engineering practice, specifically with regard to the generation of command and control (C²) systems. C² systems are a vital component of the lab mission. The area on which the project will focus is improving the correctness and completeness of such systems through the application of recently introduced theory of automatic software component generation (sometimes referred to as software composition). Component generation systems are currently limited by the underlying computational model on which

the systems are based. The most common model is termed a finite state machine (FSM). Sandia's work in the first year established that the FSM is insufficient to model the processing in typical C² systems. The anticipated contribution to the state-of-the-art will be to extend component generation systems to encompass computational models sufficient for C² systems.

Several key accomplishments characterize the first year of the project. Our focus was to analyze a large (in excess of one million lines of code) C² system built by Sandia. The first accomplishment was to establish that the current engineering methodology (rational universal modeling language [UML]) used by the engineering staff was insufficient to completely represent the system algorithms. The rational UML is based on an FSM architecture, the simplest of the formal computational models computer scientists use to study systems. Further investigation established that a much more complex model, termed a *context-sensitive grammar*, was required to concisely define the processing in one of the more problematic modules in the system. Next, we established that a tool based on the context-sensitive language could generate perhaps one-half of the module automatically, ensuring completely correct functionality. We now believe that perhaps one-half of the overall system could be automatically generated with an expanded tool. A prototype of the tool is nearing completion. The tool consists of approximately 3500 lines of object pascal.

In addition to the analysis of the problems with the large groundstation, we undertook a literature search to investigate the state-of-the-art in automatic software component generation. The result, establishing that there are classes of problems not covered by the current engineering methods (such as the popular rational UML), generated considerable interest by leading software researchers. As a result of publications and participation in conferences, this team was encouraged to act in the role of principal contractor/investigator on a major Defense Advanced Research Projects Agency (DARPA) contract proposal.

Publications

Refereed

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3512.210

Integrated and Robust Security Infrastructure

R. L. Hutchinson, M. D. Murphy, J. Espinoza, G. G. Istrail, V. A. Hamilton

The integrated and robust security infrastructure (IRSI) project has two goals: (1) a broad range of security services that are transparent to the application, and (2) public key infrastructure. Application transparency hides the details of the security services from the application. Any off-the-shelf application could use the security services for interprocess and

network communications without the need to modify the application. The goal is to develop a security layer transparent to the application that would provide data separation by user authorization level. The second goal, public key infrastructure, investigates distribution, authentication, and revocation of public key certificates. Sandia focused on a distributed trust model where a logical certification authority (CA) is distributed throughout the network. Trust is not placed in any single CA, but in a collection of CAs.

This investigation allowed the IRSI team to conclude that such a security layer is not achievable without modifying the host operating system. Our goal was to implement a broad range of security services that could be used by any application without modification to the application or operating system. It is possible to key the host and provide transparent security services over a network at a single network authorization level using security extensions for IP (IPSec). This solution does not provide interprocess security and requires a rebuild of the operating system on a UNIX platform. We implemented a secure token to store the long-term user secret. Public key cryptography systems require that a system entity maintain a long-term secret by which the entity is authenticated to the system. We implemented long-term secret storage using a smart card device. The long-term secret is never exposed to the host or system where it may be compromised. We developed models for a public key infrastructure. Using information modeling techniques, we described a public key infrastructure and the relationships between objects.

Scaled ATM End-to-End Encryption

L. G. Pierson, T. D. Tarman, L. B. Dean, II, P. J. Robertson, R. L. Hutchinson, L. G. Martinez, Jr.

This effort is to position Sandia to influence and accelerate the deployment of scalable, variable-bit-rate asynchronous transfer mode (ATM) encryption equipment needed to satisfy the Department of Energy (DOE) Accelerated Strategic Computing Initiative (ASCI) requirements for communication security. The Microelectronics Center of North Carolina (MCNC) "Atilla" prototype ATM end-to-end encryptor is the fastest known, operating at 622 Mb/s. Sandia's "Scalable ATM Encryptor Prototype" is the second fastest, operating at 155 Mb/s. The National Security Agency (NSA) "Milkbush" prototype encryptor is the third fastest, operating at about 100 Mb/s. NSA's efforts have evolved into plans to make ATM end-to-end encryptors commercially available that operate at up to 0.6 Gb/s. To meet DOE/ASCI objectives, ATM encryptors for higher data rates (2 to 10 Gb/s and even higher) are expected to soon be required. This research effort will explore techniques required to scale encryption speeds to 10 Gb/s and faster, while maintaining reliable communications synchronization.

The goal of this effort is to integrate innovative methods of key management, crypto synchronization, and key agility while scaling encryption speed. We will show viability of these methods for encryption of ATM cell payloads at the SONET (Synchronous Optical Network) OC-192 data rate (10 Gb/s), and for operation at OC-48 rates (2.5 Gb/s).

We adapted a Sandia-developed pipelined data encryption standard (DES) design for the encryption of ATM cells.

We designed and built a proof-of-principle prototype encryptor circuit board containing eleven electronically programmable logic devices (PLDs) (each holding the equivalent of 100,000 gates).

Development of this technology will accomplish the following:

- (1) Enable national defense applications requiring the secure exchange of massive amounts of data between widely separated sites.
- (2) Enable the interoperation of low-cost, "low"-speed encryptors for high-performance workstations and super-high-speed encryptors for massively parallel processing (MPP) computers.
- (3) Significantly reduce the cost of encryptors for industry standard ATM/SONET data transmission interfaces, presently costing \$30k per encryptor.

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Network Surety Modeling for Wireless ATM Networks (and Other Distributed Computing Systems)

P. E. Sholander, L. G. Martinez, Jr., B. A. Mah, L. F. Tolendino

This project has three focuses: (1) the effect of mixed wired and wireless networks on standard Internet applications, such as Web-browsing, file transfer, and video conferencing; (2) mobility management (This project examined protocol extensions to standard link-state routing protocols (such as Private Network-Network Interface [PNNI]) that support movable asynchronous transfer mode (ATM) switches. DoD applications include mobile command centers; DOE applications include temporary test and monitoring networks. Follow-on topics in this second focus area include routing in ad hoc networks.); and (3) the interaction between user mobility and the current ATM traffic management procedures. Results indicate that traffic contract enforcement may be problematic for variable-bit-rate (VBR) services such as Moving Picture Expert Group (MPEG)-2 video.

This project produced SAND report 97-0911C, on the effects of mobile ATM switches on PNNI peer group (PG) operation.

Current ATM Forum work focused on end-system mobility. However, some companies are also considering movable ATM switches. Commercial applications include local-area networks (LANs) on airliners; DoD applications include mobile command centers; DOE applica-

tions include temporary test and monitoring networks. One promising approach is protocol extensions to the existing ATM routing protocol, PNNI. SAND report 97-0911C lays out the technical problems posed by those extensions.

PNNI is a hierarchical link-state routing protocol. PGs are a key concept in PNNI. Individual switches obtain detailed information about their own PG's topology and summarize information about other PGs' topologies. As such, a PG hierarchy is conceptually similar to the (country code)-(area code)-(central office code) routing paradigm in public phone networks. There are then three core technical problems. First, how does a movable ATM switch learn about the other existing PGs? Second, how does that switch decide which PG to join? Last, how does that switch seamlessly change PGs?

The second deliverable was SAND report 97-1927C, on the effects of user mobility on usage parameter control (UPC) in wireless asynchronous transfer mode (WATM) networks.

ATM call setup entails a "traffic contract." The user requests a certain quality of service (QoS) (end-to-end delay, cell-loss, and end-to-end jitter) from the network. The network may accept that request, subject to agreed-upon traffic parameters such as peak cell rate (PCR) and sustained cell rate. In that case, the network provides that QoS to the ATM cells that conform to those traffic parameters. The generic cell rate algorithm (GCRA) is the standard conformance test. It is a filtering algorithm that ensures, for example, PCR compliance to within some agreed-upon tolerance. As such, like any filtering

algorithm, the GCRA has a finite settling time. Hence, in mobile networks, users might change wireless cells before the GCRA settles. So, if the GCRA state resets after each wireless handoff, the network can't always determine conformance. Hence, malicious or clueless users can exceed their traffic contract with impunity. This can affect the QoS for other conformant users.

SAND report 97-1927C gives explicit formulas for the relationships between a user's traffic parameters, their transit time per wireless cell, their maximum sustained cheating rate, and the GCRA's tolerance (or "limit parameter"). Results indicate that the GCRA can still police constant-bit-rate (CBR) traffic, but not some types of realistic VBR traffic. Finally, there may be no standards-based way to transfer UPC state during handoff. As such, some future public WATM networks may exclude those types of VBR traffic.

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S

ensing technologies are changing how many national issues are approached. Uses for sensors range from battlefield applications to environmental cleanup. Sensors are being developed that measure — and help researchers understand — phenomena that in the past had been unobservable. Sandia is a leader in these

areas of research:

- Chemical sensors
- Analysis techniques that combine data from multiple sensors to create a “fingerprint”
- High-resolution synthetic aperture radar
- Automatic target recognition.

Four significant technology areas are supported: (1) physical imaging techniques to view concealed or difficult-to-view objects such as landmines; (2) chemical and biological sensors that can detect minute quantities of specific chemicals in a field environment and in real time; (3) distributed sensor systems that will monitor complex systems such as battlefields or manufacturing processes; and (4) novel projects that create new applications, techniques, or skills.

Sandians are designing a new remote sensing technique called the *information-efficient spectral-imaging sensor for satellite surveillance*. The sensor offers significant improvements over existing technology by allowing passive identification of materials in a scene. One demonstrated application is the ability to differentiate between real and simulated vegetation (camouflage).

Two radar techniques are being combined to produce images not only of tree tops but also of the terrain underneath. Understanding the different images these radar systems produce will allow researchers to create an image of both the terrain and the vegetation. This information will benefit both military and commercial entities.

A three-dimensional rendering of a radar-generated height model of trees, buildings, and terrain features in the Black Mesa area south of Albuquerque, NM. Interstate 25 and U.S. 85 are prominent features of the image.

PRECISION SENSING & ANALYSIS

Superconductive Gravity Gradiometers for Underground Target Recognition

M. J. Adriaans, A. L. Sobel

One of the most formidable intelligence challenges existing in the nonproliferation community is the detection of buried targets. The physical parameter that all buried targets share, whether the target is buried armaments, a tunnel, or a bunker, is mass. In the case of buried armaments, there is an excess of mass compared to the surrounding area; for a tunnel or bunker, the mass is missing. In either case, this difference in mass generates a distinct gravitational signature.

The gravitational signature of a truck, a tank, or a nuclear warhead is infinitesimal compared to the Earth's gravity, but development has begun on a new field-deployable superconducting accelerometer to add gravity to the optical, radar, x-ray, thermal, and other methods that can help verify arms-control treaties or ferret out an enemy's armaments and underground structures.

The Earth's internal churning creates a gravitational noise thousands of times as strong as the signals being sought. By combining two accelerometers in one instrument and canceling the common-mode noise that both detect, it is possible to create a gravity gradiometer that responds only to nearby variations in the gravitational field. For example, if the two accelerometers are 15 cm apart, the Earth's gravitational noise, originating many kilometers away, will be the same at both accelerometers and will be ignored. But the mass of a vehicle a few meters away, or the absence of mass caused by a tunnel or underground bunker, affects each accelerometer differently and reveals that something is hidden.

A single-axis system (two accelerometers) for a proof-of-concept laboratory test is currently under development between Sandia and university collaborators. We fabricated the superconducting gravity gradiometer (SGG) device using the superconducting material niobium. The use of superconducting materials allows a great increase in sensitivity over other conventional gravity instruments.

Fabrication of the components of a gravity gradiometer, which are made from the superconducting material niobium,

involves intricate machining with the use of an electron discharge machine (EDM). A problem occurred in making one of the cuts on the linear accelerometer when the first cut in one of the springs warped the accelerometer. The difficulty was resolved by slightly modifying the design and changing the order in which heat treatment is performed. Fabrication of all components for the gravity gradiometer is complete.

The next major step is balancing the angular accelerometer proof masses. We measured the proof mass offset, and the first iteration of mass trimming can begin as soon as the wire EDM is finished with the linear accelerometers. We are working on the mass offset measurements to try to improve accuracy. The current numbers are satisfactory for a laboratory demonstration of the gradiometer, although it appears that an improved mass balancing setup will need to be built to achieve the performance needed for an airborne survey. Once the mass balance is complete on the angular accelerometers, the assembly can begin.

3516.030

Moving Mass Trim Control for Precision-Strike Warheads

B. R. Sturgis, M. R. Vaughn, D. M. Vanzuiden, R. H. Byrne, J. Baldo-Pulaski, C. T. Coffin

Precision-guided warheads are critical to improving the effectiveness of nuclear and conventionally armed strike systems. This research project developed a validated computer simulation tool for the design and evaluation of moving mass controllers on precision-guided reentry systems. The simulation tool includes a multiple body dynamics model, a control system model, and a guidance algorithm. Sandia designed and built a prototype moving mass controller, based on the Mk4 reentry body, and tested it for the purpose of gathering experimental controller performance data.

(1) Developed the trajectory simulation code. The first version of the trajectory code contained dynamical equations of motion of a flight vehicle under the influence of internal moving masses, the Earth's gravity field, and aerodynamic forces. The second version integrated the first version with a guidance algorithm (to

compute trajectory corrections needed to hit a target) and a control system algorithm (to compute how to move the masses to satisfy the guidance requirements). After code checkout was complete, we began studies to evaluate control system performance and vehicle stability. We realized at this point that flight vehicles may be classified into two categories. Category 1 consists of slow-spinning reentry bodies (RBs) that can steer to a target using the aerodynamic drag force and a center of mass offset provided by the moving masses. Category 2 consists of fast-spinning rocket systems that can steer primarily due to principal axis tilt resulting from the imbalance caused by the moving masses.

(2) Designed a prototype moving mass controller. Due to greater interest in category 2 vehicles, we designed the prototype for a vehicle of that type. We refined the design from a three-mass independently controlled set of masses to a two-mass master-slave ring configuration. This refinement provides the ability to fit the controller around existing components in an RB without altering the exterior (and therefore the aerodynamic properties) of the RB. The refined system is also a lower-volume, lower-power system than the first design.

(3) Built the prototype hardware and tested that hardware in the Sandia centrifuge facility. This test allowed the evaluation of hardware performance under flight-like environments (decelerations peaking around 50 Gs).

Conclusions are that (1) a moving mass control system can provide adequate control authority to improve accuracy of existing stockpile systems, (2) moving mass hardware is capable of operating in high-deceleration reentry environments, and (3) ring configurations are good retrofits to existing stockpile systems because they may fit around internal components, and they do not alter vehicle aerodynamic properties.

Publications

Refereed

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Micro-Holographic Tagging

W. C. Sweatt, D. A. Tichenor, A. K. Ray-Chaudhuri

Sandia designed and fabricated microscopic computer-generated holograms along with a highly portable readout system. We fabricated these "microtags" using the extreme ultraviolet lithography (EUVL) tool being developed at Sandia's facility. Thus one will eventually be able to mass-produce these tags quite cheaply. Microtags are 60 x 100 microns (0.0015"x0.0025") so they can be easily hidden on hardware, security cards, microchips, etc. Furthermore, the lines and spaces on the tags are only 0.15 micron wide, so they cannot be resolved with a microscope; thus the pattern cannot be easily read out.

The images created are alphanumeric characters; the first was a capital "E," which was quite clear. Underlying this image is a speckle pattern, the shape of which depends on the starting point used during the design. This could be used as a "fingerprint" to help verify the tags' authenticity.

The microtag readout system is quite simple. It includes a laser diode (633 nm) with collimating optics, a CCD camera with a liquid crystal display (LCD), and a tag holder. The whole system is battery-powered and weighs a couple of pounds.

We conceived the basic microtag concept, designed a readout system, developed the software to design the tags and fabricated several, and built a portable readout system. The experimental images and the predicted images are remarkably similar.

Microtags are extremely small computer-generated holograms (CGHs). The software developed to design them uses the standard Hertzberg-Saxton algorithm. This design scheme assumes a random set of phases in the cells and changes them until the desired image approaches. The speckle pattern associated with the final image is unique to the starting point. In later designs we also allowed the amplitude in each cell to vary. This improved the images significantly.

The microtags were exposed in photoresist using the EUVL system located at Sandia's Livermore facility. We chose this system because it can print features as small as 100 nm, as compared with today's state-of-the-art steppers that can print 250-nm lines. There was quite a learning curve associated with using EUVL. The masks are reflective. They have to be deposited on SiMo multilayer-coated mirrors that reflect the 13.4-nm EUV radiation. Photoresists for EUVL are few, and their response is not well understood in this wavelength region. Furthermore, some wall slope (on the printed features) is very good for the microtag application where it is an anathema for electronics manufacture. Hence we had to optimize some of the exposure parameters for printing microtags and could not use the general EUVL data bank.

We prototyped the readout system for microtags and rebuilt it twice, each time simplifying it and making it smaller. The final system includes a laser diode with a collimating lens, a CCD TV camera with an LCD display, the microtag holder, and a battery to run the whole system. It weighs about a kilogram.

The first tag designed, fabricated, and tested created a red "E." This 120x80-micron tag contains a 64-cell (8x8), phase-only CGH. The linewidth in this tag was 200 nm. The second tag was also designed for red light but had both phase and amplitude variations in the 64 cells. This reduced the speckle somewhat, thus improving the imagery. The third and fourth tags made were phase-only and phase-and-amplitude tags designed for reconstruction with blue light. The "blue tag" size was 80x60 microns, and the 64 cells contained 150-micron features. The images produced by all of these tags matched the predicted images extremely well. We submitted an application to the patent office covering the basic microtag.

In July we made masks for two advanced tag concepts, and in August the EUVL system went down and will not be up again until after our funding terminates. One of these tags contains two images: an "E" and an "S." These are seen from two orthogonal directions. The

other advanced tag is just a one-image, phase-and-amplitude tag designed to be overcoated with a protective plastic layer. We hope to find funding in November to make and test these tags. We submitted a Technical Advance (TA) for these ideas.

One other idea associated with this project is a condenser design for deep-UV lithography that is based on diffractive cells, just like the microtag. It allows the lithographer to switch very easily from one type of "engineered illumination" to another. Thus the stepper system can be optimized to print any specific class of features on the chip. We submitted a TA for this idea as well.

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Electrokinetic Immunoaffinity Chemical Sensors

J. S. Schoeniger, D. H. Thomas, D. J. Rakestraw, D. S. Anex

The purpose of this project is to establish the feasibility of capillary affinity electrochromatography (CAEC) with laser-induced fluorescence (LIF) detection for portable sensors of trace quantities of toxins in liquid samples. The project focuses on detection of analytes for which there is currently no portable sensor capability with adequate sensitivity and specificity, e.g., potential biological warfare (BW) agents (bacterial toxins). In CAEC, the chromatographic matrix consists of immobilized molecular recognition materials (MRMs) such as antibodies (Abs) that bind selectively to the target analyte, surpassing the specificity of capillary electrochromatography (CEC) methods that rely only on simply physical interactions. A sensor based on CAEC has the potential to combine the versatility of CEC, the high sensitivity of LIF, and the exquisite selectivity of molecular recognition.

Sandia established during the first year of this project that immunoaffinity chromatography can be performed in packed capillaries with electrokinetically driven flows. This is the first implementation of CAEC in packed matrices. Performance of these capillary columns for selective preconcentration of analyte and competitive assays is analogous to pressure-driven assays, establishing that electric field effects do not interfere with molecular recognition. To implement CAEC to detect potential BW agents, we identified a strategy for safely handling bacterial toxins (botulinum, ricin, aflatoxin, ovalbumin) and obtained Abs that bind to them. We implemented different chemistries for immobilizing Abs and applied physical and chemical techniques to characterize the resulting separation matrix. We used immobilized MRMs for both chromatography with pressure-driven

and electroosmotically driven fluid flow and compared the chromatographic results.

(1) *Identified target analytes.* Because of their level of significance in counterproliferation and food safety, we selected botulinum toxin, ricin, ovalbumin, and aflatoxin as target analytes. We determined that the safety of working with the more lethal toxins, which are often composed of two protein subunits bound together, could be greatly enhanced by working with biologically active but separately purified or recombinant subunits. We identified vendors and obtained stock of these specialized biological materials and MRMs (e.g., Abs) that bind to them. We implemented appropriate safety measures, including separate storage and work areas for particularly dangerous materials.

(2) *Defined immobilization methods for MRMs and characterization of immobilized MRMs.* We implemented systematic procedures to synthesize and analyze the properties of separation matrices with the goal of maximizing the number of binding sites (capacity), the strength of binding the immobilized MRM, reducing or eliminating nonspecific binding, and creating reproducible electroosmotic flow (EOF). The separation materials are silica microspheres covalently derivatized with MRM. Physical characterization of the silica microspheres revealed that (a) the particles were, in fact, pure silica, and that our preparation protocol, involving nitric acid wash, removed common adsorbed metallic contaminants that impede attachment and EOF, (b) the size uniformity of the particles varied greatly between vendors, and (c) the main difference between porous and nonporous supports is a surface roughness on the order of 2 nm for nonporous and 10 nm for porous, with relatively few actual pores penetrating to the interior. Because external surface area scales inversely to diameter, the limited internal surface accessibility of porous supports indicates that sufficiently small, nonporous particles will provide equivalent

surface area per volume as porous supports and better binding kinetics, but will require electrokinetically driven fluid flow, indicating that, in principle, CAEC can ultimately achieve superior performance compared to pressure-driven methods.

We characterized two immobilization procedures for Abs: (a) we treated silica beads with 3-glycidyloxypropyl trimethoxy silane (TMS), and linked Abs via Schiff base formation, and (b) treated beads with 3-mercaptopropyl TMS, washed them, and they reacted with 3-maleimidobutylsuccinimide ester (GMBS), leaving a surface of succinimide ester groups, which reacts easily with protein amides. The sulfur/GMBS linkage was more efficient than aldehyde/Schiff base. We measured isotherms for the binding of the fluorescently labeled analyte to immobilized Ab. Dissociation constants of approximately 10^{-8} molar demonstrated that the Ab binds tightly and selectively to the analyte after immobilization.

(3) *Implemented sensor system.* In a typical CAEC run, 10 kV is used to drive 5mM Tris running-buffer (pH 8.0) with EOF of 1 mm/sec through a 30-cm-length silica capillary with a 1³-cm-packed bed of Ab immobilized on silica. We electrokinetically injected sample (elution buffer) by transferring the capillary tip to the sample (elution buffer) reservoir, applying voltage for a time interval, and then stopping the voltage and returning the capillary tip to the running buffer reservoir. We detected analyte by using LIF and a photomultiplier tube.

We demonstrated for the first time that quantitative CAEC in packed capillaries can be performed in a manner analogous to pressure-driven affinity chromatography. We showed that selective concentration of the applied analyte in the eluate can be achieved. (We achieved about a 30-fold concentration for labeled biotin in the presence of interferents such as urinary metabolites.)

Information-Efficient Spectral Imaging System (ISIS)

S. M. Gentry, W. C. Sweatt, C. L. Grotbeck, S. E. Motomatsu, L. J. Krumel, M. K. Hinckley, R. J. Blake, B. R. Stallard

Hyperspectral imaging (HSI) is a remote sensing technique that is gaining significant attention for its unique ability to allow passive identification of materials in a scene. To achieve this, HSI systems acquire high-resolution simultaneous images in hundreds of spectral bands generating vast amounts of data for a single image. This makes data acquisition and processing difficult and limits the ability to do real-time target detection with HSI. Information-Efficient Spectral Imaging System (ISIS) is an optical system concept designed to reduce data rates in HSI systems and may allow on-the-fly target discrimination with limited processing overhead. ISIS allows the optical selection and mixing of key spectral image components into a small number of outputs related to target identification. Most applications could experience at least a factor of ten reduction in data rate and signal-to-noise improvements of a factor of five over traditional HSI systems with similar specifications.

We made the following accomplishments in FY97:

(1) Developed a system performance model used to compare ISIS to traditional HSI systems. We published the results of this model as a SAND report titled "Principles and Satellite Applications of the Information-Efficient Spectral Imaging Sensor," SAND97-1493.

(2) Constructed a fully functioning traditional HSI system out of existing components for laboratory- and field-scene calibration and for comparison to the ISIS sensor. Using this system, we spectrally calibrated laboratory scenery for use as an initial test-bed for materials discrimination with ISIS and developed ISIS filter-vector settings based on these measurements.

(3) Constructed a fully functioning breadboard ISIS instrument out of existing components covering the 0.5–0.75- μm region to prove liquid crystal display (LCD) spatial-light-modulator applicability to the ISIS sensor design

concept, and for laboratory use while the 0.5–1.0- μm prototype system was under design, fabrication, and testing.

(4) Demonstrated real-time materials discrimination with laboratory scenery using the ISIS breadboard system, including discrimination between real and artificial vegetation (precursor to camouflage detection). We demonstrated simulated camouflage vehicle detection using HYDICE "Western Rainbow" data, processed using ISIS filter-vector-detection methods.

(5) Completed the design and initiated procurement of ISIS prototype system covering 0.5–1.0 μm . We expect component delivery in time for integration, calibration, and laboratory testing by the end of FY97.

(6) Made initial preparations to fly ISIS on an aircraft.

Publications

Other

Stallard, B. R., S. Gentry, W. C. Sweatt, S. E. Motomatsu, C. Boye, and C. L. Grotbeck. 1997. "Principles and Satellite Applications of the Information-Efficient Spectral Imager." Sandia Technical Report SAND97-1493, 1 June. Sandia National Laboratories, Albuquerque, NM.

3516.070

Imaging of Moving Targets Using Simultaneous Synthetic Aperture Radar (SAR) and Moving Target Indicator (MTI) Radar

T. J. Cordaro, J. A. Hollowell, C. V. Jakowatz, Jr.

During the first year of this project, Sandia developed requirements and a schedule for adding a moving target indicator (MTI) capability to an existing Sandia synthetic aperture radar (SAR) system. We developed parametric modeling software for a radar operating in exocutter MTI mode. We began development of software tools for the specification and design of better MTI antennas. We modified an existing antenna to provide the two-phase centers that are necessary for

endocutter MTI techniques. We developed real-time software for collecting MTI data with an existing Sandia SAR system. We developed software for performing post-flight processing of MTI data. We conducted MTI data collection using the DeHavilland DHC-6 Twin Otter aircraft in conjunction with Sandia's modified radar system.

(1) *Developed requirements for adding MTI to an existing radar.* We developed a parametric model of a radar operating in exocutter MTI mode using the Matlab mathematical analysis package. This model computes basic algorithm performance figures (e.g., signal-to-clutter ratio) as a function of radar and aircraft operating parameters. The modeling software showed itself to be an indispensable tool for planning the flight tests that we conducted later in the fiscal year.

(2) *Modified radar software and hardware for MTI.* Exocutter MTI techniques require the radar to generate and record RF pulses at a frequency four times higher than what it was designed for. We overcame substantial technical hurdles to achieve this performance goal and to validate the operation of the radar in this mode.

Endocutter MTI techniques require the use of a displaced phase center antenna (DPCA) along with a multiplexed receiver. We modified an existing antenna and existing real-time software to provide this functionality.

(3) *Developed ground-processing software for MTI.* We used the Matlab mathematical analysis package to develop software for processing both exocutter and endocutter MTI range/Doppler radar images. This software does not have the capability to actually focus the moving targets within a scene, but it does provide a solid indication that we are recording high-quality MTI data. We used it daily during flight-testing activities to verify correct operation of the system.

(4) *Flight-tested the MTI radar function.* We collected both exocutter and endocutter MTI data using Sandia's modified radar and the DeHavilland DHC-6 Twin Otter aircraft. We conducted a total of twelve flights during the September 12–23 time frame, and every flight provided useful MTI data. Three ground vehicles were instrumented with

global positioning system (GPS) receivers and arranged in a variety of position and velocity combinations during the collection. We checked flight data daily to verify correct operation of the radar.

(5) *Developed moving target imaging requirements for linear motion.* The parametric model mentioned above facilitates MTI calculations that relate radar, aircraft, and target parameters. Some imaging requirements are included. An extension of this model will contain additional imaging requirements, but the details have not been worked out yet. We decided that the process of developing models for ground moving targets would be aided by real measurements, which we collected recently.

3516.080

Sampling and Sensing Systems for High-Priority Analytes

G. C. Frye, A. Sellinger, J. W. Bartholomew, R. J. Kottenstette, C. J. Brinker, G. C. Osbourn

This project focuses on redesigning current array-based sensing systems to optimize them for detecting high-priority analytes (HPAs) such as chemical weapon (CW) agents, CW precursors, and explosives in the presence of common interferents. Since the target HPAs have low volatility, their analysis will require modifications in adsorbent materials and surface acoustic-wave (SAW) sensor-array coatings. The team of investigators assembled to perform this project demonstrated leadership in the areas of SAW sensor systems, thin-film adsorbents and coating materials, pattern-recognition (PR) analysis, and chemical microanalysis, which makes this team uniquely qualified to take on this task. The materials and system optimization will facilitate development of low-power, microanalytical systems

(chemistry laboratory-on-a-chip) that could provide rapid, sensitive, and selective detection of these HPAs in truly miniaturized field-deployable units. Spin-off applications in environmental monitoring and industrial process control are likely for other classes of semivolatile chemicals (e.g., pesticides, sludges) that are notoriously difficult to monitor.

Accomplishments for FY97 included synthesis and testing of a new derivatized sol-gel coating for SAW sensors. We coated surfactant-modified and fluoroalcohol-derivatized sol-gel oxides onto SAW devices and tested them with volatile organic compounds (VOCs) and dimethylmethylphosphonate (DMMP), a nerve agent simulant that has a phosphonate functionality and a vapor pressure similar to Soman. We were successful in the synthesis of high-surface-area silica thin films ($> 1000 \text{ m}^2/\text{g}$) with controlled pore size ($\sim 2\text{--}3 \text{ nm}$) and site specificity for the adsorption and desorption of DMMP. We derived the thin-film surface area and pore size from the evaporation-induced co-assembly of silica and surfactant followed by pyrolysis. The DMMP site specificity results from subsequent silica surface modification with a hexafluoroalcohol (HFA) containing sol-gel monomer. In-house synthesis of this HFA monomer was a significant accomplishment. The HFA moiety is thought to serve two important purposes: (1) the hydroxyl group, having two adjacent trifluoromethyl groups, inductively promotes enhanced hydrogen bonding to P=O groups, i.e., DMMP, and (2) the hydrophobic fluoro groups significantly minimize the coating's sensitivity to water vapor as an interferent.

We performed selectivity and activity testing on the SAW devices by exposing them to low concentrations of VOCs and DMMP vapor. We significantly improved selectivity for hydrogen-bond basic compounds over our benchmark microporous oxide coating. The HFA-modified sol-gel coatings improved SAW sensitivity

to DMMP by over three orders of magnitude when compared to standard polymeric coatings such as polyisobutylene. SAW sensors coated with these materials exhibit highly sensitive reversible behavior at elevated temperatures (90°C), possibly leading to low detection levels for semivolatile analytes while remaining insensitive to volatile organic interferents.

In summary, we made great progress in both selectivity and sensitivity for modified sol-gel coatings for CW agent detection. We improved selectivity while sensitivity gains were estimated to be greater than 1000 times a nonselective yet standard polymeric coating such as polyisobutylene. Comparison to a very selective hydrogen bond acid polymer coating (provided by Pacific Northwest National Laboratory [PNNL]) indicated that the hydrophobic surfactant-templated (ST) sol-gel was 30 times more sensitive to DMMP (both sensors tested at 50°C). Thus, these films appear to have the potential to provide 10–100-fold greater sensitivities as compared with the best polymeric materials, as well as providing unique chemical selectivity based on both the surface chemistry and the size and shape of the porosity.

Publications

Other

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Automated Vegetation Height Measurement for Automatic Terrain Mapping

J. R. Fellerhoff, M. L. Yee, D. L. Bickel

Sandia demonstrated that interferometric synthetic aperture radar (IFSAR) accurately measures the tops of vegetation. A map of the tops of vegetation is sufficient for airborne users of terrain elevation information; however, troops or personnel in ground vehicles need to know the terrain below the vegetation. Many commercial and civilian map users require ground-level information rather than vegetation-top information, as well. Research from Sandia's High-Altitude Doppler Radar Altimeter (HIDRA) work shows that in many forested areas, radar altimeters receive a significant return from the top of the trees as well as the terrain underneath. We proposed to study the combination of these two radar techniques to measure not only the elevation of tree tops but also the terrain underneath.

IFSAR technology has the potential to satisfy the high demand for accurate and timely terrain data from both government and commercial entities. It is likely to become a necessary feature on most future imaging radar systems. Solving this problem could help keep Sandia in technological leadership in this extremely important area.

The understanding of the exact relationship between IFSAR and HIDRA data in vegetated areas is also an important problem for the new generation of weapon guidance systems based on imaging altimeter technology. This study will provide much insight into that relationship.

A third important result from this study will be the ability to detect, classify, and quantify vegetation regions in IFSAR elevation models. This could be important to automatic target recognition (ATR) in cueing the algorithms to use different recognition methods depending on the vegetation type and height.

In this first year we collected and processed IFSAR data from the bosque where I-25 crosses the Rio Grande near Black Mesa, south of Albuquerque. We also processed existing HIDRA data from the same flight path taken in September 1995. (HIDRA was unavailable in the first half of 1997.) Mapping the HIDRA data onto the IFSAR data showed there were many HIDRA ground returns in areas covered by trees. In a number of areas where the IFSAR data measured the tree profile, the HIDRA data provided a measurement of the underlying ground profile. We can then determine vegetation height by taking the difference of the IFSAR tree profile and the HIDRA ground profile. This demonstrated the basic capability of combined IFSAR and HIDRA data to measure both vegetation height and the terrain height underneath the vegetation.

inding technical solutions to environmental issues is a critical national challenge. The Environmental Sciences area, which emphasizes basic research, complements research on engineered processes, computational and information sciences, microelectronics and photonics, engineering sciences, and engineering with atoms.

Categories include site characterization, industrial ecology, and environmental science. Site characterization uses sensors to monitor several aspects of one environment, such as the air, water, and soil at a site. Industrial ecology projects reduce waste and harmful industrial by-products as well as increase energy efficiency without sacrificing the quality, reliability, and performance of a product. Environmental Sciences projects consist of basic research that supports breakthroughs in nuclear stockpile stewardship.

Sandians are working to develop environmentally friendly materials that will degrade into harmless components when they are no longer in use. These man-made coatings will be useful to a variety of industries. The degradable materials could be used to create nonlethal safeguard systems or in the microelectronics industry to degrade harmful waste products.

Cleanup of approximately 10,000 environmentally contaminated sites is a high priority for DOE. To optimize limited resources, researchers are developing a protocol for natural attenuation of metal and radioactive contaminants. Allowing natural processes to passively clean up contaminated sites will save time and money in this important effort.

Virtual modeling is being accomplished by meshing three-dimensional range data to produce surfaces in real time (inset). Such models enable virtual and robotic interactions in unknown or hazardous environments.

ENVIRONMENTAL SCIENCES

Development of Inexpensive Metal Macrocylic Complexes for Direct Oxidation of Methanol in Fuel Cells

D. Ingersoll

Fuel cells are being considered as alternative power sources for transportation and stationary applications. The degradation of commonly used electrode catalysts (e.g., Pt, Ag, and others) and corrosion of carbon substrates are making commercialization of fuel cells incorporating present-day technologies economically problematic. Furthermore, due to the instability of the Pt catalyst, the performance of fuel cells declines on long-term operation. When methanol is used as the fuel, a voltage drop, as well as significant thermal management problems, can be encountered, the latter due to chemical oxidation of methanol at the platinized carbon at the cathode. Though Sandia conducted extensive work on platinized electrodes for both the oxidation and reduction reactions, due to the problems mentioned above we have not fully developed fuel cells for widespread commercial use. Several investigators previously evaluated metal macrocylic complexes as alternative catalysts to Pt and Pt/Ru in fuel cells. Unfortunately, though they demonstrated catalytic activity, they found these materials to be unstable on long-term, and in some cases short-term, use in the fuel-cell environment. To improve the long-term stability of metal macrocylic complexes, we chemically bonded these complexes to the carbon substrate, thereby enhancing their catalytic activity as well as their chemical stability in the fuel-cell environment. We designed, synthesized, and evaluated these catalysts for O₂ reduction, H₂ oxidation, and direct methanol oxidation in proton exchange membrane (PEM) and aqueous carbonate

fuel cells. These catalysts exhibited good catalytic activity, long-term stability, and resistance to common poisons.

We used a procedure that we developed to synthesize several metal phthalocyanine polymer complexes (MPc). We prepared these catalysts by heating a mixture of 3,3',4,4'-benzophenone tetracarboxylic dianhydride, the metal chloride(s), and urea at 200°C for 2 hours. The complexes prepared were (CoPc), (PtPc), (Pt-RuPc), (Pt-MoPc), and (RuPc). We then mixed these materials with the carbon support, and they chemically reacted in an inert atmosphere to form a stable linkage between the carbon substrate and the macrocylic ring. We evaluated fuel cells of varying combinations of anodes and cathodes at 80°C with 30 psig H₂ and either 30 or 60 psig O₂. The anodes used in these cells consisted of either Pt-black, 10% Pt/Vulcan (0.25 mg Pt/cm²), 20% Pt/Vulcan (0.5 mg Pt/cm²), or 15% (Pt-RuPc)/Vulcan (0.035 mg Pt/cm² and 0.018 mg Ru/cm²). We assembled membrane electrode assemblies (MEAs) using various combinations of anode and cathode, and all had active areas of 40 cm². The fuel cell having the (Pt-RuPc)/Vulcan anode had slightly lower voltage than the other electrode combinations. However, because the precious-metal content is more than one order of magnitude less than in the case of the other systems, and considering the unoptimized nature of this MEA, these results are significant. At 500 mA/cm², this fuel cell with a Pt-black cathode exhibited a terminal cell voltage of 650 mV. A fuel cell built with an anode and a cathode, both composed of 20% Pt/Vulcan, exhibited a terminal voltage of 610 mV. In comparison to this, the fuel cell built with a 15% (Pt-RuPc)/Vulcan anode and a 20% Pt/Vulcan cathode has a terminal voltage only 60 mV lower, namely, 550 mV versus 610 mV. We also evaluated the performance of the cobalt

transition-metal phthalocyanine complex (CoPc) on heat-treated Black Peal 2000. The catalyst exhibits good catalytic activity for hydrogen oxidation.

We evaluated the stability characteristics of the novel catalyst in the PEM fuel cell environment using a 40-cm² MEA composed of a 15% (Pt-RuPc)/Vulcan anode and a 20% Pt/Vulcan cathode operated continuously at 80°C and 500 mA/cm². We monitored the terminal voltage of the cell as a function of time for the duration of the test. After 10,000 hours of continuous operation, there is no evidence of degradation of fuel-cell performance. We also found that periodic shutdown and restarting of the cell did not adversely affect its performance. The cell also displayed stable operating characteristics, which can be seen in the polarization behavior of this cell measured before and after 200 hours of operation.

We also studied the effect of common catalyst poisons by introducing CO, CO₂, and mixtures into the feed lines of the fuel cell after 7500 and 9600 hours of continuous operation. While we observed a decrease in terminal voltages, the fuel cell was not irreversibly harmed, unlike the behavior observed with more conventional catalysts. That is, we restored the terminal voltages to their initial value once we removed the contaminants from the feed. In addition, the performance loss with the novel catalyst is significantly less than that observed with the standard Nobel metal catalysts.

Publications

Refereed

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Designed Molecular Recognition Materials for Chiral Sensors, Separations, and Catalytic Materials

T. M. Nenoff, J. A. Shelnutt

The goal of this project is the development of materials that are highly sensitive and selective for chiral chemicals and biochemicals (such as insecticides, herbicides, proteins, and nerve agents) to be used as sensors, catalysts, and separation membranes. Sandia is using molecular modeling methods to tailor chiral molecular recognition sites with high affinity and selectivity for specified agents. The work focuses on both silicate and nonsilicate materials modified with chirally pure functional groups for the catalysis or separations of enantiomerically pure molecules. We are using surfactant and quaternary amine templating to synthesize porous frameworks, containing mesopores of 30 to 100 angstroms. We are using computer molecular modeling methods in the design of these materials, especially in the chiral surface-modifying agents. We are also using molecular modeling to predict the catalytic and separation selectivities of the modified mesoporous materials. The ability to design and synthesize tailored asymmetric molecular recognition sites for sensor coatings allows a broader range of chemicals to be sensed with the desired high sensitivity and selectivity. Initial experiments target the selective sensing of small-molecule gases and nontoxic model neural compounds. Further efforts will address designing sensors that greatly extend the variety of resolvable chemical species and forming a predictive, model-based method for developing advanced sensors.

(1) *Characterized currently available receptors.* A manuscript submitted to the *Journal of American Chemistry Society* gives a complete description of the three ester derivatives of zinc(II) tetra-cyclopropyl-porphyrin. The nitrophenyl esters of this chiroporphyrin act as a

"molecular Venus flytrap," whose different conformations can be described as "opened" and "closed." The closed form is induced when an axial group such as pyridine binds at the metal center. However, to induce these structural changes, the axial ligand must be of the correct size and shape. The resulting favorable interactions shift the equilibrium to the closed conformation, inducing a large-scale conformational change. The porphyrin macrocycle itself converts from the ruffled conformation to the domed conformation, resulting in changes in the visible absorption spectrum. The structural changes of the molecular Venus flytrap have been verified by x-ray crystallography and, in solution, by nuclear magnetic resonance (NMR) spectroscopy.

(2) *Designed, synthesized, and characterized improved chiral nonplanar porphyrins for molecular recognition.* We computationally considered many possibilities for synthesizing a highly enantio-selective molecular recognition site.

The Ni tetra(cyclopropyl)porphyrin meta-nitrophenyl ester is the first example of a nonplanar chiral porphyrin and the first chiral porphyrin with electron-withdrawing substituents that make it resistant to oxidation during catalytic oxidation reactions and increase its axial ligand affinity.

(3) *Coupled designed receptor porphyrins to silicate and sol-gel support materials by surface modification.* We completed work for our test porphyrin (which closely mimicked our designed porphyrins) and for a chiroporphyrin. The method for surface modification involves the silanol attachment of 3-aminopropyltriethoxysilane (APTES) to the surface of the pores. The porphyrin is then covalently bound to the exposed amine group of the APTES. We performed this procedure on acid-catalyzed silica sol-gel (amorphous) spheres, on the intralayer surfaces of Montmorillonite clay (2-D crystallinity) and on the pore walls of surfactant-templated mesoporous multichip module (MCM)-class materials. These are just a few of the

silicated materials that we synthesized with a variety of pore sizes; the others have differing pore size distributions, but fall into one of the three classes mentioned above.

Characterization studies included powder x-ray diffraction data (evidence that the support remains intact) and Raman data (evidence that the porphyrin remains intact). Raman studies compare the porphyrin in solution with it on each individual support. Our data show that the major peaks, indicative of the intact structure, remain the same. We carried out initial separation studies of 2-hexanol enantiomers on the supported Ni tetra(cyclopropyl) meta-nitrophenyl ester porphyrin.

(4) *Synthesized and characterized new chirally templated inorganic porous materials.* Our plan was to use chiral organic amine molecules as templates for the size and shape of pores in novel inorganic molecular sieves. Our idea was that the template would "imprint" its chirality (and size) onto the pore. Once the molecular sieve crystallized around the template, we removed the template, leaving a chiral pore in our sieve. Separations could be performed of ceramic mixtures because each enantiomer would have a different interaction energy with the pore, thereby allowing for separations of the mixture.

Working in the zinc phosphate phase space, we found that using a sugar molecule as a template, at a very defined temperature and reaction time, we can synthesize 3-D-pored structures. The mesoporous phase we synthesized is of great interest to us because of the very regular, unidirectional pore sizes.

Publications

Refereed

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Other

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3518.040

Real-Time 3-D and Heterogeneous Data Fusion

C. Q. Little, D. E. Small

This project creates a real-time world modeling method that dynamically creates and updates volumetric geometry as fast as current 3-D sensors can generate range data, while simultaneously fusing spatially registered heterogeneous data onto the surface model. This enables real-time interaction with remotely sensed data in an information-rich, 3-D environment. It also helps meet the growing demands for real-time visualization and data fusion in the areas of environmental mapping, remediation, and remote sensing.

The goal is to visualize characterization data in a 3-D setting. Such data include video image data, heat, radiation, ground-penetrating radar (GPR), synthetic aperture radar (SAR), and chemical and material makeup. Sandia began by generating 3-D maps or surface models using 3-D range sensor data. Next, we fused data from other sensors that are spatially referenced with respect to the scene with the surface model. This enabled the user to visualize and associate the heterogeneous data with its relative position in space.

This research increased the speed of geometry generation and heterogeneous data fusion to near-real-time rates. By doing so we increased the temporal relevance of the model (e.g., data that are seconds old instead of hours) and the user's ability to perceive and interpret data within the model (e.g., radiation maps made visible or calibrated video textured onto the geometry). We will be able to create a photorealistic world model as fast as the sensor data are generated. This opens up the possibilities of interacting with and visualizing rapidly changing environments.

The goal of this project was to visualize characterization data in a 3-D setting in near real time. Real time in this

sense refers to the time needed between collecting the data and presenting it to a user. Along these lines, we accomplished three main milestones: (1) to build a volumetric viewer to display 3-D data, (2) to demonstrate projecting other data, such as images, onto the 3-D data, and (3) to display both the 3-D and projected images as fast as the data became available.

We examined several ways to display 3-D surface data. The most effective to date is generating polygonal surface meshes. We are creating surface maps from this data and passing this to a commercial 3-D geometric display package.

In parallel with this, we developed a method to project real-time images onto the surface created. A key component is mapping the data to fall on the correct surfaces, which requires *a priori* positional information, along with calibration of the camera and lens system.

To achieve a continuous display, we modified a 3-D range sensor to provide a continuous stream of range data. The processing for surface rendering currently is faster than the cycle time for the range sensor (roughly 5–10 Hz). We added the projected texture independently.

We experimented with standard video images because of the ease in getting this equipment. We recently added a thermal intensity camera for a different heterogeneous data type. Other sensors that produce a 2-D image, such as a gamma camera, would be trivial to add. Sensor data from point sources, such as chemical sniffers, can be added directly as a geometric entity or mapped on the surface through a simple pseudocolor intensity scheme.

Publications

Other

Little, C. Q., and D. E. Small. 1997. "Real-Time 3-D Imaging with Heterogeneous Data." SAND Report, in progress.

Designed Synthesis of Controlled Degradative Materials

T. A. Ulibarri, M. J. Carr, S. H. Scott, J. L. Zuberky, R. S. Saunders, J. G. Curro, T. R. Guess, D. R. Wheeler

Sandia will develop polymeric materials that contain weak links that provide degradation capabilities activated only by specific keys. Weak links are specific functionalities that are susceptible to degradation and are placed within the backbone of a polymer to provide readily cleavable sites. We will generate materials for three general applications: (1) nonlethal deterrents, (2) removable encapsulants, and (3) readily recyclable/environmentally friendly polymers for structural and thin-film applications. In all three applications, a great benefit would result from the successful development of materials that can be controllably degraded into smaller components, thus providing facile removability and recyclability. In addition, we will use commercial-based polymer formulations blended with sensitizers to create another class of readily degradable systems. While these systems may not provide as intricate a key system for degradation, they should provide workable materials for large-scale applications in a more timely manner than the weak-link systems. To understand the possible property changes manifested due to the weak-link incorporation, we will combine classical density functional theory (DFT) with Polymer Reference Interaction Site Model (PRISM) calculations. We will correlate the information on polymer structure and thermodynamic properties generated through these modeling efforts

with experimental mechanical characterization. Through this correlation, we will utilize a feedback loop for the synthetic effort to optimize the production of second-generation super-slick materials. The ultimate goal of this project is to generate families of degradable materials that can be applied anywhere in nonlethal deterrent systems and as removable encapsulants to the development of process-controlled sorting of recyclable materials in the commercial market.

We successfully synthesized and characterized weak-link-containing polyethylene oxide-based polymers. These materials contain the weak-link moiety at both random and regular spacing. We determined that the most important factor is the general spacing between the weak links, not the regular or random placement, such that the degraded material is of sufficiently low molecular weight to ensure high solubility and therefore removability. The best materials synthesized to date are polymers that are susceptible to chemical or enzymatic (esterase) degradation. Modeling of the system, by both wall PRISM calculations and a more rigorous computational technique involving DFT, shows that there is a distinct change in the structure or density profile of the polymer at the interface with changing molecular weight. This change in the polymer structure is manifested as a change in the surface properties of the polymer (i.e., a change in the lubricity of the material), as measured by a torsion shear-test method developed during this program. There is a marked increase in the coefficient of friction with decreasing molecular weight. Through this year's synthesis, we generated modeling and characterization efforts of first-generation super-slick materials containing weak-link moieties.

Rapid Screening of Complex Chemical Samples via Capillary Array Analysis

D. S. Anex, D. W. Neyer, D. M. Haaland, K. M. Alam, J. S. Schoeniger

Complete characterization of complex chemical samples often requires a series of time-consuming analyses. A carefully designed parallel analysis scheme would rapidly obtain and interpret a unique chemical signature from a complex sample. To achieve this, Sandia is developing a novel approach to sample analysis based on simultaneous separations in a parallel array of capillary columns. Our main emphasis is on capillary electrokinetic (EK) techniques, which are ideally suited for implementation in an array format.

We built a column array instrument to simultaneously detect signals from each column using laser-induced fluorescence. Each particular component of a sample traverses each column in a different characteristic time. The collection of traversal times for all components on all columns constitutes the chemical signature for a particular sample. Chemometrics is required to interpret this complex signature and maximize the information obtained. It will also serve to guide the optimization of each individual column to probe a particular broad chemical characteristic of the sample.

This low-cost, compact, parallel analysis approach will lead to field-deployable devices with capabilities beyond current laboratory instrumentation. This new capability will enable rapid screening

and exacting molecular-level characterization of complex chemical samples encountered in environmental site characterization and monitoring. It will also advance industrial process control capabilities, as well as contribute to wider DOE and DoD national security missions. It will exploit Sandia's strengths in capillary separations and parallel data collection demonstrated in development of a multiple-capillary DNA sequencer and will be augmented by expertise in molecular recognition and chemometrics. This project will also be a platform for demonstrating concepts for powerful microfabricated devices, where highly parallel analysis can be implemented.

The accomplishments in the first year fell into experimental and statistical categories. Experimentally, we performed single-column experiments to test separation characteristics and to obtain dispersed fluorescence signatures. Statistical tests analyzed the stability of retention times and the need for internal standards. Also in the experimental arena, we designed, built, and tested the multiple capillary instrument. We ran a complex sample of aromatic compounds of environmental interest on the instrument with different mobile phases in each column.

The first step of the project was to develop a separation strategy for the multiple capillary instrument. We determined that the unique stationary phases to be used in the instrument will be reversed-phase, normal-phase, and cyano-derivatized. The elution order will be different on each column, with additional control of the separations obtained through optimization of the

mobile phase composition (pH and organic content, for example).

We chose as test samples mixtures of polycyclic aromatic hydrocarbons (PAHs) and nitrogen-containing aromatic compounds (NCACs). These compounds are significant environmental pollutants that have been targeted by the U.S. Environmental Protection Agency. One significant source of both PAHs and NCACs is creosote-contaminated sites. Soil extracts of creosote-contaminated soils are available for testing the power of the multiple-capillary approach.

Initial single-column studies concentrated on retention time stability and fluorescence measurements. Dispersed fluorescence studies were not in the initial project plan, but were added during the early stages of the project. We performed capillary electrochromatography (CEC) separations followed by dispersed fluorescence detection on a collection of 16 PAHs and 9 NCACs to determine individual spectral signatures. We will analyze the data using chemometrics to design the optimal set of filters to use to obtain a "second dimension" of data from fluorescence spectral signatures of the separated components as they elute from the column.

We performed chemometric analysis on an extensive data set previously collected by our university collaborators. Analysis of the retention time stability showed a systematic increase in retention time with column age (over 240 consecutive runs), but showed that internal standards can be used to correct for this deviation. Column reproducibility will also have to be challenged after introduction of "dirty" field samples. Chemometric analysis similar to these statistical studies will continue throughout the project.

We successfully designed, constructed, and tested an eight-capillary instrument. This task involved the construction of the instrument incorporating an ultraviolet (UV) laser excitation source, writing of LabView control and data-acquisition software, and initial demonstration of the simultaneous collection of data from eight open-channel capillaries.

The project then turned to the separation of neutral compounds on the multiple capillary instrument. To analyze a target test sample consisting of a mixture of the 16 PAHs and the 9 NCACs, the initial demonstration used the same (reversed-phase) stationary phase in the packed columns and varied the mobile-phase composition between them. We used organic compositions ranging from 50% to 99% acetonitrile in aqueous buffer. With this collection of mobile phases, different columns provided the best information on different ranges of retention time, with the data as a whole used to analyze the complete mixture.

We will continue to concentrate on the PAH and NCAC target compounds and actual creosote-contaminated soil extracts as the representative environmental test samples.

Publications

Other

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Mechanistic Models for Radionuclide Desorption from Soils

P. V. Brady, M. D. Siegel, D. J. Borns, G. E. Bujewski

DOE is responsible for roughly 10,000 contaminated sites, but will have the means to clean up only a fraction of these. The remainder will receive very little active remediation. Remediation efforts should be directed only toward those soils and groundwaters where natural processes are unable to attenuate contaminant toxicity. A number of technical protocols exist to quantify the site-specific potential for natural attenuation of organic contaminants, but there are no such protocols for sites contaminated with metals and radionuclides. Sandia is developing a technical protocol for natural attenuation of metals and radionuclides and is presently addressing the primary scientific data needs. Specifically, we are working to establish the fundamental controls on natural attenuation of sorbed radionuclides in soils and groundwaters by measuring (1) desorption rates of Cs from

clays, (2) U (and Pb) desorption from iron hydroxide, and (3) Sr and Am exchange from calcium carbonate minerals. We will use these results to develop a technical protocol that will ultimately provide the means to defend reliance on natural attenuation for the remediation of contaminated soils and groundwaters in the Department of Energy (DOE) and non-DOE sectors.

We measured desorption mechanisms and rates for the primary contaminant metals and radionuclides present in DOE soils and groundwaters. Specifically, we measured desorption of Cs from clays under a variety of conditions, U and Pb from iron hydroxide, Cd and Sr from calcium carbonate, and Pb from natural soils in the presence and absence of microorganisms. We are using these results to formulate a technical protocol for using natural attenuation to passively remediate DOE and non-DOE sites contaminated with radionuclides and metals. The Environmental Protection Agency (EPA) and Nuclear Regulatory Commission (NRC) have offered collaborative help in this effort. To help establish Sandia as a center for natural attenuation work, we ran a workshop that was heavily attended by a wide variety of

regulatory agencies and other national laboratories. We were also recently asked by DOE EM-40 to be the lead lab for development of a DOE complex-wide natural attenuation protocol, and to specifically coordinate the efforts of a number of national laboratories (Lawrence Livermore National Laboratory, Los Alamos National Laboratory, Oak Ridge National Laboratory, Pacific Northwest Laboratory), EPA, and NRC.

Publications

Refereed

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Other

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Brady, P. V., and D. J. Borns. 1997. "Report from the Sandia Workshop on Natural Attenuation of Metals and Radionuclides." SAND Report, draft.

The Sandia mission of stockpile stewardship requires a superior understanding of how to manage the risks and ensure the reliability of nuclear weapons and waste. This research area develops methods and tools as well as new components and systems to support the Sandia mission.

Risk and Reliability encompasses four categories of study: (1) predicting risk and reliability for systems and components; (2) studying how products and technologies age; (3) developing methods, techniques, and tools to evaluate how design changes affect reliability; and (4) developing approaches and tools to detect potential problems and to maintain equipment and systems.

Micromachines show great potential for making weapons smaller and less expensive. The failure mechanisms and reliability of this new technology must be resolved before it can function in critical weapons systems. Sandians are characterizing these aspects of micromachines. Advances in this area have great commercial as well as defense potential.

The project focuses on investigating a means of detecting when electrical components are about to fail. It has been determined that electrical devices emit signals known as failure precursors that warn of impending failure.

Understanding this phenomenon and applying it to stockpile weapons will increase the life-span and reliability of these and other critical systems that rely on integrated circuits.

A structural (metal component) failure warning of a microelectronic component's impending demise. In a world of low-volume production and use, failure precursors offer the potential to predict individual component failures.

RISK & RELIABILITY

Reliability Degradation Due to Stockpile Aging

D. G. Robinson

This project involves the development of a new method for characterizing the reliability and uncertainty of systems with time-dependent failure modes associated with stockpile aging. The aging analysis technique most often used today, Arrhenius analysis, is well known and dates back to the late 1800s. Methods of analysis such as Arrhenius have been described as deterministic, which is to say that once the system is deployed in its isothermal environment, its lifetime can be determined through calculation. That is, random effects of operating environment, material properties, etc., are considered unimportant. A major source of the error in using these very traditional reliability methods, even time-dependent methods, is that all these techniques view system operation as a go/no-go situation. The current practice is to test a system/subsystem and, if it is operating within specifications, label the test as a success. No attempt is made to monitor the degradation of the system performance characteristics as a function of system age and relate these observations to stockpile reliability. The alternative proposed here suggests that by monitoring system performance through testing, in conjunction with science-based modeling, it is possible to characterize time-dependent changes in material properties and identify

aging-related problems earlier with fewer test resources. The goals of this research are to develop a methodology that will permit time-dependent consideration of uncertainties in material behavior, processes, and operating conditions, and data from a variety of test programs to be incorporated into the analysis, and to permit engineers to identify critical performance parameters that need to be closely monitored and controlled. This will allow stockpile aging problems to be addressed in an anticipatory, coordinated effort rather than waiting for the problem to critically manifest itself.

The specific application of this effort is related to modeling the aging of electronics due to thermomechanical fatigue and corrosion. In particular, the width of aluminum interconnects in the submicron regime are now becoming common in the integrated circuit (IC) industry. This trend has brought a need to assess the reliability of these interconnects as they are affected by a failure mechanism known as *stress voiding*. Stress gradients in the metallization are caused by mismatch of thermal expansion coefficients, and these gradients are known to drive mass transport and void growth. The thrust of our work is to develop a general suite of reliability and uncertainty analysis software tools and to apply these tools to this problem and the related electromigration failure process. Progress this year involved the coding of alternative reliability analysis methodologies into a suite of Maple software routines. Specific techniques fall into the general categories of Monte Carlo and a

variety of analytical methods such as First-/Second-Order Reliability Methods, Advanced Mean Value (+), and Chen-Lind and Wu-Wirsching Fast Probability Integration techniques. We incorporated each of these methods into a generic Maple library. We validated the library routines by comparing the predicted uncertainty levels with published results from a variety of accepted test cases. In all cases, the routines matched or exceeded the accuracy of the published results. We then applied the Maple software algorithms to statistically characterize the life of a general interconnect within an IC and also to statistically characterize the time-dependent performance of a diode as atmospheric corrosion steadily degraded the diode response over time. In addition to the actual coding of the analysis algorithms, we prepared a survey report that outlines in fundamental terms the historical and technical basis for each of the analysis techniques. We used a specific application related to stress voiding throughout the survey.

Publications

Other

Robinson, D. 1997. "A Survey of Probabilistic Methods Used in Reliability, Risk, and Uncertainty Analysis-I." Sandia Technical Report, in progress.

Integrated Approach to Develop Microelectromechanical Systems (MEMS)

D. M. Tanner, W. P. Eaton, N. F. Smith,
K. A. Peterson, D. J. Bowman, S. L. Miller

The burgeoning new technology of microelectromechanical systems (MEMS) shows great promise in the weapons arena. We can now conceive of microgyros, microsiret systems, and micronavigators that are extremely small and inexpensive. Do we want to use this new technology in critical applications such as nuclear weapons? The answer to this question drives us to understand the reliability and presently unknown failure mechanisms of MEMS. By solving MEMS reliability and failure issues, Sandia serves its primary defense program customer and provides applicable solutions to industry.

We assembled an interdisciplinary team that integrated the individual research areas of failure and performance analysis, reliability characterization, and wafer-level reliability. This work has not been attempted before and will produce the knowledge essential to maintain world-class MEMS status at Sandia. The overall goals of this work are (1) to perform statistical characterization, (2) to identify failure modes, (3) to develop reliability test structures, (4) to develop reliability models that account for temperature, humidity, cycles, operating speed, etc., and (5) to develop failure analysis tools for MEMS.

We finished fabricating the first test structures in early fall. After release, the initial check verified functionality of the structures, a crucial step in our effort to test large numbers of MEMS.

Our greatest achievement this fiscal year was the development of the world's only capability to simultaneously test and acquire data from 256 micromachine devices. This system, SHiMMER (Sandia High-Volume Measurement of Micromachine Reliability), is composed of an x - y positioning table with 24-pin dual in-line package (DIP) sockets to mount the packages, a camera and microscope optics, video recorders, a monitor for

diagnostics and data storage, waveform generators to electrically stimulate the MEMS devices, and a computer with software developed to control the reliability test.

SHiMMER has the advantage of being completely flexible so that many different types of micromachines and test structures can be tested. We will use SHiMMER to identify various failure modes that are relevant to MEMS devices such as mirrors, torque converters, locks, and shutters.

Using SHiMMER we completed the first-ever reliability lifetime test on a surface-micromachined microengine. We started with a record-breaking 30 microengines, stressed the engines at 36,000 RPM, and examined functionality at 60 RPM. In the data from this test, we observed an infant mortality region, a low-failure-rate (useful life) region, and perhaps the beginning of a wear-out peak.

We decided to use the Sandia microengine, which consists of two comb-drive actuators (x and y) coupled to a gear rotating on a hub, as our test structure. Four microengines, each rotated 90 degrees from the adjacent engine, define the reticle set. To allow separation of comb-drive effects from gear effects, one of the microengines is gearless. Also, to incorporate a fiber-optic monitoring system, we notched a tooth on one of the engines.

In the design of the reliability test structures (RTS1), we actually exceeded our milestone by developing two designs with different comb-drive actuators. The second, newer design used an improved but not yet tested comb drive developed for the five-level process that we adapted to the four-level process. The choice for using the microengine as a test structure was driven by the fact that this is the actuator used on all Sandia designs. If there are any reliability issues with the microengine, it affects a broad spectrum of the Sandia MEMS program.

We identified a major failure mode that is affecting our ability to perform experiments using SHiMMER. We discovered that the packaging process causes failure in a very high percentage (sometimes 100%) of these microengines.

Traditional packaging processes were designed for microelectronics that do not have moving parts, and it is evident that some aspects of the process may be detrimental to MEMS. We performed controlled experiments that indicate there is yield loss both after die attach and again after wire bonding. We suspect that the outgassing of epoxies may be a problem, as well as the ultrasonic bonding technique and handling.

We used two new scanning-electron microscopy (SEM) techniques to study the microengines. The first was passive voltage contrast, where no external voltage was applied to the packaged part and all the pins were grounded. Contrast arose from the fact that electrically isolated elements attained a different potential, due to charge injection from the electron beam, from that of grounded elements.

The second new technique employed was active voltage contrast, wherein we applied external voltages to microengine elements as they were examined in the SEM. While the electron beam seemed to interfere significantly with a few microengines, as found in previous work, certain engines were successfully run for several hours in the SEM.

Publications

Refereed

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Precursors to Failure of Oxides and Metal Lines in CMOS Technology

D. M. Tanner, S. H. Yazzie, L. W. Irwin,
W. F. Filter

Sandia is proposing a paradigm shift away from statistical reliability toward individual part reliability. In the past, we did long-term, expensive, large-group lifetime tests to predict the reliability of electrical components. We are moving toward a model-based methodology that uses test structures to predict the reliability of components as a group. However, both of these strategies treat component reliability statistically and are valid only for large numbers of parts. This is not a complete methodology in a world of low-volume production and use. We propose to use electrical failure precursors to tell when individual devices are going to catastrophically fail. An electrical failure precursor is any electrical signal that gives warning of a component's impending demise.

Likewise, electrical precursor signals from failing microelectronics would provide similar warnings of failure, if only we were able to recognize and model them. This would result in major benefits: (1) ability to characterize individual component reliability, thereby allowing a small number of parts to be used, (2) ability to use components until near the end of life with sufficient warning to procure replacements (such as through block upgrades), and (3) ability to automate reliability surveillance, possibly resulting in components that monitor themselves or in integrated circuits (ICs) that monitor system or subsystem reliability. In a world of increasing lifetime expectations from a smaller stockpile, the understanding and implementation of a science-based reliability precursor detection and characterization scheme might allow us to have longer-lived parts with better-characterized reliability.

Therefore, our overall goal is to gain an understanding of electrical failure precursors for insulators and conductors in ICs, to model these precursors, and to create a method for predicting failure times based on these models.

We were extremely successful this year in meeting our first set of project milestones that involved detecting precursors from a wide range of samples and determining the frequency of precursor occurrence. We are now working on the electrical characteristics.

Most complementary metal oxide semiconductor (CMOS) logic and analog devices operate at 5 V or less, which translates to an electric field of 5×10^6 V/cm or less, across the gate oxide. Silicon device reliability engineers, however, routinely break down gate oxides at much higher fields, at times exceeding 12 MV/cm. The failure mechanisms at the high field are not representative of failure mechanisms nearer to operating conditions since there is no physical basis for that assumption. However, stressing near-operating conditions is typically impossible due to time constraints—the stress may take tens of years to fail the part!

The solution is to stress at high temperature and use thermionic field emission for acceleration to failure. We calculated and then verified by experiment that at low field, 5 MV/cm and below, thermionic-field (TF) emission greatly dominates over Fowler–Nordheim (FN) tunneling. The FN tunneling is the most widely used technique for evaluating gate-oxide quality and reliability, mainly because it is easier to perform experiments. However, we showed that the high-temperature technique is physically reasonable and allows stressing of oxides nearer to operating conditions.

We succeeded in detecting precursors to dielectric failures at high-temperature stressing at moderate field in the oxide, 8 V/120° or 6.7 MV/cm. We see the precursor as a change in the noise characteristics of the gate current as the capacitor nears failure. We confirmed that dielectric failures at moderate fields, close to product-operational fields, is essentially thermally activated, and the applied field merely supplies the electrons. This is an important fundamental finding.

In summary, we observed the oxide precursor signal in 86% of the failures, we observed warning periods of roughly 1% of the lifetime, and we confirmed the physics to accelerate at high temperatures.

Current best physical models of electromigration show two accelerating factors, current density and temperature. To observe the precursor signal, we performed an electromigration test on a standard National Institute of Standards (NIST) electromigration test structure. We forced a stressing current through a metal line, achieving a target stress temperature by joule self-heating. We periodically measured (approximately every 175 ms) percent change of resistance (ΔR_o) in the metal line and compared that to its initial resistance at room temperature. We used a failure criterion of ΔR_o greater than 10%; at that point, we recorded time-to-failure. As the metal line neared its failure point, we observed radical fluctuations in ΔR_o as precursors to ultimate failure.

We accumulated the data from the current CMOS6 process electromagnetic (EM) test structures (M1). Precursors were evident on all 80 samples. Seeing the precursor 100% of the time was very promising. The precursors generally occurred between 80% and 95% accelerated lifetime of the metal lines, which means we would have 5–20% of the lifetime warning.

We observed these characteristics in the precursor data: (1) the value of R_o increased in amplitude, which implies higher values of resistance as the line fails, (2) the initial change of slope at onset of the signature might be useful as a warning point, and (3) precursor resistance change was always positive, which implies higher resistance near failure.

In summary, we observed the electromigration precursor signal in 100% of our samples, and we observed warning signals of 13% of the part lifetime. This will allow us to develop the predictive models needed to apply this technique in future weapon applications.

An Extensible Object-Oriented Framework for Risk & Reliability Analysis

G. D. Wyss, R. Vandewart, R. L. Craft

To assess a system's risks, an analyst must understand the system's dynamics and structure and have expert domain knowledge (particularly viable faults and attacks). The large volume of information required can obscure the system-wide effects of changes in a given system element. This project is developing an extensible tool to support risk assessment of multidisciplinary systems. The project is establishing the requisite theoretical basis for an object-oriented risk analysis approach. In this approach, each system element is represented by a risk object that contains a "knowledge base" about the element's failure modes, support requirements, and spatial and temporal characteristics. In addition, each object contains pieces of "generic" risk models that can be automatically assembled to form system risk models. Through a blend of object-oriented system modeling, simulation, and expert decision aids, the tool will build on proven Sandia assessment techniques and will provide a framework for the capture and presentation of current and future expert risk knowledge. As every risk analysis model is currently "hand-tooled," encapsulating domain-specific knowledge into risk objects will enable risk analysts to generate studies more quickly and with greater confidence that they have not omitted important risk sources, thus spending less to obtain a better product.

The project team met with potential users of the system to develop usage scenarios and to obtain analyst input for the tool development process. The team

also evaluated several existing object-oriented analysis methodologies to determine their compatibility with the needed risk and reliability analysis methods. All existing methods were found to be wanting, but we found a combination of the Schlayer-Mellor and Rumbaugh methodologies to have favorable characteristics for this project, so we took this hybrid methodology as a point of departure for the methodology development task for this project. From here, work began on a new risk-compatible, object-oriented analysis methodology that would allow for hierarchical decomposition of a system at either design or implementation. Furthermore, the methodology should enable the analyst to embed small risk models within objects that are either deterministic (i.e., *A* causes *B* to happen) or probabilistic (i.e., *C* happens with probability *p*). A risk model can then cause a state change within this object, generate events that may cause state changes in other objects, or modify attributes within either this object or others. These goals have been largely realized in the methodology that is being finalized for implementation in software within the project.

The second part of the methodology development task is to ensure that the object methodology being developed is compatible with various common risk and reliability analysis methods. The project team concluded that there are two principal classes of analysis methods: inductive methods (e.g., Failure Modes and Effects Analysis and Event Tree Analysis) and deductive methods (e.g., Fault Tree Analysis). For both classes of methods to be usable from within this object-oriented analysis methodology, the individual objects must be able to answer two types of external interroga-

tion: (1) deductive interrogation ("Here is a condition related to your behavior that must be avoided. What are all of the ways that it can occur?"), and (2) inductive interrogation ("A new condition is being imposed upon you. What are all of the possible paths that you can follow as a result of this change?"). The methodology developed by the team meets these requirements.

We tested the methodology by handworking example systems that include aspects from a variety of technology domains. Part of the solution of these sample problems consisted of a storyboarding process where the information that will be required of the analyst is listed at each step in the analysis. We generated draft user-interface screens to determine whether methodological changes are warranted in order to best satisfy the user requests before the methodology is "cast in concrete."

The last major activity is implementation of the methodology in software. We specified a basic architecture and the high-level object design for the program infrastructure of the Automated Risk Assessment Tool (ARAT), purchased and installed software, and assembled an implementation team. We will implement the database of objects on a SUN/Solaris server platform and will provide a Common Object Request Broker Architecture (CORBA) interface to clients. The Object-Oriented Data Base Management System (ODBMS) for the application will be Versant; we held a training class for this product at Sandia in July. We generated draft functional requirements for ARAT that describe the user's conception and usage of the system. (The software will be presented to the user as a Web application compatible with current Web navigators such as Netscape.)

Risk-Based Characterization of Network Vulnerability

L. Swiler, C. A. Phillips, T. Gaylor

This project was motivated by the need for a better methodology to perform risk and vulnerability analyses of computer networks. This problem is extremely important to the military and civilian infrastructure today. The purpose of this project is to create a systematic analysis approach that can be used by persons with limited expertise in risk assessment (1) to examine how an adversary might be able to exploit identified weaknesses, and (2) to assess the universe of undesirable activities that an adversary could accomplish, given that they were able to enter the network using an identified weakness. The original project proposed extending probabilistic risk assessment (PRA) methods to systematically catalog and rank known vulnerabilities and attacks. Sandia thought that since PRA methods are able to examine how individual faults can either propagate into or be exploited to cause unwanted effects on systems, PRA could provide insights to help design secure networks.

Sandia identified some unique characteristics of networks that limit the use and applicability of traditional PRA methods such as fault trees and event trees. We now propose an approach for characterizing risks based on a state-space graph of the system, which identifies various physical and logical locations where the attacker can be present, along with the level of user access the attacker has obtained. Transitions between states are represented by attack arcs with a certain probability of success or cost. We propose to use analysis techniques such as shortest-path algorithms and simulation to calculate the risk measures of interest, such as the attack path with the highest probability of success. This report presents the work done in FY97, including the development and demonstration of our

method, the creation of a test network in the Information Technology Lab, and our current research in definition and generation of the attack graph. We also identified a future research plan.

We accomplished the following in FY97:

(1) We documented the classes of networking components (e.g., workstations, routers) and network service applications (e.g., mail services, firewalls) that are vulnerable to attack, the classes of known attacks, and the current classes of defenses that are used to deter or repel these known classes of attacks.

(2) We identified the characteristics of networks that need to be incorporated into a risk assessment (RA) method and examined the applicability of existing techniques such as fault trees, event trees, and influence diagrams for network vulnerability modeling. We constructed a list of "ideal characteristics of an RA method" for network vulnerability, including the ability to model dynamic aspects of the network (e.g., virtual topology changing), dynamic behavior of the attacker (e.g., learning), the ability to handle multiple simultaneous events or multiple attacks, the ability to represent user access controls, and the ability to represent time-dependent, ordered sequences. We constructed example fault trees for unauthorized root access, failure of a file server to provide needed data or services, and an attack on a router.

(3) Given the limitations of PRA methods, we developed a graph-based approach to model network vulnerabilities. Each node in the graph will represent a possible state that the attacker could be in. A node will usually be some combination of physical machine, plus user access level. For example, a "normal user on SUN workstation #2" could be one node. From this node, the attacker could go to the node "system administrator on SUN workstation #2" using a variety of attacks. Or, the attacker could go to other nodes, depending on the topology of the network. The arcs in the graph will represent attack methods or

normal user transitions (e.g., a user may be able to log on to another machine if he/she has a valid account on that machine).

Our method involves the generation of an "attack graph" that we will build from attack templates and the physical network topology and configuration. The attack templates will contain information about the stages or steps an attack takes. For example, a password-guessing attack could involve sniffing the password, or getting access to the encrypted password file by e-mail or ftp and then using a password-cracking program on it. These stages would be matched to the actual network and instantiated in the attack graph if present (i.e., if the network were broadcast Ethernet so one could install a sniffer). As a preliminary tool for analyzing the graph, we chose a shortest-path algorithm. If we attach a probability or cost to each arc, a shortest-path algorithm can find the attack path with lowest or highest probability of success or cost. General consensus from experts we have talked to is that this state-space analysis should work well for enterprise-level (commercial or military) networks with a system administrator who is not a security expert.

To test our ideas, we created a test network. We created a graph of an attacker trying to get access to restricted data on a file server in this network and actually tested some of the attack methods and defenses. We demonstrated how the graph approach could be used to create a probabilistic model of an attack on an individual target.

Publications

Refereed

Painton, L., T. Gaylor, J. Camp, C. Phillips, and G. Wyss. 1997. "Risk-Based Characterization of Network Vulnerability." *Position Papers for the IEEE Computer Society/CERT 1997 Information Survivability Workshop 1* (San Diego, CA, 12 February): 62-64.

Enhancing Risk Analysis Using New Mathematical Structures

A. J. Cooper

The input data for probabilistic risk or safety analyses (PSAs) can involve considerable subjectivity, especially for abnormal-environment exposure. It is particularly important that the potential for abnormal-environment exposure and the attendant input subjectivity be handled in as meaningful a manner as possible, especially in high-consequence operations. This project addressed innovative approaches utilizing new mathematical structures for enhancing conventional PSA approaches. We evaluated the approaches studied for applicability to particular types of safety situations. The intent was to provide a more comprehensive "tool box" for analysts and to provide written information and software for ease of applicability.

We began this year's work by conducting a literature search for mathematical structures that we considered for various applications and devoted considerable time to developing some of our own origination. We identified eight general structures:

(1) A "Contest" tool, which allows two or more entities to compete for success (or failure). The mathematical result is the possibility of succeeding for each entity.

(2) A "Weighted Sum" tool, which allows a weighted accumulation of factors such as safety program attribute metrics and a "sigmoid" (gradual transition)-based comparison to a goal.

(3) Fuzzy "anding," where the satisfaction of the "and" logic has a degree, rather than a crisp yes or no.

(4) Fuzzy "oring," where the satisfaction of the "or" logic has a degree, rather than a crisp yes or no.

(5) Min/Max interval length logic, where the interval bounds on a range of possible abscissa values can be "stretched" along the abscissa.

(6) Min/Max ordinate logic, where the smallest ordinate value of a collection at each abscissa point determines the result, or the maximum value at each abscissa point determines the result.

(7) Implication operators, where the implication represents what is happening implicitly in the logic at a particular gate.

(8) Composition operators, which are a mechanism to propagate fuzzy possibilities and probabilities through a logic tree.

All of these can provide possibilistic information processing as well as probabilistic (multiple-value degree membership as well as probability distributions).

In formulating inputs from engineering expertise, we incorporated the ability to portray uncertainty, the ability to portray possibility, and the ability to

weight inputs according to "expertise," and maintained logical consistency in developing a specific algorithm. The inputs are intended to be provided by expert judgment of either bounds or by possibility membership functions.

We also developed a constrained mathematics formulation that probably led to exact solutions for the bounds on uncertainties that were mathematics-dependent.

Publications

Refereed

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Other

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rojects that promise dramatic impact on national concerns — such as health care, transportation, and counterterrorism — constitute the National Grand Challenges. High-risk studies in all areas are encouraged.

The National Grand Challenge project is developing an autonomous microscale chemistry laboratory that will detect explosive chemicals. Applications for such tiny chemical sensing and analyzing units are widespread. They could include monitoring nuclear materials as well as chemical and biological weapons on the battlefield, and detecting landmines and environmental contaminants, in addition to numerous other uses.

NATIONAL GRAND CHALLENGES

Within the microchemical laboratory unit, the preconcentrator serves to collect and concentrate the chemical species of interest for subsequent detection. This device comprises a chemically selective absorbing layer (not shown) on a micro-machined suspended silicon nitride membrane with a photolithographically patterned heater and temperature sensor. After sufficient material has accumulated on the absorbing layer, the heater drives it off for analysis downstream. The thin silicon nitride membrane permits rapid heating with minimal power consumption.

Science on the Microdomain

T. A. Michalske, C. C. Wong, W. G. Wolfer, M. E. Warren, M. H. Crawford

The ability to shrink sophisticated chemistry laboratories to pocket-calculator size and smaller will revolutionize chemical detection in a manner similar to the way that integrated circuits (ICs) revolutionized information technology. Sandia can lead this field because we have the science and technology base to address all aspects of complex microsystems. We demonstrated our expertise in silicon micromachining, microsensors, and photonics, and are receiving significant external recognition for our accomplishments. However, as our recently completed Integrated Microsystems Roadmap points out, several critical scientific frontiers must be tamed before we can capitalize on the substantial military and intelligence-based business opportunities offered by this rapidly developing technology. The goal of this project is to provide the technical focus needed to ensure Sandia's leadership in the invention and application of the MicroChemLab (μ ChemLab). In conjunction with two other Grand Challenge projects, we will demonstrate the world's first mobile, autonomous μ ChemLab for explosives chemical detection.

We propose a focused laboratory thrust on the science of the microdomain. This regime of very small sizes (roughly at 0.1 mm and below) is new territory for machines where normal intuition and standard engineering models cannot be scaled to predict performance, reliability, aging, or manufacturing. This project will develop the scientific basis to understand and predict microscale processes involving micromechanics, transport, microoptics and sensing, and multivariate analyses that lead not only to the invention of mobile, autonomous μ ChemLab, but also provide the engineering foundation to address the key technical objectives of reliability, performance, and

manufacturability in future microdevice applications.

The ultimate goal of the microscale transport aspect of the μ ChemLab project is to model the concentration of solute as a function of time and position in the channel. A complete specification of the concentration profile requires as input three additional quantities: the electrical potential field, the fluid-flow velocity field, and the temperature field. The electrical potential field and in particular the electrolytic double layer plays a central role in capillary electrophoresis. In FY97 we developed methods to calculate the properties of the double layer associated with a molecule in a liquid environment, the primary physical phenomenon dominating its mobility. A 3-D coupled Quantum-Poisson-Boltzmann method was successful in determining the single- and double-layer charge distributions on the surface of a molecule of arbitrary geometry in a fluid of arbitrary ionic strength, including the electronic relaxations of the molecule created by the fluid. We then extended the 3-D Poisson-Boltzmann method to cylindrical geometries and to real discretized charge sources; potentials and fields within the cylinder reproduced analytic results.

We also developed a computer code that can predict the fluid-flow field for an arbitrary configuration of flow obstacles in a 2-D microchannel. The code couples a linearized version of the Poisson-Boltzmann equation with the governing equation for Stokes flow, and the numerical solution is obtained using the boundary element (Green's function) technique. The fluid-flow/electrical potential computations alone (i.e., without diffusional transport) provided useful insights into the optimal size, spacing, and packing fraction of flow obstacles and in the design of corners in the chemlab assembly. In addition, the calculations can reproduce the recently observed effect of recirculated flow in the open region of a capillary that is immediately adjacent to a region packed with glass beads or flow obstacles.

We also successfully modeled the temperature field generated by joule heating and investigated the temperature rise as a function of various configurations of obstacles. Several publications describing the modeling efforts outlined above are planned for the near future.

After extensively evaluating the existing designs for gas micropumps and valves, we are pursuing a valve design that uses interfacial tension (liquid droplets) for sealing. This approach is attractive because as the size decreases, surface tension dominates the sealing process, and the sealing force scales inversely with the characteristic length. We are considering two possible actuation mechanisms to induce the motion of the droplet; one is by magneto-hydrodynamics (MHD), and the other is by electrokinetics (EK). We designed, fabricated, and tested a millimeter-scale unit to explore the feasibility of developing a liquid droplet-based microvalve. In this prototype unit, a mercury droplet is driven by MHD forces into two valve seats that are 0.5-mm square. Tests on the unit demonstrated that the mercury valve effectively blocks the flow of air at pressures up to 900 Pa. With a 0.5-mm seat, the valve can theoretically operate up to 2800 Pa, and with a 5-micron seat the valve should hold back pressures of almost three atmospheres. We will explore these limits in upcoming tests and develop more complete models to aid in the optimization of actuation mechanisms and sealing designs. At this time, tests are also under way to fully characterize EK actuation mechanisms for pump and valve applications.

Publications

Other

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Autonomous MicroChem Laboratory (μ ChemLab)

G. C. Frye, D. A. Loy, J. M. Phelan, P. J. Rodacy, R. J. Simonson, R. L. Woodfin, K. R. Zavadil, M. J. Kelly, S. A. Carichner, K. Wally, M. E. Warren, R. Chanchani, C. M. Matzke, E. J. Heller, P. R. Lewis, M. C. Oborny, D. R. Adkins, R. J. Kottenstette, K. W. Schubert, D. Y. Sasaki, D. W. Arnold, S. A. Wright, J. Vitko, Jr., W. B. Chambers, T. R. Guilinger, M. X. Tan, S. H. Kravitz, D. J. Rakestraw, G. N. Ryba, D. S. Anex, S. A. Casalnuovo

This project will lead to a new generation of field-ready and compact chemical analysis devices that will have unprecedented capabilities for measuring and deciphering detailed chemical signatures. Specific goals focus on providing rapid and highly selective detection of trace (ppb) levels of target analytes in the presence of much higher concentrations of interfering compounds. At the end of three years, we will demonstrate these capabilities in an autonomous microscale chemical laboratory (μ ChemLab) that will establish Sandia as a leader in this field. This project will position Sandia to support increasing demands for detailed chemical information by current national security customers and is essential for developing new customers in nonproliferation, counterterrorism, and critical infrastructures. We will form the μ ChemLab by miniaturizing and integrating sensing capabilities, sampling and separation systems, power sources, and systems architecture. We will develop both gas- and liquid-phase analysis systems and enable microfabrication techniques parallel analysis channels to provide improved chemical discrimination. Specific system components to be developed include (1) gas-phase sample collectors and concentrators, separation columns, acoustic sensor arrays, and valves and pumps, (2) liquid-phase sample collectors, electrokinetic (EK) and electrochromatographic separation columns, and optical and electrochemical detectors, and (3) miniature fuel cells. As part of the project we will develop expertise and specialized techniques for microfabrication and packaging. We will combine the chemical

analysis chips with electronics and microprocessing capabilities into a handheld autonomous system that can detect both explosives and chemical warfare (CW) agents.

During the first three months of the program, we established a top-level concept and schedule for the three-year goals and completed a state-of-the-art technology assessment. We established a conceptual design for μ ChemLab together with requirements for major systems and subsystem components. Several approaches for microchannel fabrication for gas-phase and EK separations are under way using various materials and processing techniques. We developed techniques for sealing microfabricated components to make flow channels and are optimizing them using several materials (polyimide, solder, ultraviolet [UV]-curing acrylates). We evaluated EK pumping mechanisms demonstrating that large pressures can be generated and experimentally established simple scaling laws. We demonstrated the separation of fourteen target explosive compounds using reverse-phase EK chromatography. We demonstrated rapid (< 30 sec) gas chromatographic separation of CW agent stimulants using conventional columns and equipment. We demonstrated electrochemical detection of the explosives TNT, RDX, and PETN with carbon film microelectrodes at very low concentrations in small volumes. Design, fabrication, and testing of microgas valve and pump concepts using various designs is in progress. We completed a design for a gas-generation system, and fabrication of the first components is in progress. We completed a detailed evaluation for relevant parameters concerning (1) the chemical signatures and properties of explosive compounds present in landmines, (2) the fate and transport processes affecting movement, and (3) modeling approaches to simulate complex competing fate and transport interactions. We completed requirements and lithographic mask designs for gas-diffusion electrodes for on-chip fuel-cell power. We designed and constructed a novel reaction chamber to measure gas and water flows through the electrodes and made preliminary measurements of hydrogen and oxygen transport rates through porous membranes.

In addition to these technical accomplishments, there were several others in FY97. We established an effective management team for the overall Grand Challenge project, which includes the three project managers who established and conducted monthly video conferences to ensure coordination, communication, and teambuilding. We also initiated processes to ensure that intellectual property developed over the course of this investment is managed strategically.

Publications

Refereed

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Frye, G. C., R. J. Kottenstette, E. J. Heller, S. A. Casalnuovo, C. J. Brinker, A. Sellinger, N. K. Raman, and Y. Lu. 1997. "Optimizing Surface Acoustic-Wave Sensors for Trace Chemical Detection." *Transducers '97 Digest of Technical Papers* 2 (Chicago, IL, 15-20 June): 1323-1326.

3522.030

Cooperative, Distributed Sensing and Action Using Microminiature, Intelligent Agents

B. L. Spletzer, S. W. Reynolds, M. J. McDonald, P. C. Bennett, II, R. G. Jungst, P. R. Klarer, T. M. Weber, C. L. Lewis, J. T. Feddema, R. H. Byrne

This project will develop the technical base for modeling, simulating, designing, evaluating, developing, and deploying microminiature intelligent machines, thereby providing the architecture needed to support the deployment of multiple autonomous MicroChemLabs (μ ChemLabs) in a cooperative sensing environment. The main thrust of the project is to build hardware-verified simulation tools and to develop control systems for cooperating intelligent agents. These cooperating intelligent agents will perform a complex task in a specific area of pressing national importance. Specifically, Sandia will produce the world's first mobile autonomous μ ChemLab as part of the hardware verification to perform detection and localization of a chemical source. This project will continue to position Sandia as a leader in the community of researchers in computer science and mathematics regarding cooperative behavior and as a supplier of microminiature intelligent systems and technology.

Our accomplishments fall into four general categories: (1) determination and examination of critical subsystems, (2) development of the cooperative behavior

simulation tool, (3) construction of vehicles for hardware verification of the simulation and control algorithm testing, and (4) development of controls and behavior models for cooperative distributed sensing.

The analysis of critical subsystems revealed that the power supply is the most critical hardware subsystem in that it requires development before mobile cooperating intelligent agents on this scale can be fielded. For the scope of the demonstrations in this project, it appears that the emerging battery technologies using lithium chemistries will suffice. Some effort has been directed at examining the feasibility of these batteries and at developing a hybrid power supply where a battery provides the energy from the power system and a twin layer capacitor handles power surges. We are also investigating less conventional power supplies such as fuel cells and combustion systems to provide acceptable alternatives to battery power.

The simulation tool is functionally complete, and work is under way to develop an interface for rapid testing and modification of controls and behavior algorithms. Also, we are pursuing the incorporation of commercial software to enhance the capabilities of the tool. One area of special interest is incorporating chemical plume modeling into the simulation tool. Other areas include the development of generic interfaces to the simulation in areas such as sensor modeling, microcontroller simulation, and communication protocol simulation. These enhancements will allow many additional important facets of agent design to be tested rapidly and modified.

We completed a group of five Robotic All-Terrain Lunar Exploration Rover (RATLER)-based vehicles for use in hardware verification of the simulation tool. Each vehicle is capable of extended autonomous operation in rough terrain. The vehicles are large enough to serve as test-beds for various sensor and communication suites. The vehicles and the

simulation tool will be compatible to the extent that controls and behavior algorithms can be tested on either one with minimal changes.

The work in cooperative controls and behavior proceeded along several parallel paths. Specifically, we pursued modern control methods, variable structure control, fuzzy logic, genetic programming, and continuum analogy techniques. These efforts resulted in techniques applicable to any number of cooperating agents. We developed and coded in software mathematical models of the vehicle dynamics and kinematics, the chemical sensor, and the diffusion environment. We posed more than 20 test problems to benchmark the control algorithms. The problems vary from having full state knowledge (the vehicles' positions and orientations relative to the target) to having noisy, coarse measurements (e.g., close, medium, and far from target). We paid special attention to making sure that the algorithms are provably stable. For example, we are using variable structure control analysis to determine when to switch between simple control laws. While these individual simple control laws may not be convergent, it is possible to make the system converge by switching at the appropriate times. We are also paying special attention to the computational requirements. For instance, we are creating suboptimal fuzzy logic rules from an optimal linear quadratic regulator (LQR) design. While the fuzzy logic controller is suboptimal, the rules are simple enough to compute in an 8-bit microcontroller as opposed to the computer that the optimal control requires. Finally, we are investigating learning algorithms such as reinforcement learning and genetic programming to optimize control algorithms given several test scenarios. We tested these algorithms and many others in simulation and soon will test them in hardware.

The Focused Technologies area contains projects continuing from last fiscal year in the areas of advanced transportation and pulsed power. New projects in these technologies were incorporated into the previous system technology and solutions areas.

Projects in advanced transportation include research in the safe, secure transportation of nuclear weapons and subassemblies; transportation of hazardous nuclear materials and wastes; and advanced automotive transportation.

The pulsed power area strives to develop new capabilities in pulsed power to address nationally important problems in national defense and energy areas.

Researchers are developing electromagnetic impulse radar for the detection of underground structures. This ground-penetrating radar based on high peak power, high repetition rate, and low center frequency impulses has applications to remedial site reconnaissance for the detection of buried objects, for the detection of underground bunkers and tunnels, and as a sensor for a self-aware weapon or a height-of-burst sensor.

Ground-penetrating radar has immediate applications in environmental remediation, nonproliferation, underground structures, and unexploded ordnance detection. The transmitter system (shown here) and antenna, in the foreground, are the largest components.

FOCUSED TECHNOLOGIES

Development of Innovative Combustion Processes for a Direct-Injection Diesel Engine

J. E. Dec, D. L. Siebers, P. C. Miles

The engine for the Partnership for New-Generation Vehicle (PNGV) is one of the most critical components for meeting the goal of 80 miles per gallon. PNGV selected a small-bore, high-speed, direct-injection (HSDI) diesel as the best engine candidate, although major improvements in efficiency, power-density, and emissions will be required. The research on this project aims directly at providing the science base needed to make the necessary technological advances.

PNGV determined that the base engine configuration must have four valves per cylinder, variable swirl, and a vertical, center-mounted, high-pressure, common-rail fuel injector. Some promising new technologies for further improvements are fuel injection-rate modulation, water injection, enhanced-swirl combustion chambers, exhaust-gas recirculation (EGR), and modified fuels. This project proposes to evaluate these technologies, down-select to the most promising, develop a research engine with the capabilities of PNGV's base engine design, and conduct research to determine the viability of the most promising technologies.

We selected two promising new technologies, water injection and injection-rate modulation, and investi-

gated them in our current diesel facilities using advanced imaging diagnostics. We designed the HSDI research engine, and installation is under way. The engine laboratory will be completed as the remaining components arrive. We will conduct further investigation of the new technologies in the new HSDI engine and our current engine facilities (as necessary to ensure completion) during the coming year.

The research (optically accessible) HSDI engine lab is on schedule. In collaboration with industry, we designed an advanced four-valve cylinder head with center-mounted, common-rail fuel injection and intake-air swirl capabilities; it is scheduled for delivery shortly. We have already acquired and tested one of the prototype injection systems and will soon deliver a second, more flexible research injector. All other components are already assembled or nearing completion.

We investigated two promising novel technologies, water injection and injection-rate modulation, in our current diesel facilities using advanced laser-imaging and other diagnostics. The results show that appropriate water injection, even in relatively small amounts, can significantly reduce (by a factor of 2) soot formation rates in diesel engines. Water injection also provides the well-known effect of reducing NO_x by lowering combustion temperatures, so this technique can potentially break the soot- NO_x trade-off that currently limits diesel-engine combustion strategies.

Injection-rate modulation data show that this technique modifies the fluid dynamics of the combusting fuel jet to enhance mixing and increase the flame surface area. These investigations demonstrated that both technologies offer significant potential for improving engine performance and simultaneously reducing emissions.

Finally, we began a new multiyear, small-bore HSDI diesel Cooperative Research and Development Agreement (CRADA) with industry and DOE support. This project allowed us to take a leadership role in working with our supporting partners to develop this new research project.

Publications

Other

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Miles, P. 1997. "HSDI Diesel Hardware Status." Paper presented to the Joint Diesel Combustion and HSDI CRADA Meeting, Detroit, MI, 6-7 May.

Miles, P. 1997. "Status Update: Small-Bore Diesel Hardware Design and Acquisition." Paper presented to the Joint Diesel Combustion and HSDI CRADA Meeting, Detroit, MI, 19-20 August.

Hydrogen Production for Fuel Cells by Selective Dehydrogenation of Alkanes in Catalytic Membrane Reactors

T. J. Gardner, C. J. Brinker, A. G. Sault

Hydrogen-powered polymer electrolyte membrane (PEM) fuel cells, fueled by on-board H_2 generation from liquid fuels, represent an important technology for all-electric or hybrid-electric vehicles. Sandia has devoted much effort to the use of steam reforming or partial oxidation of liquid fuels for on-board H_2 generation, but these technologies generate large amounts of CO and CO_2 , which can poison PEM fuel cells. We propose to develop a catalytic membrane reactor system for the generation of pure H_2 via selective dehydrogenation of liquid fuels. We will achieve separation of H_2 from hydrocarbons by modification of commercial alumina membrane tubes with size-selective microporous ceramic membranes. We further propose to use hydrous metal oxide (HMO)-based ion-exchanger technology to prepare novel bulk and coated dehydrogenation catalysts. These HMO materials are superior to conventional oxide supports, such as titania and silica, in that they can be synthesized to contain high concentrations of sodium ions, which can be ion-exchanged with transition-metal ions that are catalytically active for selective dehydrogenation. By using HMO-based catalysts, we hope to increase conversions achievable with a conventional catalyst inside the membrane tube. This overall scheme offers a potential method for increasing H_2 production rates without increasing reactor size, an important consideration for transportation applications or for remote electricity generation for civilian or military applications.

This past year we successfully demonstrated the catalytic membrane reactor concept using heptane dehydrocyclization as an H_2 -generation reaction with a packed commercial catalyst bed/silica membrane system, thereby achieving a major project milestone. We found membrane performance and stability (at high temperature) for H_2 separation from other product species to be excellent, although overall H_2 -generation rates were low due to relatively low catalyst activity and selectivity combined with significant catalyst deactivation over time. The excellent selectivity of this baseline SiO_2 membrane eliminates the need to impart a catalytic functionality into the membrane to convert unreacted heptane as it passes through the membrane. HMO-based catalyst development identified Cr/HTO:Si catalysts with high heptane dehydrocyclization activity on an active metal basis. We plan further efforts to study these materials in an attempt to increase Cr loading to try to develop high catalyst activity on an overall catalyst weight basis. Membrane development activities identified new surfactant-templated SiO_2 membranes, which offer the promise of superior performance via increased H_2 permeance. We plan further experiments to improve the selectivity of these membranes for separation of small-gas molecules via molecular sieving through the use of surface derivatization techniques.

Publications

Refereed

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Hybrid Vehicle Engine Development

P. Van Blarigan, S. S. Goldsborough, N. Paradiso, Jr., J. Wu, D. V. Zanini

To meet proposed California Air Resources Board (CARB)-proposed Equivalent Zero-Emission Vehicle (EZE) standards, Sandia is developing an advanced free-piston engine. We used a double-ended free piston to compression-ignite homogeneous fuel/air mixtures as it oscillates inside a closed cylinder. Through this oscillation, we generated electrical energy in a linear alternator, which acted to control the piston motion by actively adjusting the electromagnetic forces felt by the piston. Electricity was the output of this engine, and we achieved electronic control of the compression ratio with extreme mechanical simplicity. We introduced fresh charge to the engine in a modern two-stroke cycle fashion.

A single-shot free-piston experiment is ongoing and has been tested with various fuels: hydrogen, propane, methanol, isooctane, and summer-blend ARCO regular-grade gasoline. We ran compression ratios of 24:1 to 69:1. With hydrogen fuel at an equivalence ratio of 0.32, the indicated thermal efficiency is 56% with essentially zero NO_x exhaust emissions. This compares with the 45%

indicated thermal efficiency of an optimized conventional engine. The low- NO_x emissions enable the engine to comply with CARB's EZEVE standard when fueled on hydrogen.

To test the linear alternator design, we modified a Caterpillar 3314 diesel engine to run on three cylinders, using the fourth cylinder to drive the linear alternator. We did this by cutting a 4.5-inch hole in the cylinder head and attaching a linkage from the piston through the cylinder head to the linear alternator.

To test the completed engine/alternator assembly, we are outfitting a test cell with an 1800-pound steel table to which we will mount the engine/alternator assembly. We are designing the linear alternator with the aid of MAGSOFT, a finite-element electromagnetic software package.

Publications

Refereed

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Other

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3524.150

High-Power Ion Beam (HPIB) Modification of One- and Two-Layer Metal Surfaces

T. J. Renk, M. L. Griffith, D. S. Senft, N. R. Sorensen, R. G. Buchheit

Intense pulsed high-power ion beams have been demonstrated to produce enhanced surface properties by changes in microstructure caused by rapid heating and cooling of the surface. Additional improvements can be effected by mixing a previously deposited thin-film layer (surface alloying) into any number of substrate materials. Sandia conducted surface treatment and alloying experiments with Al-, Fe-, and Ti-based metals on the repetitive high-energy pulsed-power (RHEPP)-1 accelerator at our laboratories. We produced enhanced hardness and wear resistance by treating with 440°C stainless steel, and by mixing Pt into Ti-6Al-4V alloy. Mixing a thin-film Hf layer into Al6061-T6 alloy (Al-1.0Mg-0.6Si) improved its corrosion resistance by as much as four orders of magnitude in electrochemical testing, compared with untreated and uncoated Al6061. Experiments are ongoing to further understand the microstructural basis for these surface improvements.

We used an intense ion beam to conduct surface modification and alloying experiments with various metals and bi-metal combinations. We attempted to improve surface hardness, durability, and corrosion resistance in metal alloys that have clear commercial application potential. Surface modification of 440°C stainless steel resulted in as much as a sixfold increase in hardness as measured by nanoindentation, with attendant increases in durability. We believe this is due to carbide dispersal produced by the rapid-melt and resolidification (RMR) cycle caused by the intense beam treatment. Mixing Hf coatings into Al6061 led to substantial improvements in corrosion resistance as measured by electrochemical impedance spectroscopy. Other mixed metals such as Cr and Zr also resulted in corrosion-resistance improvement. We also added Si to Al6061, resulting in improved surface hardness. Mixing a co-sputtered Pt-Ti

layer into Ti-6Al-4V alloy resulted in substantially improved surface durability. Surface performance in the Pt-Ti case, as measured by friction coefficient behavior, improved by factors between 10 and 100 over the base Ti alloy.

These are the highlights of our experiments. The microstructural basis for these surface improvements is less well understood, although the results of ongoing analyses may shed further light. We hope to complete such understanding in follow-up experiments.

In addition, we developed a knowledge base for treatment using intense ion beams that with time will resemble that of more well-established technologies such as laser processing or ion implantation. This knowledge base was developed through a collaboration; these collaborations will continue. In addition, we submitted a Technical Advance on the surface alloying that may be developed into a patent application. Efforts are beginning to further develop the commercial potential of surface alloying with Quantum Manufacturing Technologies and its established clientele, as well as with private industrial contacts directly with Sandia. This has the potential for generating a substantial revenue stream back to Sandia, both in direct company support and through the licensing agreement already in place with QM Technologies.

Publications

Other

Renk, T. J., R. G. Buchheit, N. R. Sorensen, D. C. Senft, M. O. Thompson, and K. S. Grabowski. 1997. "Surface Treatment and Alloying with High-Power Ion Beams to Improve Properties in Al-, Fe-, and Ti-Based Metals." *Proc. 11th Internat. IEEE Pulsed Power Conf.* (Baltimore, MD, 30 June).

Refereed

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A 700-kV, Short-Pulse, Repetitive Accelerator for Industrial Applications

F. J. Zutavern, M. H. Ruebush, L. F. Rinehart, M. W. O'Malley

The goal of this project was a small, 700-kV accelerator that can produce 7-kA particle beams with pulse lengths of 10–30 ns at rates up to 50 Hz for military and commercial applications in counterproliferation, materials processing, radiography, and sterilization. Sandia tested two switching technologies: (1) spark gaps and (2) high-gain photoconductive semiconductor switches (PCSSs). The spark gap-based system switches a low-impedance pulse-forming line (PFL) that drives four small linear induction accelerator (LIA) cavities. In FY96, we tested a field-enhanced diode and modified the LIA to operate continuously at 50 Hz. In FY97, we assembled the PCSS module and tested it to drive 50 Ohms, or $1/8^{\text{th}}$ of the LIA. The development of a PCSS switching module that can switch 7–10 kA of current in 180–200 current filaments on six 2-inch GaAs wafers proved more difficult than expected. On the advice of the pulse-power review committee, research focused on making one module trigger very accurately rather than initiating construction of the other modules required to drive the entire accelerator. In FY97, we succeeded in producing thirty consistent current filaments on one wafer and are presently testing six wafers in parallel at 175 kV and 6 kA. We are adjusting the optical delivery system to maximize the number of current filaments produced in the switches. We moved the LIA into place for connection to the PCSS system. However, further resources will be necessary to assemble the other modules and test the four accelerator cavities with the eight PCSS-based modulators. The LIA is also available to test other emerging technologies, such as magnetic switches. The advantages of the PCSS are lower inductance and the design flexibility of distributed

switching due to their extremely precise triggering. For the LIA and the diode, this translates to faster risetimes, more rectangular pulses, the capability of shorter pulses, and potentially higher diode efficiency.

In FY96, we operated a four-cavity LIA successfully at 30 Hz with a spark gap-based modulator. We used a wafer dielectric pulse transmission line to drive the LIA cavities and a field-enhanced diode. Although designed for single-pulse operation, we tested and modified the cavities and diode for repetitive operation to 50 Hz. In FY97, we assembled and tested a module to drive $1/8^{\text{th}}$ of the LIA with high-gain GaAs PCSS. We developed and tested an optical line triggering system that improved switch jitter and spatial control of the current filaments formed in the PCSS. We used a fiber-optic/cylindrical lens delivery system to produce approximately one optical trigger line per millimeter of switch width. On a single GaAs switch, we initiated 30 filaments simultaneously. We recorded their light emission with a high-speed, intensified, infrared-sensitive camera. Then we assembled a six-wafer module with the current-carrying capacity to drive $1/8^{\text{th}}$ of the LIA (7–10 kA). To date, that module has switched 175 kV and 6 kA with many filaments. (We presently have not photographed the switches during switching with enough spatial resolution to determine the total number of filaments.) We are still optimizing the triggering system as we increase the system voltage. By the end of FY97, we plan to test to 250 kV and 7–10 kA. If successful, further resources will be required to replicate this module and test the PCSS-based modulators on the entire LIA. We improved switch lifetime in two ways: (1) by fabricating large-scale P-type, intrinsic N-type (PIN) switches (2" wafers, 3.4-cm gaps), and (2) by triggering diffuse filaments near the switch contacts. We developed a numerical model for PCSS initiation and contact degradation to guide future design and fabrication of the GaAs PCSS.

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3524.160

Advanced 3-D Electromagnetic and Particle-in-Cell Modeling

D. B. Seidel, M. F. Pasik, M. L. Kiefer, D. J. Riley

Recent advances have led to the development of techniques to embed unstructured, free meshes into standard 3-D, rectilinear, finite-difference (FD) grids. The resulting hybrid-grid modeling capability allows the higher resolution and fidelity of modeling afforded by free meshes to be combined with the power and efficiency of rectilinear techniques. Sandia proposes to extend current particle-in-cell (PIC) methods for operation on these hybrid unstructured/rectilinear meshes. Several technical innovations are required,

including proper treatment of space-charge-limited (SCL) emission, particle transport on unstructured meshes, charge-conserving particle current/charge allocation, and proper treatment of particles in transition between structured and unstructured grid regions. This project provides the Pulsed Power Technology Initiative with a broadened simulation capability impacting the areas of nuclear weapons effects, weapon physics, and inertial confinement fusion (ICF). Critical technologies that benefit with the improved capability to simulate the details of complex, irregular structures include anode shaping for focusing of ion diodes for ICF and the design of post-hole convolutes and other high-current magnetically insulated power-flow components for advanced pulsed-power accelerators.

The goals of this project were to integrate the research and code development of the previous year's efforts into Sandia's QUICKSILVER electromagnetic PIC code and to demonstrate its utility by performing a simulation of a device or system of programmatic interest. To summarize our accomplishments, we completed the integration required to perform such a simulation. However, due to unexpected delays in debugging the software late in the project, we were not able to actually complete a demonstration simulation before the end of the project.

There were several important accomplishments throughout the year associated with the integration of hybrid grid particle handling into the QUICKSILVER code. We developed a subsystem to push particles on the unstructured grid in a manner compatible with QUICKSILVER's standard particle handler. We completed and tested the code that transitions particles back and forth as they move between the structured and unstructured grids. We also implemented modules to allocate charge and current on the unstructured grid, as well as to ensure the conservation of charge. In addition, we modified several features of QUICKSILVER's structured grid solver to accommodate the inclusion of unstructured grid regions, including a reordering of the operations in the timestep loop and

the addition of a time-averaging technique for the suppression of particle noise. We modified the unstructured grid preprocessor/solver to support mirror symmetry, which is necessary for most particle applications. The extension to periodic symmetry, while not complete, is straightforward. The most difficult and time-consuming task in the integration has proven to be the development and testing of the modules that properly couple the state variables of the system at the interface between the structured and unstructured grid regions; debugging these modules, more difficult than anticipated, ultimately prevented the accomplishment of completing a simulation of programmatic interest. Other important, nonphysics-related accomplishments this year included new development required for integrated data visualization as well as the conversion of the code to use dynamic run-time memory management.

In addition to not meeting our goal of successfully performing a programmatically relevant simulation, one significant integration goal was not accomplished: the inclusion of SCL particle emission from unstructured boundaries. While this is not needed for many applications of interest, it will eventually be required.

Publications

Other

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Electromagnetic Impulse Radar for Detection of Underground Structures

G. M. Loubriel, J. F. Aurand, W. D. Helgeson

The goal of this project was to develop and demonstrate a ground-penetrating radar (GPR) based on high-peak-power, high-repetition-rate, low-center-frequency impulses. Sandia discharged a transmission line, charged at 100 kV, with high-gain GaAs photoconductive semiconductor switches (PCSS) into a matched antenna. We also achieved a repetition rate of 1 kHz. We used the system to observe targets behind large (2-foot-thick) concrete structures.

We accomplished the following tasks:

- (1) Performed low-voltage transmitter tests*
- (2) Constructed the high-voltage switch assembly and transmission line*
- (3) Built and tested a modulator capable of 100-kV, 1-kHz operation*
- (4) Designed a mask, procured GaAs wafers, and fabricated the PCSS*
- (5) Designed and built the receive antenna*
- (6) Installed diagnostics and laser diode array in the laboratory*
- (7) Assembled the transmitter with laser diode and fiber*
- (8) Pulse-charged the pulser and test diagnostics*
- (9) Assembled and calibrated receive antenna*
- (10) Measured radiated-pulse waveform*
- (11) Measured return waveform from target in air*
- (12) Measured return waveform from "buried" target*
- (13) Published final SAND report.*

The goal of this project was to develop and demonstrate a GPR that is based on high-peak-power, high-repetition-rate, low-center-frequency impulses. We discharged the transmission line, charged at 100 kV, with high-gain GaAs PCSS into a matched antenna. We used the system to (1) measure penetration of the transmit pulse through large (2-foot-

thick) concrete structures, (2) measure returns from targets in air (no penetration), and (3) measure returns from targets obscured by concrete. The enabling technology for the transmitter is high-gain GaAs PCSS. These switches are optically triggered with small laser diodes and laser diode arrays, can hold off high voltages, and have fast risetime and low jitter.

We made the following accomplishments:

(1) *Modulator.* We built a modulator with a risetime of 270 ns, peak voltage of 100 kV, and full width, half maximum (FWHM) of 425 ns. The modulator can run up to a repetition rate of 1 kHz. To eliminate a switch longevity problem, we used diode stacks between the modulator and the pulse-forming line. The diode stack holds the voltage on the line even after the modulator's pulse is extinguished. Thus, when the switches are triggered, only the short-duration current is produced. In this project, we designed a 180-kV diode stack.

(2) *Pulse-forming line.* We designed and tested a pulse-forming line that incorporates two PCSSs and a capacitive voltage probe. The line is capable of producing either bipolar or unipolar pulse (of either positive or negative polarity), depending on whether two (bipolar) or one of the switches is fired. As part of the pulse-forming line, we designed and tested an integrating capacitive voltage probe.

(3) *Antenna.* We tested the existing antenna to determine its characteristics, especially at low frequencies. We used different techniques (frequency-domain and time-domain) to characterize both the input reflection and the transmitting/radiation performance of the antenna. The antenna does not radiate effectively below 70 MHz (the frequency roll-off). As part of this work we built an impedance-matching section that connects the pulse-forming line to the antenna. We also built and calibrated a voltage divider to measure the voltage in the antenna (at the feed point).

(4) *Calculations of electromagnetic (EM) penetration into soil.* We developed a model for GPR in which we can vary the initial voltage pulse into the antenna,

including the measured antenna transfer function, the transmission of the EM waves on entering (and exiting) soil, attenuation and dispersion by the soil (real soils with varying water content), and the cross-section of the target. The model assumes normal incidence into soil and target. The model showed that high-peak-power impulses do penetrate into soils with some water content in such a way that targets buried down to 10 m could be detected.

(5) *Jitter.* After building the system, we quickly discovered that we could not radiate a bipolar waveform with the PCSS. The problem was that only one or the other switch seemed to trigger, even though both of them were activated. At the start of tests, we achieved only a bipolar waveform once every 10 pulses. By the end of the project, we obtained very reproducible waveforms at every pulse. We achieved this through a combination of stronger laser diode triggering and using glass rods as cylindrical lenses to form lines on the switch instead of round spots that are the typical pattern from the optical fibers.

(6) *Tests of system effectiveness.* We measured radiated pulses, reflected pulses from targets in air, measured penetration through concrete, and returned waveforms from targets behind concrete walls.

Publications

Other

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S

tudies address issues of urgent concern to the Department of Energy and Sandia. For example, energy production is a vital national concern; therefore, Sandia has developed a technology to monitor drill parameters. This technique improves the existing technology by at least two orders of magnitude. Called *surface-area*

modulation telemetry, it was designed for oil production in a cased well. The device has applications in complex drilling environments such as in the petroleum, geothermal, and environmental industries.

Sandians are also developing a compact, high-resolution, room-temperature gamma-ray sensor. Sensors currently available are of limited efficiency and performance. A more sensitive gamma-ray detector would find immediate application in safeguarding stored nuclear materials and detecting nuclear smuggling in weapons facilities, in controlling arms and verifying treaty operations, in detecting land mines and unexploded ordnance, and in monitoring environmental and remediation activities.

RESERVE

Here the response of a CZT radiation sensor to a weak radioactive source is tested. Compact field instruments based on CZT sensors can be used to uniquely determine the presence of a wide range of isotopes, including special nuclear materials.

Computational Methods for Predicting the Response of Critical As-Built Infrastructure to Dynamic Loads (Architectural Surety)

R. V. Matalucci, D. S. Preece

Significant internationally recognized computational mechanics capabilities reside at Sandia. This project provided an opportunity to assess the applicability of this technology to the analysis of explosive/structure interaction. We performed four different example calculations demonstrating this technology and are presenting the results of these calculations to potential customers. These example calculations are (1) explosive barrier wall simulation using PRONTO-3D, (2) brick explosive barrier wall simulation using PRONTO-3D, (3) brick explosive barrier wall simulation using ZAPOTEC/CTH/PRONTO-3D, (4) centrifuge experiment of explosive detonation in a tunnel, and (5) implementation of explicit rebar-reinforced concrete model.

We made four computer simulations of situations involving explosive/structure interaction:

(1) *Explosive barrier wall simulation using PRONTO-3D.* We simulated a solid explosive barrier wall using PRONTO-3D, which is a transient dynamics finite-element (FE) computer code. We modeled the wall using 3-D solid FEs with a concrete material model. We modeled the detonation of the explosive using smoothed particle hydrodynamics (SPH),

a gridless method that accurately treats gases and fluids. Results from this simulation include pressure on the wall induced by the explosive as well as stresses and strains in the concrete wall. An examination of the stresses and strains indicated that the explosive charge used would destroy the wall by breaking off one corner. The velocities induced in the wall showed it also moving and beginning to tumble at the end of the calculation.

(2) *Brick explosive barrier wall simulation using PRONTO-3D.* We accomplished a simulation similar to that reported above using masonry bricks instead of a solid concrete wall. The calculated pressure induced on the wall by the explosive as modeled by the SPH gas particles was identical. Each brick was composed of many FEs, which makes the bricks deformable and also able to break when subjected to extreme loading. The discontinuous nature of the bricks caused the wall to respond very differently from the solid wall. The bricks in the area of the wall with the highest explosive pressure began to move almost immediately, with that corner of the wall disintegrating. This calculation yielded the launch velocity of the bricks and demonstrated the ability of the codes to perform a simulation of a brick wall. This capability is important in calculating the response of civilian structures to explosive loading.

(3) *Brick explosive barrier wall simulation using ZAPOTEC/CTH/PRONTO-3D.* Another option for performing these types of calculations is a new computer code named ZAPOTEC,

which couples the Eulerian code CTH with the Lagrangian code PRONTO-3D. CTH is a Eulerian Sandia hydrodynamic code used extensively for shock-wave physics simulations, including explosives. In this simulation the explosive is modeled with CTH and the bricks in the wall with PRONTO-3D, similar to the previous case. The advantage of ZAPOTEC is that it can always be applied to the latest versions of CTH and PRONTO-3D, leaving these two codes free to evolve separately from each other.

(4) *Centrifuge experiment of explosive detonation in a tunnel.* This and another project, with the objective of performing an explosive experiment on the Sandia indoor centrifuge, were synergistic in that both involved application of computational mechanics codes to predict the effect of explosives on structures.

(5) *Implementation of explicit rebar-reinforced concrete model.* An explicit rebar-reinforced concrete model was implemented into PRONTO-3D. This model treats the effects of the concrete confinement on the behavior of the rebar, such as the slip.

Publications

Refereed

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An Advanced Unmanned Vehicle for Remote Applications

B. J. Pletta, J. T. Sackos

An autonomous mobile robotic capability is critical to developing remote work applications for hazardous environments. The ability of the remote platform to sense and maneuver within its environment is a basic technology requirement that is currently lacking. This enabling technology will open the door for force multiplication and cost-effective solutions to remote operations.

This work integrated Sandia's scannerless range imaging (SRI) sensor with a small exterior mobile robotic platform based on the surveillance reconnaissance ground equipment (SARGE) design, which we recently delivered to the DoD. We redesigned the computing and control system on the SARGE platform and upgraded it to a multiprocessor system to handle the increased computing demands of the autonomous control system.

The SRI was developed from the previous lab prototype to a field prototype unit capable of withstanding the abuse of a mobile environment. Further enhancements in the illumination source and data acquisition hardware now provide daylight operation and increased range resolution.

This work integrated Sandia's SRI sensor with a small exterior mobile robotic platform based on the SARGE design that we recently delivered to the DoD.

We redesigned the computing and control system on the original SARGE platform and upgraded it to a multiprocessor system to handle the increased computing demands required for autonomous control. The upgraded SARGE design replaces the previous platform and provides a Sandia-owned test-bed for future experiments in autonomous navigation.

The SRI is a unique type of imaging optical radar sensor. We designed and built a small portable version of the SRI for use on a mobile robotic vehicle under

this effort. This development required customization, miniaturization, and ruggedization of both the laser light source and the SRI processor electronics.

We designed the SRI processor subsystem around a commercially available, 200-MHz, Intel Pentium-based, industrial-type, single-board computer. We also implemented a 10 Base-T Ethernet data connection within this subsystem to provide a means for efficiently passing continuous acquisitions of range and reflectance imagery collected from the SRI system to the robotic vehicle's control computer. To produce a relatively eye-safe laser-based transmitter that provided good range-imaging performance out to 50-foot ranges in daylight environments, we constructed our first distributed-array laser transmitter. This device is composed of 180 lasers at the 904-nm wavelength, which are spatially distributed over approximately a 25-square-inch area.

We met our primary goal of developing a modern test-bed for research in autonomous navigation technology that will provide an invaluable tool for developing new programs in this research area with external customers.

3530.050

Cosmic Rate of Expansion from the Ambient Temperature's Observed Relaxation (CREATOR)

M. J. Adriaans, R. D. Moyer, P. D. Thatcher

The Cosmic Background Explorer (COBE) was launched on November 18, 1989, to measure the effective temperature and the anisotropy of the cosmic background radiation (CBR). COBE was a great success, posing many more questions than it answered. Cosmologists would like to fly another mission with much higher-temperature resolution. High-resolution thermometer (HRT) technology, developed for use in precision superfluid helium

physics experiments based on board the space shuttle, offers a unique opportunity for astrophysical radiometry. COBE was able to observe the large-scale temperature anisotropy of the CBR and made an observation of the microwave background quadrupole moment of the Universe. These measurements, however, were very near the limits on their thermometry and have large uncertainties associated with them. A next-generation mission, PLANCK, a European Space Agency (ESA) mission expected to launch in 2005, will improve temperature resolution to approximately 3 mK, an improvement of a factor of 30 over COBE. The temperature resolution and stability of current, space-proven HRTs is 0.1 nK.

The goal of the cosmic rate of expansion from the ambient temperature's observed relaxation (CREATOR) is to make use of this very precise thermometry and redevelop it for use in astrophysical instrumentation. There are two key areas where the HRT technology is most applicable. The first is in the development of a radiometer for detecting the CBR with an effective temperature sensitivity of 10 nK near 2.7°K. Second is the development of an ultra-stable blackbody calibrator. Sandia will test both the radiometer and the calibrator in a highly stable low-temperature instrument. We will also complete a "phase A"-type scientific definition study of a possible mission.

We completed a study investigating the feasibility of using the paramagnetic material, used in current HRTs, as the sensing material for an astrophysics radiometer. We found that, due to the high heat capacity of the material and their nonrobustness, paramagnetic salts were probably not the best solution to a radiometric sensor (although they can still be used for the blackbody calibrator). However, we are currently conducting a materials study to investigate the properties of special alloys with "giant moments." We have already performed a test of such an alloy, palladium iron (PdFe). Although this material displayed a reasonable temperature resolution, it also exhibited hysteretic behavior and longtime constants, making it inappropriate

ate for use as a thermometer. A similar alloy, palladium manganese (PdMn), will be the next material investigated.

We completed some of the initial work on BRAMS. The students assisted in establishing a laboratory at UNM, which included setting up a pumping station, a low-temperature dewar, and support electronics, and modifying a basic low-temperature probe for testing high-resolution thermometers. We completed an initial temperature-sensitivity test of bulk PdFe in the low-temperature probe. The next project involved work on the development of an HRT in a new geometry for use as the blackbody calibrator. Most elements of the thermometer were constructed and assembled, but there was not sufficient time to perform the experiment. The final project involved a study of making a thin-film HRT using the "giant moment" alloys.

3530.070

Productivity Enhancements for Analysts

J. A. van Berkel, N. H. Irwin, H. M. Koller

Data visualization is an emerging technology with high potential for addressing the information overload problem. This project extends the data visualization work of the Navigating Science project by coupling it with more traditional information-retrieval methods.

Sandia augmented a citation-derived landscape with documents using a text-based similarity measure to show the viability of including datasets where citation lists do not exist. The resulting hybrid landscape, showing hills where clusters of similar documents occur, can be navigated, manipulated, and queried.

The capabilities of this tool provide users with an intuitive explore-by-naviga-

tion method not currently available in today's retrieval systems.

We successfully loaded a nuclear science and technology subset of the ISI (Institute for Scientific Information) Science Citation Database, 1991-95, into an Oracle database and displayed it using VxInsight, formerly called EigenVR.

We purchased two SGI computers, one for development and one to use for demonstrations of the software, and loaded them with the VxInsight and related software and datasets. We connected one workstation to a local-area network (LAN); the other is a standalone.

We developed algorithms to select a nuclear-related subset, 1994-96, of FBIS (Foreign Broadcast Information Service) documents.

We then developed algorithms to measure similarities based on text matching between each FBIS document and every ISI document. We converted the similarity measures to x,y coordinates so that we could insert the FBIS documents into the ISI-based nuclear science and technology landscape. Since using text as the matching element between the two record types resulted in ambiguous placements on the landscape, it was necessary to develop an algorithm that chose one location from several possible locations, rather than just letting the ordination software place the text records equidistant from each of the possible placement sites.

We modified the VxInsight visualization software to accommodate abstracts for ISI records, to differentiate (through color) FBIS and ISI records, to allow structured query language (SQL) queries of the text fields, and to display full-text FBIS records using a Netscape browser.

Eight proliferation analysts tested the landscape, prepared a narrated videotape demonstrating the capabilities of the nuclear science and technology landscape, and wrote a final report.

The analysts' evaluations provided validation of the navigation concept and interesting insights into areas for improvement. In general, the analysts enjoyed being able to visualize a large set of data all at once and were interested in exploring the data through navigation. However, several analysts expected every record within a "peak" on the landscape to be on the same topic. Because the basic landscape was not formed by topic analysis, but rather by citation analysis, this was not the case. Therefore, the labels generated by the software for the peaks were not as representative of the content of the records contained within the peaks as the analysts expected. In addition, many of the analysts found the crosshairs indicator for navigation confusing.

In summary, the FBIS/ISI nuclear science landscape achieved a proof of concept. It demonstrated that it is possible to integrate records without cited/citing relationships into a VxInsight landscape that was formed based on those relationships.

The method developed by this project to integrate FBIS records into an ISI landscape could be used in other domains as well. For example, one could add epidemiological database records to a basic biomedical ISI landscape. In addition, the analysts' evaluations produced strategies for future development of VxInsight.

Publications

Other

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Web Vulnerability Demonstration

T. Q. Thai, K. L. Harrison, J. W. Walkup

The Web is one of the most popular places these days for information query and exchange. The number of new Web sites on the Internet has grown significantly in the last few years. As the Web becomes more important for business, its security increasingly draws considerable attention. This project examines the vulnerabilities, threats, and possible exploitations of the Web servers and clients running Intel-based PCs under Microsoft Windows 95 and NT operating system (OS). The vulnerabilities, threats, and possible exploitations do not include those found in the open literature. The study focuses on three areas: (1) the ActiveX technology, in particular ActiveX controls running under the Internet Explorer (IE) browser, (2) the authentication process of ActiveX controls, and (3) the Windows NT security on ActiveX controls. Details of vulnerabilities, threats, and possible exploitations are reported in a separate, classified report. The general conclusion is that casual Web-browsing activities to a malicious site under certain conditions can indeed present a serious problem to the user's computer and pose a serious compromise to the network to which his/her computer connects.

The focus of the study is the vulnerability (V), possible threats (T),

and exploitations (E) on Web servers and clients using the ActiveX technologies on an Intel-based computer running Windows 95 and NT OS. Although the involved technologies are still evolving at a rapid rate, we identified and demonstrated many underlying VTEs. Details of the VTEs are reported in a separate classified document. The following summaries highlight some key findings:

(1) Downloadable ActiveX controls from a Web server can be a serious VTE to an internal network because they will pass through firewalls and proxies and run in the context of the browser with current user's privilege.

(2) The authentication and verification process of ActiveX controls is dependent on the OS configuration. Thus, the process can be weakened or even bypassed under certain OS configurations.

(3) The highly flexible architecture of the IE browser, which is built upon software components based on the Component Object Model (COM), is also dependent on the OS configuration. Thus, the browser can also be a source of VTE under certain OS configurations.

The general conclusion is that casual Web-browsing activities to a malicious site under certain conditions can indeed present a serious problem to the user's computer and pose a serious compromise to the network to which his/her computer connects. We developed demonstration software of some found VTEs and showed it to potential external customers.

System of Labs Direct Fabrication Technology

M. E. Schlienger, V. Tikare, J. E. Smugeresky, M. Essien

This project is a cooperative effort between Oak Ridge National Labs (ORNL), Idaho National Engineering and Environment Lab (INEEL), and Sandia Labs. The project seeks to capitalize on the combined expertise of these three Lockheed Martin facilities. This effort is targeted toward combining the metal spray-forming technology being developed at INEEL with the laser-engineered net shaping (LENSTM) technology being developed at Sandia in an effort to produce a new compound direct fabrication technology. In addition to these process development efforts, ORNL is evaluating microstructures and developing alloys that are particularly suited for these direct fabrication technologies.

The ultimate goal is to arrive at a technology package that provides an agile new direct fabrication technique, along with the appropriate alloys to enable the maximum utilization of the technology. Although many potential applications exist, this work will target tooling. Tooling, as might be used for injection molding, represents a challenging application for traditional technology. This challenge arises from the difficulty in processing tool steels via conventional techniques. Both the INEEL and Sandia processes have no difficulty processing tool steels and, as such, the production task should be greatly eased. In addition, the rapid solidification that occurs within these technologies provides an additional opportunity for improved part performance; it is this performance increase that ORNL is addressing.

The INEEL spray-forming process involves the production of a part by impinging a molten metal spray onto a nonmetal preform. This allows the very quick deposition of material, but does not allow tailored material properties at

different locations, nor does it support the production of parts with high-aspect ratios. The Sandia LENS™ process addresses these limitations.

This project is targeted toward developing and characterizing a combined direct fabrication process. Toward this end, we are developing a process combining the INEEL spray-forming capability with Sandia's LENS™ technology.

Sandia's specific accomplishments associated with this project include (1) the development of improved powder flow measurement techniques, (2) the modeling of gas dynamic powder containment schemes, model-based powder focusing techniques, and (3) accurate characterization of the LENS™ powder feed system as a function of motor velocity and gas flow. These results impact this and other programs by identifying the path required to further improve process control, repeatability, surface quality, and ultimately microstructural control. Joint efforts include the design of a demonstration part, the deposition of LENS™ deposits onto spray-formed substrates, and the analysis of such composite deposits at INEEL, ORNL, Sandia-NM, and Sandia-CA.

Analysis shows that tool steels processed in this fashion may have advantages when contrasted to more conventional processing techniques. Specifically, preliminary information seems to indicate that INEEL/Sandia parts may be processed to the desired material characteristics with an aging heat treatment, as opposed to a conventional, higher-temperature, austenizing heat treatment. This result is of significant importance as it means that the process being developed may not only provide for the very rapid development of complex tooling, but also may allow ultimate properties to be achieved without the distortion associated with the typical thermal processing required. However, metallography reveals the presence of small cracks at the interface

between the spray-formed and LENS™ deposits. Such cracks, though small, may ultimately lead to tool failure. As such, it is desirable to determine the mechanisms associated with their formation and what, if any, mitigation techniques can be developed. To this end, we designed experiments to determine whether process modifications such as pre-LENS™ or *in situ* heat treatments may provide an effective mitigation scheme. We have produced the spray-formed deposits necessary for this study. The samples we received are H13 tool-steel spray deposits, which we then subjected to heat treatment and aging processes. The next step is to deposit LENS™ material onto these substrates under a variety of conditions and then evaluate the interface.

In addition to the above work, ORNL provided some nickel aluminide powder for LENS™ deposition. It is important to note that the alloy developed at ORNL may represent a new high-performance material. However, the nature of the material may result in an alloy that can be processed only via LENS™ or some similar process. As a result, this aspect of the project may be very exciting.

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3531.040

In Situ Optical Photoreflectance During MOCVD

W. G. Breiland, H. Q. Hou

Sandia successfully explored the use of normal incidence photoreflectance as an in situ tool for measuring n-type doping levels in metalorganic chemical vapor deposition (MOCVD)-grown GaAs materials. The technique measures phase and frequency shifts in Franz-Keldysh oscillations measured on 300-nm-thick, uniformly doped films. Doping concentrations from 5×10^{16} to 3×10^{18} can be measured at temperatures below 130°C. We developed a method to include photoreflectance as the last step in our pregrowth in situ calibration procedure for MOCVD thin-film structures. This combined capability now enables us to rapidly and accurately determine growth rates, composition, and doping levels necessary to generate a recipe to fabricate complex optoelectronic compound semiconductor devices.

We successfully explored the use of normal incidence photoreflectance as an *in situ* tool for measuring n-type doping levels in MOCVD-grown GaAs materials. The technique measures phase and frequency shifts in Franz-Keldysh oscillations measured on 300-nm-thick, uniformly doped films. We found the shifts to be monotonically related to impurity doping levels. Doping concentrations from 5×10^{16} to 3×10^{18} can be measured at temperatures below 130°C. The photoreflectance signal rapidly disappears above 130°C, which caused us to change our strategy for measuring doping levels. We developed a method to include photoreflectance as the last step in our pregrowth *in situ* calibration procedure for MOCVD thin-film structures. This combined capability now enables us to rapidly and accurately determine growth rates, composition, and doping levels necessary to generate a recipe to fabricate complex optoelectronic compound semiconductor devices.

Cold-Cathodes for Sensors and Vacuum Microelectronics

M. P. Siegal, D. R. Tallant, T. A. Friedmann, N. A. Missert, J. P. Sullivan, J. C. Barbour, P. A. Schultz

The development of robust, cold-cathode electron emitters will have significant implications for modern technology and may launch a new industry: vacuum microelectronics (VME). The potential impact of VME on Sandia's national security missions, such as defense against military threats and economic challenges, is profound. VME enables new microsensors for applications such as chem lab-on-a-chip and intrinsically radiation-hard ME. Amorphous carbon materials, developed in part by Sandia, demonstrate the required emission properties. Our challenge is to understand the emission mechanism in order to optimize materials for stable, robust device structures. The nature of the topological carbon-carbon bonding structures in these materials is poorly understood and remains a requisite for modeling more complex behavior such as emission. The emphasis of this project is therefore to study the structures in these films by both experimental measurements and first-principles theoretical calculations.

Amorphous carbon (a-C) thin films grow via energetic deposition processes and consist of a mixture of threefold and fourfold coordinated carbon atoms. We expended effort studying topographical carbon-carbon atom bonding structures, both theoretically and experimentally, measuring and modeling electronic transport, and measuring electron emission from a-C films.

Obtaining topographical models representative of a-C is fundamental to developing an understanding of the observable properties of the material. We systematically investigated the effects of basis set quality on the prediction of representative structures. In fully self-consistent first-principles calculations, variations in the quality of the basis set result in significant variations in predicted structure. Notable is how little rebonding and energy separate a-C structures that have qualitatively different

densities of threefold C atoms. This work provides new insights into potential a-C structures that affect interpretations of experimental data.

We primarily used pulsed-laser deposition (PLD) for the energetic growth of a-C films. We measured films with Raman spectroscopy, x-ray reflectivity, and Rutherford backscattering spectrometry (RBS) to provide structural information. In general, film density increases with increasing growth energetics. Films grown under the most energetic conditions result in densities about 3 g/cm³. Detailed analysis of Raman spectra suggests that the film-substrate (usually silicon) interface consists of a different a-C variety than the bulk of the film. The nature of the surface of the film may also be different from the bulk. Understanding these structural features is critical for interpreting other measured properties such as electrical transport, optical transparency, and electron emission.

While a-C films grow with several GPa residual stress, we find that they can be totally relaxed via short-duration thermal anneals at temperatures near 600°C, well within the ~800°C stability region for a-C. The ability to create stress-free a-C films that are akin to "amorphous diamond" opens up many new possible (and exciting) applications. We modeled this relaxation by a series of chemical reactions that led to conversion of some fourfold coordinated C atoms into threefold coordinated C atoms. Increases in electrical conductivity also occurred following annealing. The results indicate that the increase in conductivity and stress relaxation originates from the same bond conversion process and that electrical transport is dominated by a hopping conduction process.

The onset of electron emission in a-C is typically preceded by a "conditioning" process where the material is stressed by an applied electric field. We simulated this using the spatially localized electric field of a scanning-tunneling microscope (STM) tip. Such conditioning creates observable modifications in the films, with changes in both surface and electronic structures. Spatially resolved electron energy-loss

spectroscopy indicates that the conditioning causes a change in the surface region from fourfold to threefold coordinated C atoms.

Emission measurements on a-C films find turn-on fields > 20 V/micron. Once initiated, the emission of electrons twinkles (turns on/off). We can model this from a tunnel barrier existing in the film surface consisting of wide-bandgap material that can trap positive charge states. The lifetime of these states is long, but can be neutralized by recombination, possibly accounting for the observed emission site twinkling.

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3531.060

Micromachined Contact Fuses for Earth-Penetrator Applications

B. R. Davies, J. J. Sniegowski, S. Montague, V. C. Rimkus

The acceleration environment experienced by the sensors and electronics in an earth-penetrator weapon is extreme, with average accelerations in the 20,000-G

range and peak transient accelerations up to several hundred thousand Gs. Earth penetrators often contact earth, concrete, rocks, or other hard materials while traveling at thousands of feet per second. Sensors must be able to survive both penetrator launch and contact and penetration while distinguishing between each.

Sandia developed designs for suspended high-G and low-G plate mass sensors as part of this project. We developed the high-G sensor design to directly measure acceleration and shock during earth-penetrator operation. We developed the low-G sensor design to begin coupling multiple fuse functions into a single, integrated device in order to reduce size, power, and cost while increasing reliability and performance.

We use high-G acceleration measurement to determine target contact, target composition (density and/or hardness), and launch velocity. In some cases, weapon fusing is based on contacting a physical structure (weapon hits the ground or other target). In other cases the weapon fusing is based on discriminating between multiple layers of different materials (like sand, gravel, concrete, steel, air, etc.) while it is passing through each.

Low-G acceleration measurements are necessary to accurately measure velocity and distance traveled of weapons traveling through air or water. Velocity and distance information relevant to weapon fuse operation might then be determined using the low-G accelerometer. Velocity and distance information is relevant to weapon fusing to ascertain such important parameters as safe separation distance, weapon position and orientation, safe fusing velocity and direction, impact velocity, and target proximity.

The first prototype suspended-mass high-G accelerometer design showed promising results up to 14 kg, but was not suitable for higher acceleration levels. We developed a second-generation series of designs to improve and correct those factors that contributed to the unsatisfactory performance of the first prototype. These second-generation prototypes include two different mechanical designs and three different electronic circuit designs. We are currently

fabricating the second-generation prototypes, which should be ready for testing in the next few months. We developed a low-G accelerometer design that is compatible with the new integrated microelectronics, three-level polycrystalline silicon process. The low-G accelerometer is suitable for use in a high-G environment as a fuse component.

We could redesign the high-G accelerometer device for different sensitivity ranges by changing the geometry of the proof mass suspension springs. We will correlate future test results to spring length, deflection measurement, and finite-element (FE) analysis predictions to develop an algorithm for spring length design of high-G accelerometers. We could theoretically modify the high-G device to act as a switch by adding conventional microelectromechanical system (MEMS) "dimples" to the proof mass and modifying the spring geometry. We could use integrated low-G accelerometers to count both the number of rotations and the rotation rate of a spinning weapon. Additionally, we could design a purely mechanical pendulum-spring device to count revolutions of a spinning weapon. We could design MEMS relays to accommodate many of the switching and triggering functions, with certain voltage and current limitations.

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Novel Thermoelectrics for Next-Generation Power Sources

T. L. Aselage

Thermoelectric devices can be used to generate power from a temperature difference. Thermoelectric power generation requires no mechanical parts and is both reliable and long-lived. Thermoelectric devices can also provide a reliable, purely solid-state means of cooling. The foundation of a thermoelectric device is the Seebeck effect. The Seebeck coefficient is the electromagnetic field (EMF) across a material induced by a temperature differential. Efficient thermoelectric devices require materials with large Seebeck coefficients. The Seebeck coefficients of conventional materials are large only when the carrier density is low. However, thermoelectric devices also require the active materials to be at least moderately good conductors. Hence, conventional thermoelectric materials compromise between having low enough carrier densities to having large Seebeck coefficients and high enough carrier densities to be reasonable conductors. Sandia's research has unearthed a novel effect by which Seebeck coefficients of some unconventional materials, e.g., boron carbides, can be large even when their carrier densities are large. This novel enhancement of the Seebeck coefficient arises from a local lattice softening produced by the polarizabilities of charge carriers localized at multi-atom sites. These softenings can be particularly large when charge carriers, as in boron carbides, form pairs that can redistribute among degenerate molecular orbitals of the site. Boron carbides' electrical conductivities and Seebeck coefficients are consistent with expectations based on the effects of carrier-induced softening. Na-doped Si clathrates, the focus of experimental efforts in this study, do not meet the conditions that we now find for large softening effects. It is thus unlikely that these solids would be good thermoelectrics based only on softening

enhancements of the Seebeck coefficient. We have not as yet successfully synthesized bulk clathrate samples to test this hypothesis.

The goals of this exploratory effort were to develop a better understanding of the local softening enhancement of the Seebeck coefficient and to apply this insight to the pursuit of unconventional thermoelectric materials. The experimental effort focused on clathrates since these solids have structural similarities to the boron carbides.

Local softening is a general feature of self-trapped carriers, called *polarons*, arising from the polarizabilities of their electronic states. We endeavored to understand why softening can be particularly large in certain solids, e.g., boron carbides. Charge carriers in boron carbides form singlet pairs, called *bipolaronic holes*, associated with twelve-atom, boron-rich clusters. The ground state of a boron-rich cluster with two unfilled states among the degenerate frontier orbitals is a triplet, in accordance with Hund's rule. We find that a singlet pair can be stabilized by a symmetry-breaking deformation of the cluster. The stabilization of the singlet state can also produce a particularly large carrier-induced softening. Both effects are driven by large differences between the Coulomb repulsions of pairs occupying the same molecular orbital and the Coulomb repulsions of pairs on different molecular orbitals.

Carrier-induced softening makes two contributions to the Seebeck coefficient. The first contribution arises from the increase in the solid's entropy associated with decreasing local vibrational frequencies. The second contribution comes from the net transport of vibrational energy associated with the hopping motion of a charge carrier. We showed that the temperature dependence and magnitude of the sum of these two contributions are consistent with our experimental measurements of boron carbides' Seebeck coefficients and electrical conductivities.

We also wish to exploit this novel Seebeck coefficient enhancement to

develop new, unconventional thermoelectric materials. Na-doped Si clathrates contain multi-Si-atom cages that surround Na ions. The number of Na dopants sets the carrier density. Because of their structural similarity to boron carbides and the indications of hopping motion between Na-containing cages, we initially hypothesized that clathrates were good candidates for carrier-induced softening. Two problems must be overcome to synthesize bulk Na-doped Si clathrates: the large disparity in melting temperatures (Na: 98°C, Si: 1412°C) and the high vapor pressure of Na. We attempted direct synthesis from the elements in a Ni vessel we designed to contain Na vapor at high temperatures. Although the vessel was moderately successful in containing the Na vapor, the molten Na did not wet the Si powder under any of our conditions (400°–900°C). Thus, we observed little to no reaction between the Na and Si. We altered our strategy and will attempt to synthesize samples directly from the melt (> 1420°C) in electron-beam-welded crucibles. This appears to be the most promising approach to obtain a bulk clathrate sample of desired stoichiometry.

In summary, we achieved a better understanding of conditions that can produce a large Seebeck coefficient enhancement through carrier-induced softening. We showed that such effects are consistent with our experimental observations in boron carbides. The conditions under which we now expect large softening effects are not likely to be found in clathrates, where localized carriers do not appear to form pairs and where the orbitals associated with motion between Na sites are *s*-like and non-degenerate. Indeed, our measurements of powder clathrate samples obtained from a collaborator find small Seebeck coefficients. Successful synthesis of bulk clathrates can provide a test of our current understanding. More promising candidates for carrier-induced softening are systems where charge-carrier pairing occurs and *d*- or *f*-like orbitals are involved: other boron-rich solids or transition-metal compounds.

Advanced Stress-Sensing Assembly Test Chip Design

J. N. Sweet, A. H. Hsia, D. W. Peterson

The goal of this program was the design and test of an advanced piezoresistive test chip for use in measuring packaging-related stresses at the die surface. Sandia completed an integrated circuit (IC) layout of a chip with a group of candidate circuits in a 0.7-micron complementary metal-oxide semiconductor (CMOS) technology. The area density is about four times greater than the existing ATC04 chip, and the new stress-sensor piezoresistors have taps that enable measurement of sections of a resistor. We added transmission gating of all measurement buses to individual piezoresistors to improve high-temperature performance. Additionally, we designed new ring oscillator circuits to improve both sensitivity to environmental stressing and ease of measurement. This work resulted in an ATC4.x die design with a simpler addressing scheme, reduced leakage currents, better isolation, and a tapped resistor structure, plus redesigned oscillators, stress cells based on new materials, and overlaying bondpads. All of the above enable the ATC4.x for use as an investigative vehicle for higher-temperature applications, new fabrication processes, and novel stress applications. Difficulties in the design phase caused project delay, but a contract has been placed to fabricate some of the new test die for future evaluation.

We designed and simulated a new version of the original ATC04 stress measurement chip and laid it out for fabrication. We designed the new chip in

a 0.7- μm feature-size *N*-well CMOS process. This second-generation design addresses many of the shortcomings found in the ATC04 chip and incorporates some new and some modified structures for measuring die surface stress in a variety of conditions. We designed the layout carefully to make it portable to Sandia's CMOS6 rules for layout.

We designed and simulated new electronics using the SPICE (a program for electronic circuit analysis) simulator software. The logic density of the chip is approximately four times that of its predecessor, and we customized the majority of the local circuitry around each stress cell to fit area and layout constraints. The result is a portable stress cell whose orientation can be specified independently of the circuitry while maintaining the same simple addressing scheme. The previous version required a convoluted addressing scheme to access the stress cells in the desired order.

All of the new stress cells use a tapped piezoresistor scheme where up to four different subsections of each resistor can be addressed separately and measured. This design allows for a finer measurement resolution and will help as an investigative tool to determine which resistive range is best suited for different applications. Despite the additional circuitry and taps, the resulting cell is smaller in area than the original and requires less wiring to address it.

We also designed a series of three ring oscillators for use in package life-test evaluations. Each ring oscillator bridges or connects from inverter-to-inverter stage in a different metal layer; the first in first-level metal, the second in mid-layer metal, and the last in top-layer

metal. We resized all three ring oscillators to fit a target frequency of around 20 MHz. In the original version, we obtained very little information from one of the ring oscillators because its high frequency made it difficult to measure reliably. In addition, the output buffer circuitry was inadequate to drive off-chip measurement instrumentation. We enhanced this buffer circuitry to alleviate that problem.

We added CMOS transmission gating of all of the measurement buses to the individual piezoresistors to help isolate the resistors and cut down on junction leakage currents. The ability to make *in situ* measurements of thermal stress requires that the resistors function without leakage at high temperature.

We designed a customized standard cell library for use in creating digital logic blocks. We made this library with an eye toward reuse in the Microelectronics Development Laboratory (MDL) CMOS6 process, thus facilitating the transfer of the design to a full-production version.

We designed stress cells using different IC materials to enable a comparison of the piezoresistive effect commonly in these materials. This list includes polysilicon, polysilicide, silicided diffusion, and standard nonsilicided diffusion. We also made a bondpad structure overlaying these various stress cells in order to look at the effects that package wirebonding has on the die surface stress distribution.

This work resulted in an improved piezoresistive cell design with a simpler addressing scheme, reduced leakage currents, better isolation, and a tapped resistor structure. In addition, we redesigned the ring oscillators to facilitate measurement with laboratory equipment.

Cat's-Eye Modulator Fabricated in GaAs

M. E. Warren, M. G. Armendariz, W. C. Sweatt

The "cat's-eye" modulator is a reflectance modulator design for free-space optical communications with a remote optical transmitter that is capable of retroreflecting a signal back to the transmitter without using a corner cube reflector, which is the usual retroreflection approach. The advantages of a "cat's-eye" retroreflector are much simpler packaging and easier alignment of the modulator to the optics. Sandia developed an optical design that increases the collecting area for the "cat's-eye" modulator by a factor of about 20. We chose a "landscape lens" design where the lens is a diffractive element. With this architecture, the modulator can be a flat reflector—a diffractive element does not have to be etched on its surface. We examined and rejected numerous other families of optical designs.

(1) *Optical design.* We studied several families of optical designs that would increase the collecting aperture of this system, which would then increase the range over which it could be used. We increased the aperture from a diameter of about 0.5 mm to 2.2 mm; the useful range should scale similarly. The retroreflecting image quality of the final system is very good over a 100-mr acceptance angle. Finally, the best system does not require that a grating be deposited on the modulator.

We studied several families of optical designs, including refractive lens, diffractive lens systems, mixed refractive/diffractive systems, focusing designs with field lenses, triplet designs, and finally, the winner—a diffractive landscape lens. A landscape lens for our

application is simply an aperture stop placed one focal length in front of the lens. This causes the light bundle to be telecentric in image space, a condition that allows the light to reflect off the modulator (which is located at the focal plane of the lens) and pass back through the aperture as it exits the system. The diffractive element is radially symmetric and should be easy to make, though it has the properties of a fairly exotic aspherical refractive lens. The modulator can be a flat reflector with all of the beam bundles from various field positions incident on it as close to normal as possible. This maximizes the modulator's efficiency.

Other designs suffered relative to the landscape lens concept. The triplet is far more complicated and would probably have only marginally better image quality. We studied the lens plus field-lens concept extensively. The image quality is not as good, it is more complicated, and a diffractive element would have to be etched on the face of the modulator. We also studied all-refractive designs. The optics required are so small that they would be quite expensive to fabricate and mount. The diffractive system described is somewhat more expensive when made with lithographic technology. However, if mass-produced in plastic, it would be very inexpensive.

(2) *Fabrication.* We converted the "landscape lens" design to a photomask layout for fabrication of the diffractive optical element. We accomplished this conversion with software specifically written for this project. We will soon use the photomask layout for fabrication of the structure with direct-write electron-beam lithography. Since the design does not require changes to the modulator, the prototype demonstration does not require new modulator fabrication, and we can use existing devices developed for external customers.

Interfacial Charge Removal for MOVPE-Grown pHEMTs by In Situ Cleaning

H. Q. Hou

Sandia identified the problems of metalorganic vapor phase epitaxy (MOVPE) manufacturing of pseudomorphic high-electron mobility transistors (pHEMT) and proposed novel processes to solve these problems. In situ thermal cleaning process developed through this project proved to be very effective and reliable in removing the interfacial charges. We achieved record high-performance pHEMTs (0.5 W at 35 GHz). We also developed an in situ chemical process using AsCl₃. This approach is very promising for on-chip integration of a variety of devices for circuit applications. Overall, we exceeded our expectations for this project significantly.

MOVPE is widely used for preparing a variety of III-V compound semiconductor devices. One of the vexing problems with MOVPE is the presence of the interface charge at the substrate-epilayer interface. This is particularly harmful for pHEMT as the interface charge increases the leakage current, lowering the breakdown voltage, and yielding poor pinch-off characteristics. As a result, MOVPE has not yet achieved comparable success to molecular beam epitaxy (MBE)-grown structures because of Si, O, and C impurities on the GaAs substrate surface that cause bypass leakage channel in pHEMTs.

In this project, we proposed *in situ* processes to remove the interface charges. The novelty of the proposed work lies in the *in situ* process of etching. The etched surface will not be exposed to air or unclean ambient; therefore, very minimal contamination will occur.

We employed two novel approaches to solving the interfacial charge problem. The first approach is to thermally clean the interfacial charges in the growth chamber prior to the epitaxial growth. We "soaked" the substrate in a high arsine flow (~300 sccm) at an elevated temperature (~750°C) for an extended period of time (~20 min). Depth profile analysis by secondary-ion mass spectroscopy

copy (SIMS) shows that the Si, O, and C concentrations are below the detection limit for thermally etched samples. We achieved high-electron mobility ($\sim 6500 \text{ cm}^2/\text{Vs}$) for a pHEMT design with a sheet carrier concentration of $2.5 \times 10^{12} \text{ cm}^{-2}$. This result is comparable to the best results achieved from MBE growth. Although it was not scheduled in the original proposal, we sent the thermally etched samples to a commercial foundry, M/A COM, for pHEMT fabrication. The complete test results are still pending, but the preliminary high-speed measurements show a record high performance for MOVPE-grown pHEMT structure, namely 0.5 W power at 35 GHz. This is extremely important for Ka band microwave communications.

The other approach is to chemically remove the surface impurities prior to the epitaxial growth. The first chemical precursor we used is trisdimethyl-aminoarsenic ($\text{As}(\text{N}(\text{CH}_3)_2)_3$, or TDMAA). TDMAA is a novel arsenic precursor. This makes it a very attractive precursor for both etching and surface passivation during etching. It was shown to etch GaAs and the native oxide under certain conditions during MBE growth. However, we found that TDMAA does not etch the GaAs substrate effectively in MOVPE process. This might be due to the low partial pressure of TDMAA in MOVPE process, although the detailed mechanism is not clear at this point.

We then looked into another etching precursor, AsCl_3 . Since the original milestones were satisfactorily accomplished by the *in situ* thermal etching process, we emphasized the application of AsCl_3 for the regrowth on AlGaAs. This subject is very closely related to the pHEMT manufacturing, and the work we did offers a promising process for integration of pHEMTs with other devices on the same chip.

In summary, we identified the problems of MOVPE manufacturing of pHEMTs. *In situ* thermal cleaning process developed through this project proved to be very effective and reliable in removing the interfacial charges. We achieved record high-performance pHEMTs. We also developed an *in situ* chemical process using AsCl_3 . This approach is very promising for on-chip integration of a variety of devices for

circuit applications. Overall, we exceeded our expectations for this project significantly.

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3531.110

Infrared Quantum-Well Intersubband Photodetector Development

T. J. Drummond, S. R. Lee

Infrared Quantum-Well Intersubband Photodetectors (IR QWIPs) relevant to this project are intended to detect light with a wavelength in the range of 1-2 microns. The semiconductor materials of choice are InGaAlAs alloys with an InAs mole fraction of 0.40. There is no suitable substrate material for this alloy having the same lattice constant. The solution is to start with a GaAs substrate and epitaxially prepare an alloy buffer layer with the lattice constant graded from that of GaAs to that of the desired InGaAlAs alloys. The buffer layer must be of high crystalline quality and have a surface lattice constant matching that of InGaAlAs. In an ideal buffer layer (1) the surface lattice constant is stable under continued growth and subsequent device processing, (2) the buffer layer thickness is minimized, and (3) the buffer layer surface is globally smooth on the order of a few atomic-layer thicknesses.

At the outset of the project it was possible to synthesize buffers with high crystalline quality and a stable surface lattice constant matching that of the device

material. The goal was to simultaneously minimize layer thickness and improve surface smoothness without compromising structural stability in the buffer. Recently published results found in the relevant literature suggested that our previous design thickness could be reduced by a factor of three to four. The published report was not conclusive.

We prepared and partially characterized samples. Available results support the hypothesis. Thinner layers are smoother than thicker buffer layers. Control of the surface lattice constant degrades for a full factor of four reduction in buffer layer thickness, as expected. Final analysis of the intermediate layer thickness samples will define the maximum layer thickness reduction that may be achieved.

To achieve an appropriate buffer layer for the subsequent growth of an InGaAlAs QWIP, the standard approach is to fabricate a step-graded buffer structure of InGaAlAs. We increased the InAs mole fraction by 0.03 per step out to the target composition; we increased the AlAs mole fraction step in equal increments to attain an InAlAs ternary alloy in the final step; and we adjusted the GaAs mole fraction to achieve stoichiometry in each step. Conditions for the growth by molecular beam epitaxy (MBE) were previously optimized for 300-nm-thick steps. Results reported elsewhere suggest that this thickness could be reduced to about 75 nm per step without seriously compromising the structural integrity of the buffer structure.

We grew a series of layers under nominally optimal conditions with layer thicknesses as small as 50 nm. The sample with the thinnest layers was smoother than all other layers but did not achieve the target surface lattice constant. All other layers (above the critical 75-nm thickness) had a comparable surface smoothness. Thicker layers had the desired target lattice constant. Characterization of the thinner layers approaching the critical thickness from above have not been fully characterized. However, assuming that the surface smoothness correlated with structural relaxation and the achievement of the target surface lattice constant, the hypothesis appears to be valid. This implies that high-quality buffers can be grown in less time and at a lower cost.

Advanced Quantum-Well Structures for Improved Modulator Performance

I. J. Fritz, S. A. Casalnuovo, J. F. Klem

Semiconductor vertical-cavity optical modulators typically employ square quantum wells (QWs) in their electrooptic active regions. The resultant modulation then depends on Stark shifts that are quadratic in applied voltage, leading to a highly nonlinear response and low-voltage sensitivity. To improve sensitivity and reduce nonlinearities, Sandia investigated the electrooptic properties of asymmetric QW structures. To obtain operation near 1300 nm, we studied QW structures utilizing alloys in the InGaAlAs materials system, grown on GaAs substrates with an intermediate strain-relieving buffer layer from the same material system. We employed tunneling-resonance calculations to determine the low-lying energy levels and their dependence on electric field for ten different asymmetric QW structures. From these results, we chose two structures with strong linear components to their Stark shifts for experimental investigation. We grew these structures by molecular beam epitaxy (MBE) in the form of p-i-n diodes to allow application of external fields. We investigated the electric-field dependence of the band-edge position and linewidth with photocurrent and electroreflectance spectroscopies. We found that a residual background doping in the intrinsic region caused nonuniform fields in these initial structures, making evaluation of the electric-field effects somewhat uncertain. Making appropriate corrections for these nonuniformities, we observed Stark shifts that are in reasonable agreement with the theoretical calculations. These structures show promise for improved vertical-cavity modulator applications.

Semiconductor vertical-cavity reflectance modulators typically employ square QWs in their electrooptic active regions. The resultant modulation then depends on Stark shifts that are quadratic in applied voltage, leading to a highly nonlinear response and low-voltage

sensitivity. To improve sensitivity and reduce nonlinearities, we investigated the electrooptic properties of asymmetric QW structures with band-edge wavelengths near 1300 nm. Due to the reduced symmetry, these structures have a linear leading-order term in the dependence of their bandgap on applied field.

To obtain operation near 1300 nm, we studied QW structures utilizing alloys in the InGaAlAs materials system, grown on GaAs substrates with an intermediate strain-relieving buffer layer from the same material system. The QW structures were formed from multiple layers of the InGaAs and InAlAs alloys that are lattice-matched to the buffer. By varying the duty cycle of the layer thicknesses in a multilayer structure, it is possible to effectively produce a continuous change in the semiconductor bandgap to produce active regions with arbitrary potential profiles.

We employed tunneling-resonance calculations to determine the low-lying energy levels and their dependence on electric field for ten different asymmetric QW structures. From these results, we chose two structures with strong linear components to their Stark shifts for experimental investigation. The first of these is a structure that has a (effective) sawtooth-shaped potential repeated multiple times. The sloped potential profile in such a structure acts as a built-in pre-bias, thereby leading to a linear component in the Stark shift. The second structure chosen for investigation has three QWs with slightly different bandgaps, with the triplet being repeated multiple times through the structure. With increasing applied electric field, the ground-state energies of such structures degenerate, leading to level-repulsion effects (Stark delocalization) that produce rapid shifts of the bandgap.

We grew the two structures discussed above by MBE in the form of p-i-n diodes to allow application of external fields for studies of their Stark shifts. We investigated the electric-field dependence of the band-edge position and linewidth with photocurrent and electroreflectance spectroscopies. We

found that a residual background doping in the intrinsic region caused nonuniform fields in these initial structures, making evaluation of the electric-field effects somewhat uncertain. The photocurrent spectra exhibited a marked broadening with increasing applied voltage and only very small peak shifts. On the other hand, the electroreflectance spectra, depending on the derivative of the absorption edge, exhibited distinct peaks at the bandgap energy. We estimated the magnitude of the Stark shifts from the field-dependent positions of the lowest-energy electroreflectance peaks. We roughly estimated the electric fields by measuring all voltages relative to the voltage at which definite shifts began to appear. With these approximate corrections for the nonuniformities, we observed Stark shifts that are in reasonable agreement with the theoretical calculations.

These structures show promise for improved vertical-cavity modulators for applications involving both fiber-based systems (utilizing the low-dispersion wavelength regime of silica fibers) and for free-space applications utilizing commercially available lasers near 1320 nm.

3531.130

High-Temperature Stereolithography Female Molds for Small-Lot Composite Manufacturing

J. A. Emerson, C. L. Atwood, M. W. Donnelly, P. A. Cahill

Manufacturing needs direct-fabricated tools generated by stereolithography that require high-temperature (> 150°C) processing for a wide range of applications, including molds for injection molding, tooling for composite layup, and under-the-hood applications. In a previous project, Sandia directly fabricated female molds by stereolithography for use as tooling for composite layup. We chose near-room-temperature curing prepreg materials

because of the limited end-use temperature of the stereolithography materials. If the molds stereolithographically produced could be used at higher temperatures, there would be a wide range of applications in the aerospace industry. Our idea could be extended into other areas; for example, the time for direct fabrication could be greatly reduced by building only a skeleton structure in the machine and with processing further to make the finished, full-density part.

The motivation of this work is to increase the service temperature of stereolithography-generated parts, particularly for female molds used in small-lot applications such as composite construction or encapsulation. A skeleton structure was fabricated in the stereolithography, infiltrated with an anhydride-cured epoxy, and thermally cured. This new material becomes the matrix, with former skeleton material being integrated. Sandia found that the properties of the final part exhibit the properties of the cured matrix material. From the dynamic modulus data, the stereolithography-generated skeleton has modulus of about 2 MPa at 70°C, whereas the filled skeleton has modulus of 100 MPa at 70°C. The modulus at 140°C was about 60 MPa for the filled part. We estimated the skeleton material modulus to be 2 MPa at 140°C. This increase in modulus doubles the service temperature of the conventional stereolithography-generated molds. Further refinement in the epoxy chemistry (change in curing agent and cure temperature) would extend the use temperature for required applications. To test this idea, we increased the cure temperature to 170°C instead of the normal 100°C. The glass transition temperature (T_g) of the matrix material did not increase, and modulus of the final part was about the same as for the 100°C cure. The point made here is that we can extend the service temperature to 170°C without any deleterious effects on the skeleton or matrix material. This work demonstrates that molds made by stereolithography can be enhanced both in higher operating temperatures and in toughness.

3532.040

Modeling the Atmospheric Entry Physics and Terminal Explosions of the Anomalous October 3, 1996, Bolide Swarm

M. B. E. Boslough

This project involved three main thrusts: (1) determine the trajectory and heliocentric orbit of one of the October 3, 1996, bolide events, which by proxy yields the orbital elements of the entire swarm, (2) develop new code and programs to assess the capture hypothesis and analyze the possibility of aerobraking and capture of a meteoroid into Earth-orbit, and (3) combine atmospheric entry, opacity, and terminal explosion modeling to synthesis observational data to provide interpretations and deeper understanding of atmospheric explosions that are observed by global monitoring instruments. Sandia made significant progress in all three areas.

(1) *Summary of October 3 trajectory determination.* We extracted the velocity history and trajectory of the October 3 bolide from a videotape record. This required two trips to El Paso to take calibration photographs with university collaborators. We modeled the ballistic flight to determine the heliocentric orbit and used winds aloft Radiosonde data to determine its darkflight path and predict its impact location in Texas. This result eliminates our initial capture hypothesis, but strongly supports our subsequent swarm hypothesis. Of the sixty infrasonic events of October 3 and 4, this is the only event for which a trajectory determination was possible, and its orbit therefore applies to all the other events of the swarm.

(2) *Code development.* We developed a computer program to calculate the trajectory and evolution of an ablating, fragmenting bolide as it passes through a planetary atmosphere. The computer model indicated the difficulty associated with having a bolide fragment at relatively high altitude (as the physical observations indicated), with some pieces ablating in the atmosphere while others managed to temporarily escape and re-enter at a later location.

A related project involved adding a potential field solver to Sandia's shock physics code, CTH. The addition of this piece of code to CTH allows for the computation of a gravitational potential and can be easily modified to compute electrostatic potentials as well. We can use these potential fields to compute the trajectory and influence of bolides passing through the Earth's atmosphere.

(3) *Bolides and holes in the far-ultraviolet (FUV) dayglow.* We coupled hydrodynamic bolide simulations to atmospheric radiative transport models with collaborators to provide an explanation for holes in the FUV dayglow that were observed by two UV satellites. This combines atmospheric entry, opacity, and terminal explosion modeling to relate these emission holes to the normal flux of meteorites in the Earth's upper atmosphere, and potentially provides a method to unambiguously discriminate bolides from other atmospheric explosions.

Publications

Refereed

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Chemical Feedstocks for the Future: Oxidative Dehydrogenation

N. B. Jackson, J. E. Miller, A. G. Sault, T. M. Nenoff

Oxidative dehydrogenation (ODH) is a potential chemical process for producing olefins such as ethylene and propylene—the organic chemicals with the largest production in the U.S.—from alkanes. Small alkanes are readily available from nature—from natural gas and petroleum—and as major by-products from refinery operations. However, the building blocks for all economically important chemicals are olefins. At present, these small olefins are produced by a direct dehydrogenation process used by all the major chemical companies for decades. Direct dehydrogenation is an inefficient, energy-consuming, endothermic process that creates large amounts of carbon deposits on reactor walls that must periodically be burned out, resulting in stress of reactor walls and CO₂ emissions. ODH is an exothermic process that produces heat and has the potential, with a properly designed catalyst, to minimize waste, energy consumption, and CO₂ production. The production of olefins is a highly competitive business. Due to economic and environmental concerns, industry has begun to be open to a step change in olefin production technology. We are targeting the work in this effort toward understanding structure-activity relationships of potential ODH catalysts made of mixed metal phosphates and oxides. In particular, we are directing our attention to the lattice oxygen of the catalyst and its reactivity versus the selectivity of the catalyst. The “trick” is to identify the traits of a catalyst that will activate the alkane and oxidize it to the olefin, yet will not combust the product olefin to CO₂.

We constructed a reactor capable of safely testing catalysts for ODH of both ethane and propane. An integral part of this system is an online analysis capability for evaluating the reaction products. Using this reactor we began to study ODH of ethane over perovskite catalysts. Perovskites are a class of compounds comprising the structure ABO₃. At high temperatures, or when defects (primarily oxygen vacancies) or substitutions are present, the crystal structure is strained, and the oxygen conduction increases. The conducting ability of oxygen and therefore the availability of oxygen on the surface of a perovskite is a function of its composition and temperature. To better understand the relationship between the availability of oxygen on the surface of a catalyst and the reactivity/selectivity of the catalyst for ODH of ethane, we chose a perovskite system, the BaCeO₃-based ceramic doped with Nd, La, Y, or Ca for study. This was the first catalytic study of this system.

Since oxygen mobility is more significant in perovskites at higher temperatures, it is not surprising that these materials were all more active at high temperatures (> 873°K). However, upon closer analysis, we discovered that under the more severe reaction conditions where the reactivity and selectivity are best, the perovskite structure is not retained in any of the materials yet analyzed, and a mixture of carbonates and oxides is formed, as revealed by x-ray diffraction (XRD). X-ray photoelectron spectroscopy (XPS) shows strong enhancement of the Ba signal at the expense of Ce after reaction. Dopants affect this enhancement, with Y causing a depletion of Ce before reaction, while for BaCeO₃ and the Ca-doped material, Ce levels decrease only after reaction. We also observed a strong enhancement of the oxygen signal after reaction suggesting the formation of BaO₂ at the surface.

While both the Ca- and Y-doped materials showed enhanced total combustion activity below 873°K, only the Ca-doped material displays enhanced ethylene production at 973°K. This gives some indication that the strong and plentiful oxygen on the surface of the catalyst above 873°K leads to complete oxidation of the ethane to CO₂. For all the catalysts studied, CO₂ is a major product. The ready formation of CO₂ is most likely associated with the reactive and available oxygen on the surface of the oxygen-conducting perovskites. The perovskites are acting as oxidizing catalysts, but are too oxidizing to be desirable.

We also synthesized mixed metal phosphate catalysts, including Zr/Ta/PO₄, Ta/PO₄, Ta/Ce/PO₄, Zr/Ti/PO₄, and sulfated versions of all metal phosphates. University collaborators synthesized Zr/Nb/PO₄, Ti/Nb/PO₄, and Nb/PO₄ analogues, both sulfated and nonsulfated. We characterized the majority of these catalysts for their acidic strength, crystal character, and surface area. We tested the activity of these catalysts for ODH or other relevant reactions. Although the ODH activity of these catalysts has been low, some have shown remarkable selectivity. Another interesting point is that these materials deactivate in a unique way, with carbon deposition occurring on the Lewis acid sites during certain reactions. However, these sites do not necessarily affect the activity for desired reactions.

Publications

Other

Jackson, N. B., T. M. Nenoff, S. Thoma, D. A. Rakestraw, and D. Kambhampati. 1997. “Mixed Metal Phosphates as Solid Acid Catalysts.” Paper presented to the North American Catalysis Society Meeting, Chicago, IL, 22 May.

Global Approaches to Infrastructural Analysis (GAIA)

D. Engi, T. E. Drennen, R. P. Thomas, D. M. Jeppesen, D. L. Harris

Our country (and, in fact, the global community) is vulnerable to significant costs (in both dollars and human lives) associated with stresses arising from sources that are both manmade (e.g., war, terrorism, and political disruptions) and natural (e.g., hurricanes, tornadoes, earthquakes, droughts, and floods). There is currently a need for a comprehensive, integrated suite of information that would be of value in helping identify opportunities for technological responses to these stresses. This project is directed toward the development and deployment of a decision support system (DSS) that will provide timely, accurate, and high-impact information. The context for this information is the international arena with an emphasis on the technological aspects of responses to these stresses.

This proposal is motivated by Sandia's recognition that enhancing our nation's ability to manage vulnerabilities of global infrastructures is necessary to maintain our national security. We recognize the technical challenges of creating an integrated infrastructure DSS and propose a strategy consisting of architecture, process, and metrics to address these challenges. We propose to create an architectural framework to support the system, methods for specifying modeling and analysis, integration of new commodities into the system, and metrics for measuring the utility of the knowledge provided. Integrating the computer modeling and simulations of diverse commodities, explicitly considering the international arena as the system, and combining the judgment of international subject matter experts are innovations now possible due to the advent of high-performance computers and the global information infrastructure.

We accomplished three major modeling tasks and produced significant analytic results during FY97: (1) developed dynamic simulation models of four critical infrastructures (water, agriculture, energy, and greenhouse gas), (2) integrated these models into a single critical infrastructure model, and (3) developed a World Wide Web (WWW) page and implemented a graphical user interface (GUI) to access the infrastructure model over the Web. We presented analytic results based on these models as a part of the input to Vice President Al Gore.

The infrastructure models that we implemented followed three general design constraints. We identified the commodity flows between models during the initial infrastructure analysis and implemented these flows to allow the models to be integrated into a single dynamic system model in a straightforward fashion. Second, we constrained the models to be executable from a Web-based server engine. Finally, we designed each model to be robust so it could be applied to a variety of geographic regions by changing only the model data base; the model dynamic should not have to change based on the particular region of interest.

Each of the four models that we developed provides the capability to simulate the flows of a commodity through their respective infrastructures. We integrated these models to view the dynamics of a more complete system and to simulate the impact of changes in one commodity flow on the flows of other commodities. We have several examples of this integration. We integrated the energy infrastructure model with the greenhouse gas model so we could observe the changes in the greenhouse gas loading due to increased energy production. We integrated the agronomic model with the greenhouse gas model, allowing us to model the gas loading due to methane production from the decay of biomass in rice paddies and the enteric and anaerobic emissions from agriculture animal populations. In addition, we

integrated the agronomic model with the water model to determine the ability of a water region to supply the agriculture end-use sector with sufficient water to produce grain. These examples illustrate some interdependencies between infrastructures. These examples also reinforce a basic premise that, although we modeled these infrastructures independently, we must integrate the models in order to simulate the effects on one commodity from changes in another.

We then executed the integrated model through the year 2025. We presented the results of the simulation illustrating the changes in the flows due to changes in their basic drivers and the interactions between commodities. The results of these simulations provide information that policy planners and decision makers, such as Vice President Gore, can use when managing these critical infrastructures.

We also installed a WWW server and created Web pages that include documentation describing the results of the model simulations. In addition, we installed a Web-based model execution engine on our Web server and created a GUI to allow the execution of the model and presentation of the simulation results over the Web. Use of the Web and Web-based technologies has improved the capability for collaborative decision making and policy planning. People anywhere in the world share the same model results and simulation data in real time, with the Web providing a communication medium for sharing information, discussion, and evaluation of model results.

Publications

Other

Thomas, R. P., S. H. Conrad, D. M. Jeppesen, and D. Engi. 1997. "Understanding the Dynamics of Water Availability and Use in China." Sandia Technical Report SAND97-1626, 1 July. Sandia National Laboratories, Albuquerque, NM.

Advanced Subterranean Warfare (ASW) for Deep Underground Structures

G. E. Sleepe

Under this project, Sandia applied advanced subterranean warfare (ASW) methods to the problem of monitoring deeply buried facilities. The project utilized a combination of seismic modeling, signal analysis, and experimental test verification to assess the feasibility of monitoring seismic emissions from deep facilities. This three-pronged approach provided the basis for establishing system design requirements and sensor placement rationale for characterizing and locating underground activity. We performed a deep-tunnel experiment at the Nevada Test Site (NTS) p-tunnel; signal processing demonstrated the ability to detect and identify deep activity. Furthermore, we developed a preliminary 3-D seismic propagation model, which provided insight to the problem and potential solutions.

This project focused on establishing the feasibility of monitoring deeply buried facilities using geophysical methods. We performed a system architecture study and established a methodology for utilizing surface seismic sensors and near-portal acoustic sensors. Based on this system study, we designed an experiment for the p-tunnel at the NTS. The experiment involved placement of seismic sensors on the surface (approximately 300 m from the tunnel to the surface and up to 400 m offset) and acoustic sensors near the tunnel entrance portal. Furthermore, we deployed equipment representative of deeply buried facilities to determine if the equipment could be monitored on the surface and near the portal. The equip-

ment included generators, jack-hammers, small explosives, and a man-train. We performed the experiment in two phases such that the second phase incorporated lessons learned from the first phase. We analyzed the collected data using advanced signal processing methods.

The analysis demonstrated that the equipment could be successfully detected and identified from the remote sensors.

We also applied signal processing methods for estimating the location of the equipment, but met with less success due to the complex tunnel structure and local geology. We used 3-D seismic-wave propagation modeling to study this problem. Code enhancements were required to properly model this buried structure problem. Successful enhancements included the brute-force incorporation of topography, tunnel structure, and complex seismic sources. The modeling effort additionally required the use of effective absorbers at the model boundaries to reduce reflection artifacts. We successfully incorporated such absorbers into the code but could not complete extensive case studies using the new model by the end of the fiscal year. In summary, this project successfully demonstrated the feasibility of detecting and identifying activity within deep facilities. We identified localizing such activity as a challenging task, and the seismic model developed under this project should prove useful in future efforts in this area.

Publications

Other

Sleepe, G. E., G. E. Elbring, H. D. Garbin, and M. D. Ladd. 1997. "Advanced Subterranean Warfare (ASW) for Deep Underground Structures." SAND Report, in progress.

Dispersive Measurements of Velocity in Heterogeneous Materials

L. C. Chhabildas, W. M. Trott

The purpose of this project is to develop new experimental techniques for validating material response at the mesoscopic level. This approach will allow unprecedented abilities to develop physically-based material models that can be used for true predictive capabilities in a wide variety of applications, including stockpile stewardship, energy, and industrial purposes.

We anticipate this project to be a research effort involving close collaborations between theoretical and experimental capabilities existing at both Sandia and several universities. In the initial phase, we defined the overall project and evaluated the feasibility of performing the experimental and theoretical investigations.

We held several working meetings at Sandia involving researchers from our university collaborator and team members from Sandia. These meetings resulted in the following definition of a phased approach to resolving the research issues for this project:

(1) The first phase of the experimental project will evaluate experimental parameters for measurements of particle velocity in heterogeneous materials subjected to shock loading. These efforts will include evaluation of the spatial and temporal resolution possible with the proposed experimental technique.

(2) We will perform theoretical modeling efforts to determine the critical parameters necessary for validating numerical simulations of shock-wave

propagation in heterogeneous materials. Initial indications are that the average particle velocity and several spatial and temporal moments of the velocity may be the appropriate variables to measure. These variables are not presently attainable in normal shock velocity measurements and will require several specific modifications to existing techniques to achieve.

(3) We will conduct experimental studies with a university collaborator in the first year to evaluate the ability to measure these critical parameters and to compare them with predicted response. The initial studies conducted this year defined the overall experimental hardware, the need for advanced data-reduction software, and the general experimental facilities needed to carry out these experiments. In particular, we intend to use nonsequential ray tracing code to evaluate the optical components of a line-imaging velocity interferometer system to optimize the interferometer's design and performance.

(4) We acquired specialized and appropriate optical lenses to enhance the imaging performance of the velocity interferometer system. This is intended to improve the spatial and temporal resolution of the instrument.

(5) We initiated activities this fiscal year to transfer the technologies for performing both the experimental investigations and the numerical simulations to our university collaborator. We accomplished these through individual visits by members of the team that will be working on this project. In addition, we identified two other universities that have unique theoretical and experimental capabilities of benefit to this project. We arranged with the appropriate investigators at these universities to hold future discussions related to specific tasks in support of this project.

3533.030

Ceramic Membranes for Electrically Driven Ionic Separations

E. R. Lindgren, M. G. Hankins, T. J. Boyle

The goal of this project was to investigate a novel, electrically driven, ionic separation scheme that uses sol-gel-treated ceramic as ion-selective membranes. The postulated physics for the separation studied was electrical conduction along the pore surface, which is fundamentally different from the separation physics studied in other investigations. Ceramic membranes have previously been considered for ionic separations, but the separation physics depends on the physical dimensions of the pores, which result in ionic exclusion in very small pores (0.05 μm). Ionic exclusion in porous media is known to occur in pores of sufficiently small size when the net surface charge or zeta potential prevents ions of the same charge from entering the pore. Ceramics that have an average pore size in this range, however, are prone to fouling, which can lead to inefficiency.

We treated porous ceramic tubes (3.5 inches OD, 3 inches ID, and 3 inches long) with an average pore size of 0.6 μm and 35 vol% porosity with various sol-gels using methods already developed by Sandia. Pores of this size are considered too large to exhibit any ionic exclusion. The sol-gel coating constituents tested were alumina, zirconia, and titania for positive zeta potentials and silica for negative zeta potentials. We treated one ceramic with a quaternary amine (cetyltrimethyl ammonium hydroxide), which produces a positive zeta potential surface. We tested the treated ceramic by measuring the electroosmotic flow (as indicated by liquid level changes) and voltage drop through the ceramic with an applied constant current of 200 mA. We analyzed samples collected from both sides of the ceramic by ion chromatography to identify the ions carrying charge through the ceramic and thus determine the selectivity of the ceramic. We used buffers with carefully

chosen compositions on both sides of the ceramic to allow the determination of the zeta potential and ion selectivity.

We conducted a number of conduction experiments using porous ceramic treated with silica, which should produce a uniform negative zeta potential surface, and alumina, titania, zirconia, and a quaternary amine, which should produce a uniform positive zeta potential surface. The silica produced the negative surface as expected, and the quaternary amine coating produced a slightly positive surface. The alumina, zirconia, and titania did not produce positive surfaces as hoped. The results of ion chromatography analyses for the silica-coated ceramic suggest that cations carried most or all of the applied current into and out of the ceramic, supporting the surface conduction hypothesis. This is best illustrated by the fate of the lithium and chloride ions initially present in the ceramic pore space. A significant amount of lithium appeared in the cathode chamber, and a negligible amount of chloride appeared in the anode chamber. The charge balance between the anionic species and the cationic species in each compartment is an important measure of precision of the analytical method and was generally greater than 90%. In the anode compartment, there was a significant loss of sodium ions, which represents over 90% of the applied current. There was only a slight increase in the moles of anions present, which could account for at most 7% of the applied current. The overall balance between the amount of current applied and the apparent change in charge was 97% and is a measure of the relative accuracy of the current measurement method and the analytical methods. Note that while the moles of the buffering ion used in each compartment remained relatively constant, the concentration actually changed due to the volume changes caused by electroosmosis. Solution level changes due to electroosmosis can also be used to estimate a zeta potential of -21 mV, which is quite reasonable.

Policy and Resource Allocations in Risk Management

R. G. Knowlton, D. M. Boak, P. I. Pohl

Sandia developed an approach to assist U.S. Department of Defense (DoD) and U.S. Department of Energy (DOE) organizations in prioritizing environmental cleanup (disposition) activities. This approach draws on Sandia's capabilities in risk and decision analysis to (1) assist in formulating performance objectives and metrics and (2) establish risk-management procedures to plan and prioritize an effective national-level cleanup effort. The approach accounts for the complex nature of the problem to be solved, ever-increasing pressure from Congress to accomplish more with less funding, and the need for agencies to demonstrate clear project progress. The DoD alone has 17,000 sites potentially requiring cleanup encompassing 25 million acres that must be screened, evaluated, and dispatched. The assessment and management challenges of environmental cleanup are thus of national interest. We designed the management oversight tools to help the high-level manager identify potential problem areas before they affect project progress, minimizing programmatic risks.

This year we focused on the policy decisions and risk-based resource allocations in environmental cleanup. We used the approach we developed to (1) screen sites on the basis of human health risk, (2) systematically develop risk-management options based on cost, risk, and benefit trade-offs, and (3) manage the site disposition process. This approach is intended to assist the environmental program manager responsible for hundreds of sites and budgets with hundreds of millions of dollars in ensuring that, despite uncertainties, real health risks are being identified and resolved in a demonstrably cost-effective and timely manner. The approach also describes management oversight tools based on an adaptation of well-established statistical quality-control methods. We designed the management oversight tools to help the high-level manager identify potential problem areas before they affect project progress, minimizing programmatic risks.

Publications

Refereed

Boak, D. M., R. G. Knowlton, and W. Beyeler. 1997. "Policy Decisions and Risk-Based Resource Allocations in Environmental Cleanup." Sandia Technical Report SAND97-2925, November. Sandia National Laboratories, Albuquerque, NM

3533.040

Developing On-Line Process-Monitoring Capabilities

D. S. Blair

The on-line use of chemical characterization systems for process monitoring and control has experienced tremendous growth in the past decade. From environmental remediation to process control, higher-quality product at a significantly reduced cost can result from obtaining accurate chemical information of a process. Within the DOE complex, applications for process-monitoring systems include real-time characterization of caustic waste sludge prior to formation of high-level waste (HLW) glass logs, pipeline slurry for the GAAT-TS tank waste disposal, and a broad range of industrial applications. Available monitoring technologies can be divided into two classes: chemical sensors and analytical instruments. Appreciable research dollars have been spent designing and building analyte-specific chemical sensors. While sensors can be relatively inexpensive, they cannot compete with the reliability, stability, and breadth of information provided by analytical instrumentation. This is due to the decades of research dollars spent developing the existing lines of commercial instrumentation. A similar time frame could be expected for chemical sensors to reach this state of maturity. Today's research environment does not allow ample time to design and build application-specific sensors that are reliable enough for online monitoring. We are asked to provide solutions to existing process characterization problems with extremely short time constants (typically < 2 years). This is difficult to do with chemical sensors since they cannot satisfy overall system requirements for accuracy, precision, and

reliability due to the limited research time available.

We modified and upgraded an infrared spectrometer for research in the area of process analytical chemistry. We designed, built, and evaluated a flowthrough sample cell in conjunction with various waveguide samplers to examine useful sampling formats for process analytical chemistry.

We met with researchers from Los Alamos National Laboratory (LANL) to investigate possible collaborative interactions between both of the laboratories, specifically in the area of process chemistry. From that, we organized a Process Analytical Chemistry Symposium with LANL to investigate possible collaborative interactions on a larger scale.

3533.050

SAM Telemetry for Measurements While Drilling

S. Ballard, D. E. Gallegos, R. G. Keefe

The objective of this project is to determine whether Sandia's surface area modulation (SAM) wireless telemetry technology is viable for measurement-while-drilling and logging-while-drilling applications. A field test of the system was conducted during which Sandia deployed the system in line electrode mode on both coated and uncoated tubing. In addition, we tested coaxial mode using uncoated sucker rods. We thoroughly characterized the performance of the system under each of these conditions.

SAM telemetry utilizes existing oilfield tubulars, such as casing and drill pipe, to create a grounded electrical circuit capable of transmitting high-quality data streams from a position near the bottom of a well to the surface. By controlling, or modulating, the effective electrical length of the drill string from a downhole position, the current flowing through the circuit changes throughout the circuit and can be detected with instruments on the surface. Modern electronics and military communication standards allow detection of the minute changes in the circuit that encodes the transmitted data.

Since the drill string is in contact with the earth, it is termed an *earth-*

immersed electrode, which leaks current to the earth along its length. However, since the drill string is a much more conductive current path than is the earth, some percentage of the source current will make it to the bottom of the drill string. If this downhole current is as little as 1% of the source current, the downhole electronics package will be able to encode the data in a manner that can be decoded at the surface.

The downhole electronics package utilizes serial and frequency modulation (FM) communication techniques to transmit sensor and package diagnostic data to the surface. The package can also detect data encoded at the surface, resulting in a half-duplex telemetry system.

During a recent test of this system, we obtained a wealth of diagnostic information that allowed us to gain important insights into the behavior of the system. We are still analyzing the results to extract all information possible. A very important observation was that coating the tubing with an electrically insulating material vastly improved the performance of the system. It also appears that most of the electrical signals do not propagate through the earth, as we previously hypothesized, but rather travel up the source electrode to the surface data-acquisition system. We are currently investigating techniques designed to exploit this new insight.

3533.080

Applicability of a Metalloprotein Toxic Heavy-Metal Detector to DOE Production and Waste

T. F. Luera, Jr., R. J. Lipinski, D. J. Bragg, Jr., D. E. Bodette

A kidney protein called metallothionein (MT) is the basis for a heavy-metal detection system. MT binds to and controls the trace elements of Zn and Cu in the body. MT also binds to other metals (e.g., Pb, Hg, Cd, Bi, Ag, and Au) and does so with differing affinities. The MT protein is chemically bound to a trace amount of a radioisotope and is immobilized on a filter column for support. When a solution of a heavy metal with a greater affinity for the protein than the metal radiotracer is

poured through the filter, a mechanism similar to ion exchange displaces the radiotracer. A gamma-ray counting instrument readily detects the displaced radiotracer in the filter column's effluent.

The main objective of this study is to determine whether this system has adequate sensitivity and selectivity for detecting heavy metals in aqueous solutions. Prior experiments did not yield the same sensitivities as reported by others. Sandia performed tests to verify experimental parameters and results from previous work. We performed further tests to determine the specific affinities of metallothionein for the metallic species of most concern to DOE: mercury, lead, and chromium.

The conjectured deficiencies of prior experiments were investigated and determined to not have influenced our results. One of the major concerns was that the metal solution concentrations were unverified. It was possible that some of the metal might have precipitated, leaving the metal concentration in solution much lower than expected. An independent lab quantified the metal concentrations using an inductively coupled plasma (ICP) technique. The measured concentrations were within 6% of the nominal expected concentrations and so were not the problem. Another concern was that the residence time in the filter columns was too short. We made changes to increase the residence time by about a factor of 100 and repeated the tests. The longer residence time yielded essentially the same results as before. The source of the discrepancy with published data is as yet unknown.

The threshold sensitivity of the metallothionein-radiotracer (MT-RT) system for detecting heavy metals is at the ppm level. The measured threshold concentrations of detectability were, in descending order, mercury (147 ppm), lead (16 ppm), iron (11 ppm), cadmium (10 ppm), and chromium (10 ppm). The toxicity characteristic leaching procedure (TCLP) regulatory limit for mercury is 0.2 ppm, for lead 5.0 ppm, for cadmium 1.0 ppm, and for chromium 5.0 ppm. Based on our current results, therefore, the MT-RT detection method is not acceptable for mercury or silver and is not necessary for iron, but it might be useful as a general positive/negative test for lead, cadmium, and chromium.

Discussions with several experts in the fields of environmental characterization, monitoring, and treatment revealed that most field characterization technologies are quite sophisticated and costly, and that quick, inexpensive, qualitative screening methods would be of great value in the environmental market. Additionally, there were no highly desirable technologies available for automatic sensing applications, such as process effluent monitoring. The major client of environmental firms seems to be the government, especially the agencies associated with the Department of Defense and the Department of Energy. Commercial entities and the Environmental Protection Agency both require some environmental products and services, but the government represents by far the largest market potential. If this system were to perform with the optimal specificity and sensitivity, it would be of significant value.

The technique we used to bind the MT onto a polyacrylamide bead bed is a standard practice in affinity chromatography (AC). AC makes use of the fact that proteins preferentially bind to specific ligands. There are over 50 companies that provide a range of different synthetic supports, MT proteins, and binding ligands to the AC community. The well-developed technologies associated with AC, if applied to the MT-RT system, could provide significant gains in the sensitivity. Gains are also possible through simple process optimizations, such as pH and temperature variations. The MT-RT detection method demonstrated sensitivity at the ppm level to toxic heavy metals and can be turned into a commercial product through a focused research program.

Publications

Other

Randles, K. E., D. J. Bragg, D. E. Bodette, R. J. Lipinski, and T. F. Luera. 1997. "Applicability of a Field-Portable Toxic Heavy-Metal Detector, Using a Radioisotope-Tagged Metalloprotein, to DOE Environmental Remediation and Waste Minimization Initiatives." Sandia Technical Report SAND97-2367, in review. Sandia National Laboratories, Albuquerque, NM.

Dynamic Simulation Models and Geographic Information Systems

T. E. Drennen, J. H. Ganter, L. A. Malczynski

The goal of this project is the development of a tool that combines dynamic simulation modeling (DSM) and geographic information systems (GIS) software to allow geographic visualization of policy options for a wide range of applications. As part of this project, Sandia performed a series of experiments to see if GIS data and possibly displays can be combined with DSM and applied to subjects like climate change, international energy flows, and global resources. We selected Powersim as the DSM for these experiments because of its open design OLE/OCX (object linking and embedding/OLE custom control) interface. We selected MapObjects™ over an initial client/server approach using ArcView. We spent the majority of the second year of this project dealing with integration issues.

During the second year of this project, we successfully completed a prototype demonstrating the concept. The prototype developed links to a very simple Powersim model on population dynamics in China at the provincial level.

A key component of the overall prototype is SandView, which we developed as part of this project using Visual Basic 4 and 5. The main purpose of SandView is to provide most of the user-interface functionality necessary for the prototype.

While we achieved the majority of our technical goals, there are several outstanding technical issues that were not resolved.

Publications

Refereed

Drennen, T. E., and J. H. Ganter. 1997. "DSM-GIS: An Application that Links MapObjects™ to the Powersim Dynamic Simulation Modeler." *Proc. 1997 ESRI*

User Conf., <http://www.esri.com/base/common/userconf/proc97/home.html> (San Diego, CA, 9–11 July).

Ganter, J. H. 1997. "SandView: A View Document Object for MapObjects™." *Proc. 1997 ESRI User Conf.*, <http://www.esri.com/base/common/userconf/proc97/home.html> (San Diego, CA, 9–11 July).

3533.070

Design-for-Manufacturability Applied to Photovoltaic Modules

J. M. Gee, S. E. Garrett, W. P. Morgan

Sandia is applying design-for-manufacturability (DFM) principles to photovoltaic (PV) module manufacturing. Current PV modules use discrete crystalline-silicon (c-Si) solar cells. The assembly process is over 20 years old, uses serial low-throughput process, and is difficult to automate. Through application of DFM, we are developing a new module assembly process that electrically connects and encapsulates all the c-Si PV cells in a module in a single step. The new assembly process (1) uses back-contact c-Si cells, (2) uses a module backplane that has both the electrical circuit and the encapsulation material in a single piece, and (3) uses a single-step process for assembly of these components into a module. This new process reduces module assembly cost by reducing the number of steps, by eliminating low-throughput (e.g., individual cell tabbing, cell stringing, etc.) steps, and by using planar processes that are easy to automate. We refer to this process as "monolithic module assembly" since it translates many of the advantages of monolithic module construction of thin-film PV modules to wafered c-Si PV modules. Simplifications in the module fabrication are estimated to reduce the cost of module fabrication by up to 50%, which corresponds to a reduction of around 25% in the total manufacturing cost for the module.

(1) *Examined and documented a set of assembly options.* We developed a total of four different assembly options and surveyed a wide variety of materials. The options included one-step, two-step, and three-step assembly procedures, and the materials included a variety of electrical attachment (conductive epoxies, conductive adhesives, and solders), backsheet (screen mesh, Tedlar™, and a proprietary polymer sheet from a U.S. PV manufacturer), and encapsulation (ethylene vinyl acetate and proprietary encapsulants from two U.S. PV manufacturers) materials.

(2) *Presented assembly options in a design review.* We documented these options and presented them in design reviews to four U.S. PV module manufacturers. Based on the design reviews, we selected two options for further development.

(3) *Assembled mechanical prototype.* We assembled mechanical prototypes and began thermal cycling testing. The thermal cycling tests found potential problems with our initial selection of a conductive-adhesive-coated copper tape for the electrical attachment. We are now examining conductive epoxies, which we believe to be much more reliable but also more costly.

(4) *Developed electrical prototype.* The work was sufficiently promising that we submitted a Technical Advance Disclosure (S-88,532/SC-6012, Photovoltaic Modules Using Back-Contact Crystalline-Silicon Solar Cells). We will complete electrical prototypes, pending successful completion of the thermal cycling tests.

Publications

Refereed

Gee, J. M., S. E. Garrett, and W. P. Morgan. 1997. "Simplified Module Assembly Using Back-Contact Crystalline-Silicon Solar Cells." *Proc. 26th IEEE Photovoltaic Specialists Conf.*, accepted.

Enhancing Energy Security Through New Routes to Petrochemical Feedstocks

A. G. Sault, T. J. Gardner, A. Martino

Sandia synthesized a series of hydrous titanium oxide (HTO)-supported Cr catalysts with Cr loadings ranging from 1.76% to 3.14% by weight. Surprisingly, the nearly twofold increase in Cr loading resulted in no systematic increase in activity for propane dehydrogenation. Conversions ranged from 6.6% to 7.7% under standard reaction conditions, with selectivities to propane exceeding 95%.

We also synthesized several Pt-based catalysts formed by encapsulation of Pt nanoclusters within both alumina and silica aerogels and xerogels and tested them for propane dehydrogenation. Pt loadings are less than 1% by weight for all samples. We used both transmission electron microscopy (TEM) and hydrogen chemisorption to investigate Pt particle size, resulting in particles on the order of 4 nm for all samples. Propane dehydrogenation activity is highly dependent on treatment history for these materials, with rapid deactivation observed for all samples. Reactivation is possible through a combination of oxidation in air to remove carbonaceous residues followed by hydrogen reduction. Furthermore, activation behavior appears to be highly dependent on the nature (aerogel versus xerogel) and identity (silica versus alumina) of the support, making valid comparisons between the various Pt catalysts difficult. The best Pt catalyst achieved a maximum propane conversion of 5.6%, but we observed conversions as low as 0.5% for some catalyst/pretreatment combinations. In general, selectivities to propane fall in the range of 65–85%.

We synthesized a series of supported Cr catalysts by ion-exchange of Cr(III) onto HTO ion-exchange materials. Cr loadings of 1.76%, 2.04%, 2.34%, and 3.14% resulted in propane dehydrogenation conversions of 6.8%, 7.7%, 7.7%, and 6.6%,

respectively, with selectivities to propane exceeding 95% in all cases. Thus, while we succeeded in increasing Cr loading through modifications to the ion-exchange procedure, we observed no corresponding increase in activity. This surprising lack of sensitivity to Cr loading is not well understood, and an explanation will require more extensive catalyst characterization than was possible under the limited scope of this project. The results to date suggest, however, that Cr/HTO catalysts may not be particularly promising candidates as improved selective dehydrogenation catalysts, since testing of a commercial Cr catalyst under identical reaction conditions results in equilibrium-limited propane conversions of ~30%.

As an alternative to the Cr/HTO catalysts, we also synthesized several Pt-based catalysts formed by encapsulation of Pt nanoclusters within alumina and silica aerogels and xerogels and tested them for propane dehydrogenation. In general, we prepared the samples by addition of an organic solution containing Pt nanoclusters stabilized inside inverse micelles, to a silica or alumina sol, followed by gelation of the sol. After gelation, we analyzed the samples by thermogravimetric analysis (TGA) to determine the temperatures required to completely oxidize unreacted organic material (surfactant, metal alkoxides). Based on this TGA analysis, the samples were calcined in air at appropriate temperatures to ensure complete removal of organics prior to activity testing. We studied four samples: (1) 0.26% Pt/silica xerogel, (2) 0.78% Pt/silica aerogel, (3) 0.252% Pt/alumina xerogel, and (4) 0.30% Pt/alumina aerogel. The reported Pt loadings are for the calcined materials. We used both TEM and hydrogen chemisorption to investigate Pt particle size in the calcined catalysts, revealing particles on the order of 4 nm for all samples. We observed slightly smaller particle sizes by TEM for the uncalcined materials, indicating some particle growth during calcining. Propane dehydrogenation activity is highly

dependent on treatment history for these materials, and all samples deactivate significantly over a period of 30 minutes to one hour. Partial reactivation is possible through a combination of oxidation in air to remove carbonaceous residues followed by hydrogen reduction. Furthermore, activation behavior appears to be highly dependent on the nature (aerogel versus xerogel) and identity (silica versus alumina) of the support, making valid comparisons of the various Pt catalysts difficult. The best Pt catalyst achieved a maximum propane conversion of 5.6%, but we observed conversions as low as 0.5% for some catalyst/pretreatment combinations. In general, selectivities to propane fall in the range of 65–85%. Further studies will be necessary to achieve a systematic understanding of synthesis parameters on activity and to determine the prospects for further development of this class of catalysts. For example, gelation of the sols can be performed prior to or after addition of the Pt nanoclusters, and Pt cluster formation can be initiated in the presence of the sol rather than in a separate solution. Furthermore, techniques need to be explored to improve the Pt loadings of the catalysts, and the addition of stabilizing promoters such as Sn must be explored to improve catalyst stability.

Publications

Other

Martino, A., A. Sault, J. Kowala, E. Boespflug, and C. J. Brinker. 1997. "Encapsulation of Metal Nanocluster Catalysts in Xerogel and Aerogel Materials via an Inverse Micelle/Sol-Gel Synthesis." Paper presented to the AIChE 1997 Annual Meeting, Los Angeles, CA, 18 November.

Martino, A., A. Sault, J. Kowala, E. Boespflug, and C. J. Brinker. 1997. "Encapsulation of Metal Nanocluster Catalysts in Xerogel and Aerogel Materials via an Inverse Micelle/Sol-Gel Synthesis." Paper presented to the Materials Research Society Fall Meeting, Boston, MA, 2 December.

Cathodic Protection of Zero-Valent Iron-Reactive Barriers

D. C. Marozas, M. G. Hankins

Chemical reduction of environmental pollutants by zero-valent iron-permeable barrier treatment is moving beyond pilot-scale research into commercial deployment. In 1995-96 alone, Sandia completed seven commercial installations. Despite the acceptance of the advantages of this environmental remediation approach, evidence of future problems is overwhelming. A reactive barrier pilot installed by Sandia at a site in Colorado plugged after seven months; Oak Ridge National Laboratory obtained similar results at Portsmouth. The problem is that the reactive-iron media can rust and plug with iron salts. This project investigated the feasibility of using cathodic protection to improve the lifetime of iron barriers. The project included laboratory experiments of cathodic protection, computer simulation of a field deployment of cathodic protection using boundary element analysis, and a compilation of the current deployment costs of zero-valent barriers without longevity improvements.

Laboratory studies using electrochemical cells to simulate iron-reactive media indicate that contaminant removal rates by cathodically protected iron were comparable to rates without cathodic protection. While there was no evidence of corrosion of the iron in experiments that utilized cathodic protection, with unprotected iron, corrosion was rapid and is apparent within minutes of the experiment's initiation. These experiments support the hypothesis of this study that cathodic protection can be used to minimize rust and salt formation.

Reactive barrier systems are not currently designed with cathodic protection. Because there is no information currently available on how to design a cathodic protection system for reactive barriers, simulation models must be utilized to aid in the design. The boundary element model developed partly by this study is a first attempt at discerning which variable will be most significant when designing a fieldable system.

This study investigated utilization of cathodic protection to improve the longevity and performance of zero-valence iron-permeable treatment walls. Iron in treatment walls is quickly consumed, not only in the conversion of contaminants to harmless by-products, but also in the reduction of water and oxygen. By general agreement it is believed that corrosion of the iron will limit the barrier lifetime and restrict certain applications. This project included laboratory experiments of cathodic protection, computer simulation of a field-scale deployment, and a study of the current costs and performance of zero-valent barriers.

Cathodic protection of iron structures eliminates or significantly reduces corrosion. In the case of iron-reactive barriers, it is important that the application of this technology not interfere with the reductive capabilities of the barrier. We conducted laboratory experiments to test whether iron maintains its reductive capacity when protected from corrosion by the application of a sacrificial anode. We manufactured electrochemical cells that simulate cathodically protected reactive barriers on a small scale for this purpose. We used steel wool and a 4.0-mM Cr (chromium) (VI) solution in the cathodic half-cell. We used a sodium chloride solution and sacrificial anode (zinc or magnesium) in the anodic half-cell. The half-cell solutions were separated by a Nafion membrane, and the electrodes were connected by a copper wire. We monitored the rate of Cr VI reduction with other parameters such as pH and current. Under the conditions of the experiment, complete reduction of chromate occurred within 24 hours using either zinc or magnesium anodes. The rate of chromate reduction and the pH changes were comparable to the rate of reduction without cathodic protection. However, there was no evidence of corrosion to the iron in experiments that utilized cathodic protection. In experiments with unprotected iron, corrosion was rapid and is apparent within minutes of the experiment's initiation.

Reactive barrier systems are not currently designed with cathodic

protection. Because there is no information presently available on cathodic protection systems for reactive barriers, simulation models could be utilized as an aid in their design. A boundary element method model was developed partly by this study as a first attempt at discerning which variables will be most significant in the field. In addition to corrosion protection of the barrier, the model showed that it may be possible to design specific reduction potentials for the treatment zone through the use of impressed currents at the anode. Previous study showed that some organic contaminants like carbon tetrachloride are very slow in undergoing reductive dehalogenation under the potential of iron alone. Other studies show that the electrolytic dehalogenation of chlorinated organics like carbon tetrachloride and trichloroethane can be promoted by ensuring that the potential of the treatment zone is maintained in a certain range, i.e., between -0.6 and -1.0 V for carbon tetrachloride and -.71 and -.93 for trichloroethane. The model suggests that it may be possible to design a range of potentials in the treatment zone. This model would be a first step in determining if this is a cost-effective approach for difficult contaminants. To further improve the model, polarization data such as rates of galvanic corrosion, corrosion potential, and current densities for cathode protection for the materials involved should be incorporated. The permeable nature of the cathode makes it a unique material. In the model the cathode was assumed to behave as a continuous material, but the nature of a permeable material may make more detailed study of the interface between the cathode and the ground an important consideration.

Publications

Other

Hankins, M. G. 1997. "Developments in Reactive Barrier Technologies at Sandia National Laboratories." Paper presented to the TIE Conference, Idaho Falls, ID, 27 August.

Modeling Interdependence in the U.S. Infrastructure

D. C. Marozas, R. S. Longenbaugh

The U.S. infrastructure is a complex system of interdependent elements whose continued operation is vital to the security and well-being of the U.S. As interdependency between infrastructure elements builds, it is becoming apparent that additional steps must be taken to identify potential cascading impacts that could occur during failure. This project initiated the development of a model of infrastructure interdependencies.

Sandia used results from the 1997 Prosperity Games on U.S. Infrastructure Assurance and other resources to identify key infrastructure vulnerabilities. A survey of infrastructure models and modeling algorithms resulted in the identification of key models and modeling approaches (i.e., dynamic simulation and agent-based modeling) that could provide a framework for developing a combined infrastructure interdependency model. The modeling effort eventually focused on one agent-based model of the electric power and gas utilities (ENERGY 2020) that can be combined with commercially available economic models or with Sandia's agent-based model of the banking and finance infrastructure (Aspen). ENERGY 2020 is a detailed, all-fuel, dynamic energy demand and supply model that combines causal, behavioral, and engineering simulation to determine how infrastructure systems evolve. The model also utilizes a gaming module that is primarily used for gaming of the rules to advantage one company and disadvantage competitors. This gaming for profit is conceptually identical to the "gaming" that could be part of a destructive attack on the energy system.

A final modeling effort focused on using computer simulations to investigate the impact of disruptive events on the electric power infrastructure. One detailed analysis focused on the economic impacts of two examples of purposeful disruption to

the electric utility system in a single metropolitan area (Houston) and analyzed the impacts of the disruption on the local economy, the state, and the U.S.

The U.S. infrastructure is a complex system of interdependent elements whose continued operation is vital to the security and well-being of the U.S. Previous experience shows that a loss of service in one infrastructure element can produce indirect but potentially severe collateral damage to any of the other infrastructure elements. As interdependency between infrastructure elements builds, particularly between the telecommunications, banking/finance, and energy generation and distribution industries, it is becoming apparent that additional steps must be taken to identify potential cascading impacts that could occur during failure events. This project initiated the development of a model of infrastructure interdependencies.

We used results from analyses of the 1997 Prosperity Games on U.S. Infrastructure Assurance and other resources to identify key interdependent infrastructure vulnerabilities. Second, a survey of infrastructure models and modeling algorithms resulted in the identification of key models and modeling approaches (i.e., dynamic simulations and agent-based modeling) that could provide a framework for developing a model of combining infrastructure interdependencies. The modeling effort eventually focused on one agent-based model of electric power and gas utilities (ENERGY 2020) that can be combined with commercially available economic models (i.e., REMI—Regional Economic Models, Inc.) or Sandia's agent-based model of the banking and finance infrastructure (Aspen). ENERGY 2020 is a detailed, all-fuel, dynamic energy demand and supply model. It combines causal, behavioral, and engineering simulation to determine how people and the infrastructure systems actually evolve. The utility sector includes financial, accounting, capacity expansion, production, transmission, and rate-making simulations. The demand sector provides end-use detail for the

residential, commercial, and transportation infrastructures, including cogeneration and technology decisions. The model also utilizes a gaming module that is used primarily for gaming of the rules to advantage one company and disadvantage competitors. This gaming for profit is conceptually identical to the "gaming" that could be part of a destructive attack on the energy system.

A final modeling effort focused on using computer simulations to investigate the impact of disruptive events on the electric power infrastructure. One detailed analysis focused on the economic impacts of two illustrative examples of purposeful disruption to the electric utility system. This effort looked at a single metropolitan area (Houston) and analyzed the impacts of premeditated disruption on the local economy, the state, and the U.S. One scenario simply assumes an event that brings down the Houston electric power grid for two days. The second scenario represents four events that bring down only a fourth of the city for one day each. The impacts are quite different for each scenario. In the first example, it is a single significant event that has minimal long-term impact on the public. Industry responds only modestly to the event, like an insurance company to a first-time car accident. It makes minor changes to its day-to-day operations to limit the impacts of any possible reoccurrence (a 0.1% increase in costs for the non-electric utility industries and 1% increase for the electric utility). The second case, however, is like a series of airplane sabotages that have a semipermanent impact on how people act and do business; the industry must change the operation to accommodate a real possibility of another event. These actions increase the total business cost by 0.5% into the foreseeable future. The "targeted" electric system sees its costs increase by 5% as it modifies its system design to limit the impacts of future sabotage acts. For both scenarios, we calculated the impact on total employment, gross regional product (GRP), and consumption.

Consequence-Based Rationale for an Infrastructure Assurance Program

G. D. Wyss, T. T. Brown, R. G. Cox

For more than 20 years Sandia has approached nuclear reactor safety analysis from a consequence-based perspective in which the analyst first identifies the system-level consequences to be avoided and then proceeds to systematically decompose the events that cause those consequences into their fundamental causes.

The probabilistic risk assessment (PRA) method accomplishes this task and allows system designers and operators to view their design and protection decisions in light of an "acceptable" level of residual risk. These methods have not, however, seen significant application to infrastructure systems analysis. This project sought to bridge this gap by first identifying the classes of consequences that must be avoided to provide assured performance for a few representative classes of U.S. infrastructure, then, through a scoping analysis, to identify how existing PRA techniques can be used to find dominant system failure modes (both internal and external to that infrastructure). The project will also examine how PRA techniques can be applied to identify the interdependencies between classes of infrastructure. The project documented the advantages and disadvantages of various PRA methods for selected prototypic infrastructure architectures.

We began by conducting literature searches to determine the distinguishing characteristics of several classes of infrastructures. From this survey the project distilled the many possible types of distinguishing characteristics into a few key indicators by which these infrastructures can be categorized. These indicators include the geographic extent of the network, one-way versus two-way flow, individual pairwise connections versus single-commodity distribution, interdependencies, centralized versus

distributed control, and public versus private ownership.

The literature search also identified an extensive list of potential consequences that might arise given the failure of various classes of infrastructures and sought to determine the degree to which these consequences can be quantitatively predicted given current modeling techniques. In addition, the project identified classes of hazards that might cause disruption of various infrastructure services and initiate a sequence of events that might lead to the identified consequences.

The project also surveyed common PRA methods both within and outside of the laboratory and examined the advantages and disadvantages of using each method to assess the surety of particular classes of infrastructures.

Finally, the project developed a framework for selecting which types of models are required to assess the surety of selected infrastructures. The framework begins by considering the type of decision that is of concern and leads the analyst to consider which types of consequences would be relevant to that decision and which general classes of hazards are to be considered within the scope of the analysis. It then helps lead the analyst to the most appropriate types of simulation and risk-based modeling techniques to identify the failure modes and accident sequences that are most important to that decision.

Publications

Other

Brown, T. T., R. G. Cox, and G. D. Wyss. 1997. "Consequence-Based Approach for Infrastructure Assurance." Sandia Technical Report SAND97-2956, December. Sandia National Laboratories, Albuquerque, NM.

Wyss, G. D. 1997. "Risk and Reliability Assessment of Communications Networks." Paper presented to the Risk Management for Critical Infrastructures Conference, Albuquerque, NM, 26 August.

Surety of North American Electric Power Transmission Network

D. G. Robinson

The North American Power Grid is an extremely complex dynamic system critical to the economics and safety of over 380 million people. It has been recognized by the U.S. President's Commission on Critical Infrastructure as being vulnerable to disruptions from natural causes and sabotage. In addition, the system will undoubtedly be impacted as the regulatory environment is restructured from a rate-based exclusive franchise to a competitive energy-production environment. To understand the implications of the changing environment on the adequacy and security of the electric power grid, a new approach is needed. The objectives of this study are to estimate some of the important effects of deregulation and a shift in competitive energy markets on power grid reliability at the bulk power level for a representative power pool and to evaluate the modeling approach for evaluating power grid adequacy and security. Sandia addressed two major aspects of the problem: (1) the effect of deregulation at a demand sector/fuel source level, and (2) the effect on the overall reliability of the bulk power system. The power pool chosen for this study is the Electric Energy Council of Texas (ERCOT); the base conditions studied are those prevailing for 1997. ERCOT is particularly appropriate since the state of

Texas is currently deregulating the bulk power system. ERCOT covers approximately 70% of the geographic area of Texas and about 90% of the population.

To understand the higher-level impact of deregulation on power grid reliability, we constructed a dynamic simulation of the control area fuel shares and generation capacity. Using the fuel share information obtained through the Energy Information Administration, we constructed a high-level model of the control area fuel shares and generation capacity. This portion of the overall model allows the user to set ERCOT-wide generation of power by fuel source to meet projected demand. This model consists of several arrays and vectors defining fuel shares and power capacity for each control area. For further detail at a more localized level, we expanded the model to include fuel share control information in one specific control area. We selected the Houston Light Power (HLP) control area as our focus because it is geographically small, densely populated, and includes a variety of power plants as well as one nuclear power plant. This portion of the model interacts with the Control Area Fuel Source Model to simulate the impact and response to varying fuel source selection at the ERCOT level and couples it with impacts and responses at the local level. The user can adjust generation capacity to simulate bringing down a power plant, then watch the resulting cost of compensating with power plants using other fuels. The user demand is simulated with

projected data entered through a spreadsheet or table.

To investigate the impact of deregulation on power grid reliability, we considered ten ERCOT control areas. We modeled each area as a single-point generation and load and investigated two loss-sharing scenarios. First, we assumed that areas within ERCOT share capacity resources during emergencies only up to the point of area surpluses and that there was no impact on loading in areas with surpluses to minimize pool load loss. The second loss scenario assumed that areas within ERCOT shared resources during any emergency to minimize the pool loss of load. Load shedding may occur in the interest of minimizing overall pool loss of load. Within each of these scenarios, we investigated four different scenarios for generation unit commitment (economic shutdown of uncommitted units is again assumed for cases 2-4): (1) all units in continuous operation except for planned outages (traditional planning assumption), (2) units committed to satisfy area peak load plus operating reserve from company commitment priority lists, (3) units committed to satisfy pool peak load plus operating reserve from pool commitment priority lists, but with ISO (independent system operator)-enforced control of transfers with consideration of transmission limitations and protection of pool reliability (similar to environment expected under new regulation structure), and (4) generating units committed to satisfy pool peak load plus operating reserve pool commitment priority lists without regard for area protection or

transmission limitations. The results are conservative in that they address only the impact of peak loading. Alternatively, they are optimistic in that the transmission lines are assumed to be in continuous operation. In summary, the results indicate that, under the current operating guidelines, there is approximately one day per year when peak electrical requirements can not be met. However, under the conditions expected to prevail under restructured generation and transmission regulations, there will be over thirty-seven days when peak load requirements can not be met. This initial study indicates that the reliability of the electric power grid will suffer under the ensuing economic pressures unless the effects are understood and appropriate actions taken. In addition, while the modeling and analysis techniques emphasized the effects of deregulation, the modeling approaches used are equally applicable to assessing the impact on the grid from a variety of sources, including physical and cyber-based sabotage.

Publications

Other

Robinson, D. G., A. D. Patton, and C. Singh. 1997. "Electric Power Grid Reliability." Paper presented to the Risk Management for Critical Infrastructures Conference, Albuquerque, NM, 26 August.

Protective Coatings for Concrete

K. L. Nagy, A. Sellinger, C. J. Brinker, R. T. Cygan

*Sandia applied the new two-layer protective coating developed for monuments constructed of limestone or marble to highway cement and to tobermorite, a component of cement, and tested it in batch dissolution tests. The goal was to determine the suitability of the protective coating in retarding the weathering rate of concrete construction. The two-layer coating consists of an inner layer of aminoethylaminopropylsilane (AEAPS) applied as a 25% solution in methanol and an outer layer of A2** sol-gel. In our previous work, this product resulted in a lowering of the rate of calcite dissolution by a factor of ten and was shown through molecular modeling to bind strongly to the calcite surface, but not too strongly so as to accelerate dissolution. We performed batch dissolution tests at 22°C of tobermorite (1.1-nm phase) and of powdered cement, both coated and uncoated. We also calculated the binding configuration and energy of AEAPS to the tobermorite surface for comparison with previous calculations on calcite.*

The research included convening a workshop that focused on identifying key issues in the area of concrete preservation, dissolution tests on cement materials, and molecular calculation of the binding energy of the passivant layer to tobermorite, a primary component of Portland cement.

The workshop included a number of participants: the Sandia researchers, researchers from our university collaborators, researchers from a national laboratory, and a building preservationist for the State of New Mexico. The ten presentations generated much discussion. Key issues discussed included precise identification and quantification of cement phases in Portland cements, the uncertainty of material behavior resulting from variation in local sources of concrete aggregate, effects of freeze-thaw and salt crystallization on mechanical stability, the alkali-silica reaction in concrete, natural weathering that rapidly produces surface coatings of carbonate phases such as calcite, and the potential of sol-gel materials for preservation.

We performed batch dissolution tests on coated and uncoated tobermorite ($\text{Ca}_{4.5}\text{Si}_6\text{O}_{15}(\text{OH})_3 \cdot 2\text{H}_2\text{O}$) and powdered Portland cement at 22°C. The coating consisted of one layer of AEAPS (25% in methanol) and one layer of A2** sol-gel. We put 25 g of sample in 125 g of deionized water and shook it periodically. We monitored concentrations of dissolved Ca and Si over a period of 24 hours. Starting pH was about 6.5; final pH ranged from 9.9 to 11.8. In all comparisons of uncoated versus coated material, dissolved Ca was reduced in the coated sample experiments by a factor of 0.25 to 0.75. However, dissolved Si increased for the coated samples by a factor of 1.5 to 9. The coating itself may be dissolving in the high-pH environments generated by the aqueous cement system. The final pH for the coated cements was typically one pH unit lower (~10.7) than for the uncoated cements (~11.8). The change in pH for the coated versus uncoated tobermorite was insignificant: final pHs = 9.8 to 9.9. Further investigation into the saturation state of these solutions with respect to all solid phases present in the system is necessary.

We calculated the binding energy of AEAPS to the (001) surface of tobermorite by first energy-optimizing the AEAPS as a free gas-phase molecule, then docking it onto a molecular cluster representation of the fixed tobermorite substrate. The binding energy was 165 kcal/mol. Further refinements of the calculation would be expected to change this by 25–30%. Compared to the calcite substrate, AEAPS appears to bind three times more strongly to tobermorite, although still much less strongly than other charged anionic passivants investigated in the previous study that actually contributed to increased calcite dissolution. This calculation suggests that AEAPS is well-suited as a sealant for tobermorite.

In summary, the calculation and experimental results on Ca-release rates suggest that the two-layer protective coating holds some promise for sealing and protecting concretes. However, evaluation of the behavior of the alkoxysilane sol-gel itself in the high-pH environments generated within wet concrete is necessary. Also, any secondary-phase formation should be monitored closely to completely address the observed changes in chemistry. Although

the Si release-rate data indicated that the sol-gel may be unstable, longer-term experiments are needed to investigate the extent of dissolution of the sol-gel both at the high pHs found within cement and at the pHs of concrete surfaces exposed directly to the environment.

3534.020

Low-Cost Cadmium Zinc Telluride Radiation Detectors Based on Electron-Transport-Only Designs

R. B. James, J. C. Lund

The goal of this project is to utilize a novel device design to build a compact, high-resolution, room-temperature-operated semiconductor gamma-ray sensor. We will construct this "smart" sensor from a cadmium zinc telluride (CZT) crystal. It will be able to both detect radiation and determine the particular isotopes responsible for the emitted radiation. CZT detectors produced today have excellent electron charge carrier collection, but suffer from poor hole collection. For conventional gamma-ray spectrometers, both the electrons and holes must be collected with high efficiency to preserve energy resolution. The requirement to collect the hole carriers, which have relatively low lifetimes, limits the efficiency and performance of existing experimental devices. By implementing novel device designs such that the devices rely only on the electron signal for energy information, the sensitivity of the sensors for detecting radiation can be increased by a factor of 100 or more. The availability of new CZT sensors with enhanced sensitivity would find immediate application in the safeguarding of stored nuclear materials, detecting nuclear smuggling and weapons facilities, improving arms-control and treaty-verification operations, detecting land mines and unexploded ordnance, and improving environmental monitoring and remediation activities.

The overall goal of this project is to develop a new type of gamma-ray radiation detector with improved performance over existing devices. In particular we intend to develop a detector system based on CZT detector elements with much better energy resolution than any other room-temperature gamma-ray detector system. We will achieve this goal

by utilizing a novel new device design that makes use of the motion of electrons only within the sensor (as opposed to the motion of electrons and holes). The dominant source of energy resolution broadening in existing room-temperature sensor systems is a phenomenon known as "hole tailing." Hole tailing arises because of the poor transport properties of holes in room-temperature semiconductor materials. The new design being developed during this project completely eliminates hole tailing. During the first year of the project we achieved some of the best energy resolution ever achieved from a room-temperature device and intend to surpass this result during the second year.

Accomplishments during the first year focused on three areas: (1) characterizing and selecting appropriate crystals for device fabrication, (2) fabricating and testing electron-only gamma-ray sensor elements, and (3) developing computation methods for designing optimized sensor elements.

We made major progress in the fabrication and testing of sensor elements during the first year of the project. In addition to fabricating devices using conventional fabrication techniques (vacuum and electroless deposition of gold contacts), we also discovered methods for making usable contacts with metallic deposition. We found that conductive rubber contacts could be used for the grid contact of the device. The significance of this development is that we can achieve substantial acceleration in design verification because the rubber grid contacts can be readily removed and replaced on the surface of the device. This substantially decreases the design verification/test cycle because a new device does not have to be fabricated for each design iteration of the grid; instead, the grid can simply be moved to the new location and the device retested. We also developed new methods for automatically testing the new devices during the first year of the program. The automatic testing is necessary with these devices because they are three terminal devices, and the phase-space of operational variables is very large.

Perhaps the most significant technical development in the first year of the project was that of computation tools for predicting the performance of these new devices. Prior to the development of

these tools, we relied on intuition to design the position of the contacts on the device, but now we can quantitatively predict many aspects of the device's behavior in advance and use these predictions to optimize device performance. In particular, we solved Poissons equation using numerical methods (finite element relaxation) for a variety of different device geometries. Solution of Poissons equation yields the weighting potential as well as the electric field distribution within the device. Once the weighting potential and field distribution are known, electron trajectories from gamma-ray interactions can be computed and optimal device geometries defined. During the second and final year of this project, we will use these computational methods to design optimized device structures, and we will also extend these techniques to full 3-D device modeling. Now that we have coded numerical solutions to the potential distribution, we can use these computing methods to design optimized devices.

Publications

Refereed

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3534.030

LIGA Micromachining

J. M. Hruby

This project focuses on developing the infrastructure to perform LIGA micromachining at Sandia. LIGA is an acronym derived from the German words for lithography, electroforming, and molding. The tasks include mask making, electroplating in high-aspect-ratio channels, scanner design and fabrication, product realization software development, and exploration of alternative exposure methods. To support the mask-making task, we developed software and began parametric evaluation of the mask gold thickness. We accomplished the high-

aspect-ratio electroplating task by completing the feasibility testing of new plating methods. The scanner design and fabrication task included initial evaluation of scanners designed and constructed by others. The product realization task proceeded nicely with an architecture defined to communicate and share design definition in real time.

This project focused on developing the infrastructure to perform LIGA micromachining at Sandia, a process used to make high-aspect-ratio metal micromachines. In this project, we outlined five tasks: mask making, electroplating in high-aspect-ratio channels, scanner design and fabrication, product realization software development, and exploration of alternative exposure methods.

Under the mask-making task, we developed software to simulate the exposure conditions and to perform parametric evaluation of mask gold thickness for various synchrotrons. These calculations will lead to the establishment of parameters for "standard" LIGA masks. We also purchased and installed a plasma cleaner, an optical microscope, and a profilometer that we will use to examine masks once they are fabricated.

We accomplished the electroplating task by completing the feasibility testing of a new plating method that looks promising, but we still need to establish details associated with the plating bath chemistry and compatibility with the electrodes. This method offers the potential to eliminate plating inhomogeneities that cause a decrease in yield of LIGA parts.

The scanner task was also unsupported but included evaluation of the scanners designed and constructed by other LIGA groups. We also evaluated potential software control packages to use to communicate with the scanner. We purchased a water chiller and computer to use in the new scanner system.

The product realization task proceeded nicely with an architecture defined to communicate and share design definition in real time. This software is compatible with standard drawing packages and will be deployed on machines of both the primary process engineers/scientists and the primary designers.

Chemistry and Physics of Microfluidics

P. H. Paul, E. B. Cummings

During FY97, Sandia embarked on the first year of a project in microfluidics. The aim of this project is to develop expertise in microfluidic actuation and patterned-bed design, both enabling technologies for the "chemistry-lab-on-a-chip" project. We created and equipped the Applied Microfluidic Physics Laboratory (AMPL). In addition, we are examining means of fluid actuation other than electrokinesis (EK), e.g., dielectrophoresis and electrostatic streaming that may complement electrokinesis in microfluidic devices on a chip.

The principal technological hurdles that we overcame relate to device fabrication. The group at Sandia that is working on the "chemistry-laboratory-on-a-chip" recently developed techniques for sealing cover plates on microfabricated channels and found silicon substrate coating procedures that withstand high voltages (~ 1 kV) in the presence of aqueous solutions.

The ability to seal the channels permitted us to study the flow in unpacked (unpatterned) microchannels that were etched in silica. We are employing a unique imaging tool that we developed to study microscopic flows in capillaries for these studies.

We developed numerical models of pressure-driven and EK flows in 2-D, rectilinear geometries. We are also studying other techniques of actuating and controlling liquids and molecules in solution that could be effectively integrated into a microfluidic circuit.

Combinatorial Peptides for Chemical Sensing

J. S. Schoeniger

Combinatorial peptides (CPs) are a new class of molecular recognition material. CPs are small molecules that can be engineered to bind tightly and selectively to a designated analyte. The purpose of this project is to explore the utility of CPs for chemical sensing of complex analytes in aqueous solutions containing multiple-background chemical species. The goal is to show proof-of-principle that CPs can be incorporated into compact, sensitive flow-through sensors using laser-induced fluorescence (LIF) detection of the analytes. The analytes of particular interest are proteins of importance as potential warfare agents or contaminants in biotechnology process streams.

Sandia designed and synthesized peptides that will bind selectively to a protein target for use in proof-of-principle experiments in affinity chromatography. We based these peptides on previously isolated and published sequences known to bind to Ribonuclease S. Custom-synthesized peptides obtained have modifications that facilitate different chemistries for attachment to silica chromatography supports. A collaborating university group is developing peptide that bind selectively to ovalbumin, a protein of interest in biological warfare (BW) counterproliferation. We are currently evaluating the efficiency of attachment chemistries and the affinity activity of the immobilized peptides.

Pulser in a Chip

G. M. Loubriel, H. P. Hjalmarson, W. D. Helgeson, A. G. Baca

The over-arching goal of this project is to study whether laser diode-triggered photoconductive semiconductor switches (PCSS) can be used to activate electrooptic devices such as Q-switches and Pockels cells and to study possible laser diode/switch integration. The PCSS switches Sandia used were high-gain GaAs switches because they can be triggered with small amounts of laser light.

The specific goals of the project were to demonstrate the following: (1) that small laser diode arrays that are potential candidates for laser-switch integration will indeed trigger the PCSS switch, and (2) that we can use high-gain GaAs switches to trigger optical Q-switches in lasers such as the laser to be used in the X-1 Advanced Radiation Source. This technology is the prime candidate for triggering the Q-switch in the multiple lasers in the laser trigger system of the X-1 Advanced Radiation Source. As part of the project we will develop a commercial supplier. To study laser/switch integration we tested triggering the high-gain GaAs switches with edge-emitting laser diodes, vertical-cavity surface-emitting lasers (VCSELs), and transverse junction stripe (TJS) lasers. The first two types of lasers (edge-emitting and VCSELs) did activate the PCSS but are harder to integrate with the PCSS for a compact package. The TJS lasers, while easier to integrate with the switch, did not trigger the PCSS at the TJS laser power

levels we used. We used the PCSS to activate the Q-switch of the compact laser to be used in the X-1 Advanced Radiation Source.

The goals of this project were to demonstrate that (1) small laser diode arrays that are potential candidates for laser-switch integration will indeed trigger the PCSS switch, and (2) we can use high-gain GaAs switches to trigger optical Q-switches in lasers such as the laser to be used in the X-1 Advanced Radiation Source. This technology is the prime candidate for triggering the Q-switch in the multiple lasers in the laser trigger system of the X-1 Advanced Radiation Source. As part of the project, we were to develop a commercial supplier.

We made four major accomplishments in FY97:

(1) *Demonstrated that the high-gain PCSS can properly activate the optical Q-switch of the laser for the X-1 accelerator.* This task is the most crucial one in this project since it impacts the laser trigger system of the X-1 Advanced Radiation Source. Prio to receiving the laser, we demonstrated electrooptic control of a Pockels cell with a PCSS switch. We performed this demonstration by charging a cable and discharging it to the Pockels cell via the PCSS. When we received the laser from AlliedSignal, we demonstrated that its Q-switch could be triggered with a high-voltage pulser based on a high-gain GaAs PCSS. In particular, the high-gain GaAs-based pulser reduced the optical system jitter

(2) *Demonstrated the capability of VCSELs to trigger high-gain PCSS switches for parameters compatible with task 1.* We

demonstrated that high-power VCSELs are capable of triggering a high-gain PCSS. This is a significant result because it demonstrates that the PCSS can be triggered with the types of optical output of microlasers that may be monolithically integrated with the PCSS. It is also important since (a) the PCSS was triggered with a record low energy of 2.1 nJ, (b) the VCSEL is 75 microns by 75 microns (5600 microns squared) in size with an active area of about 3200 microns squared, and (c) the price of VCSELs is significantly lower than that of edge-emitting lasers. The PCSS discharged a transmission line charged to 3.5 kV, producing a 45-Å pulse of about 3-ns duration. The peak optical energy density produced by the VCSEL is 0.65 J per square meter.

(3) *Demonstrated the capability of edge-emitting lasers to trigger high-gain PCSS switches for parameters compatible with task 1.* In the past, we triggered high-gain PSS with edge-emitting lasers. In this project we wanted to trigger the switches with edge-emitting lasers that are compatible with monolithic integration of switch and laser. We originally considered two options: using existing TJS lasers (preferred) or using edge-emitting lasers with waveguides. Because of the difficulty in obtaining lasers with waveguide structures in a short amount of time, we tested only the TJS lasers. They did not trigger the PCSS.

(4) *Developed industry collaboration.* Two companies expressed an interest in using high-gain, optically triggered, GaAs switches for driving Q-switches and Pockels cells in lasers. The president of a small company that manufactures

electrooptic modulators and Q-switches; ultra-high-speed, high-voltage pulse generators; Q-switch drivers; high-speed electrooptic switching systems; and electronics for modulators, among other products, visited Sandia to study this system and discuss future options. They are very interested in the Q-switching application we demonstrated.

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Ultra-High-Pressure EOS Studies on Metals and ICF Ablators Using PBFA-Z

C. H. Konrad, B. F. Clark, W. M. Trott

This project will provide the first accurate pressure-volume measurements of the ultra-high-pressure equation-of-state (EOS) obtained with pulsed-radiation sources in the multi-Mbar regime. This new capability will enable a user-friendly capability at Z for a variety of EOS, thermomechanical, physical, and surface property measurements. These data will have comparable accuracy to other experimental methods obtained from gun technology, overlapping their pressure regime, and extending it into a new higher-pressure area. In addition, these data will be critical to both the weapon physics and inertial confinement fusion (ICF) programs for validation of material models used in the design and analysis of non-nuclear, nuclear, and ICF system performance. The ability to perform these experiments in the laboratory for the first time versus underground tests should result in substantial new business for Sandia.

In an effort to optimize our dedicated EOS experiments, we ran pressure profile simulations to predict the capabilities of Z as a source to drive EOS experiments. In addition, the codes aided in identifying optimum target and Z-drive configurations for dedicated EOS experiments that we conducted in the fall.

We accomplished installation and interface into the Z environment of EOS instrumentation consisting of a Velocity Interferometer System for Any Reflector (VISAR) and associated equipment. This involved designing and fabricating a new optical probe for VISAR measurements. Characterizing the probe, lithium fluoride windows, and optical fibers for both fluorescence and optical darkening, we completed two conditions that are side effects of the Z environment, both in laboratories and at Z. In addition, we identified unacceptable levels of noise and localized them to the laser required for VISAR experiments. A new laser configuration and addition of a screen box solved the problem. We used the probe design and fibers on Z experi-

ments, and they performed successfully. We modified the VALYN VISAR system to remove three photomultiplier units (PMT) and installed a fiber-optic (FO) coupler to output the VISAR data to a streak camera. We designed and fabricated a FO coupling cable with 30 data fibers for interface to the VISAR and shock breakout data to the streak camera.

We developed a shock breakout system and will use it in the upcoming dedicated EOS experiments. We tested the shock breakout probes in the laboratory utilizing laser-accelerated flyer plates, impacting an aluminum target foil, and recording the change in reflectivity of the foil surface due to shock wave. We resolved problems involving fluorescence of the breakout fibers caused by Z radiation overdriving the return data light by passing the return light through narrow (1 nm) bandpass filters and increasing the input light energy through the use of a pulsed dye laser. We were able to increase the light into the FO splitter from 2 watts cw to kilowatt laser pulses.

We tested the VISAR as "add-on" instrumentation to several existing experiments. We recorded time-resolved pressure data in aluminum that correspond to predicted values. We developed a shot plan for the Z experiments and ordered hardware.

Publications

Refereed

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Flocking Small Smart Machines

B. L. Spletzer, C. L. Lewis, P. R. Klarer

The purpose of this work was to investigate and demonstrate cooperative behavior among a group of mobile robot machines. The specific goal of this work was to build a small swarm of identical machines and control them in such a way as to show a coordinated movement of the group in a "flocking" manner, similar to that observed in nature. Control of the swarm's individual members and its overall configuration are available to the human user via a graphic man-machine interface (MMI) running on a base station control computer. Any robot may be designated as the nominal "leader" through the interface tool, which then may be commanded to proceed to a particular geographic destination. The remainder of the flock follows the leader by maintaining their relative positions "in formation," as specified by the human controller through the interface. The formation's configuration can be altered manually through an interactive graphic-based tool. An alternative mode of control allows for teleoperation of one robot, with the flock following along as described above.

(1) *Mobile platform.* The mobile platform design chosen for use as a test-bed for this work was a scaled-down version of Sandia's Robotic All-Terrain Lunar Exploration Rover (RATLER), due primarily to the RATLER's excellent performance characteristics in moderate to rough terrain. The original RATLER was a 1-meter vehicle weighing 100 kg, whereas the SWARM-RATLERs used in this work are approximately 40 cm long and weigh 12 kg each. We configured the vehicles to allow integration of sensing and other payloads to be as flexible as possible, with plenty of unused payload space, power, and signal path capacity. The platforms are built entirely of carbon-epoxy composite; the wheels have a tread pattern molded/bonded to the outer surface in high durometer polyurethane.

(2) *Onboard power, computing, control, and sensing.* The onboard power system provides 24 V raw DC power from the battery system and regulated power at 12 V, 9 V, and 5 V at 2 A, 2 A, and 3 A, respectively. Each of the SWARM-RATLER vehicles is fitted with a PC-104-based computing system utilizing an Intel 80486 CPU running at 66 MHz and 4 MB RAM with onboard SVGA capability and two Type-III personal computer memory card interface adapter (PCMCIA) slots for mass data storage. Data-acquisition channels provided include 16 each 12-bit analog inputs, 16 each digital inputs/outputs (transistor-to-transistor logic [TTL] level), 2 each 12-bit analog outputs (used for drive motor control), and 6 each RS-232 serial ports, of which only about 20% have been used. We can add additional input/output (I/O) channels very easily.

We control the drive motors through the analog output channels and a pair of integrated H-bridge servo drives (one for each side) running in torque control mode. The motors are conventional brushed DC gearhead units, one for each of the four wheels.

Sensors onboard include pitch and roll for each chassis body, compass heading, raw three-axis magnetometer flux, ambient temperature, and differentially corrected global positioning system (GPS)-based latitude, longitude, and elevation.

(3) *Control station and control software.* The control station is a laptop PC running Windows NT and the application control interface software. The application control software provides a graphical user interface (GUI) to the swarm of robots, allowing a swarm pattern to be arranged as a set of points (individual robots) with separation distances and orientations along a curve or line using the mouse. A menu-driven interface allows the user to select a particular robot to control, and also allows the user to choose either a teleoperation mode or an autonomous mode of operation for that robot. In teleoperation mode, a "virtual joystick" is displayed in a window and is controlled using the mouse. In autonomous mode, a

geographical destination point is specified for the "leader" as a goal toward which to proceed. Either by driving the designated "leader" robot or by commanding it to proceed toward a specific location, that vehicle begins moving when directed by the user, and the remainder of the swarm follows that vehicle's movements by maintaining the separation distance and orientation with respect to the leader as specified by the user. Each vehicle is modeled internally as a mass in a spring-mass system, where the "springs" describe the "interconnections" of the swarm's individual robots. Manipulating the parameters of the masses and springs allows the flocking behavior to be tuned and optimized for a particular vehicle/terrain combination.

To date the swarm consists of four identical robots, which we tested individually for functionality. We controlled individual robots in teleoperation and autonomous modes and tested the flocking control algorithm in simulation. We are ready to begin testing the flocking control algorithm with the actual robot hardware.

3535.050

Development of Explosive-Event Scale Model Testing Capability at Sandia

N. T. Davie, J. J. Calderone, T. C. Togami,
T. K. Blanchat, R. A. Benham, D. S.
Preece

Geotechnical structures such as underground bunkers, tunnels, and building foundations are subjected to stress fields produced by the gravity load on the structure and/or any overlying strata. These stress fields may be reproduced on a scaled model of the structure by proportionally increasing the gravity field through the use of a centrifuge. We can then use this technology to assess the vulnerability of various geotechnical structures to explosive loadings. Applications of this technology include assessing the effectiveness of earth-penetrating weapons, evaluating the vulnerability of various structures,

counterterrorism, and model validation. This project describes the development of expertise in scale-model explosive testing on geotechnical structures using Sandia's large-scale centrifuge facility. This study focused on buried structures such as hardened storage bunkers or tunnels. We used data from this study to evaluate the predictive capabilities of existing hydrocodes and structural dynamics codes developed at Sandia (such as Pronto/SPH, Pronto/CTH, and Alegria).

Centrifuge experiment of explosive detonation in a tunnel. Computer modeling was a critical part of this project for assurance that the explosive loading of the experiment on the centrifuge would be large enough to be meaningful but would not damage the centrifuge. This and another project were synergistic in that both involved application of computational mechanics codes to predict the effect of explosives on structures. The centrifuge experiment chosen was an aluminum tunnel liner buried in an engineered soil with a decoupled explosive detonating inside. A uniform acceleration field of 100 Gs on the tunnel/soil model effectively scales the behavior for the 1.5-inch-diameter centrifuge model to 150 inches. We performed a computer simulation of this experiment with a computer code named Alegria, which is an arbitrary Lagrangian Eulerian (ALE) code. Alegria also accurately treats the explosive/structure interaction. We performed pre-test calculations on the centrifuge tunnel experiment with the calculated explosive-induced plastic outward displacement of the aluminum tunnel liner being within 10% of that measured after the experiment. This experiment and the corresponding computer simulation together are an important benchmark.

Publications

Refereed

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Application of SAR Vibrometry to Distributed Seismic Sources

C. V. Jakowatz, Jr., J. P. Lauffer

Sandia collected synthetic aperture radar (SAR) data on scenes having seismic excitation and investigated a potential technique for measuring seismic vibration.

We collected the database at Sandia Area III and made ten passes of an open site near the large sled-track facility. Seismic excitation was provided by a vertical LRS315-S vibrator, rated at 40,000-pound peak-to-peak force. We conducted tests at 9, 15, and 30 cycles per second. We measured ground truth via triple-axis accelerometers from 10- to 200-foot range.

We made an additional six passes of the cluster of buildings surrounding the Large Centrifuge Facility (LCF). Seismic excitation was provided by a 100,000-pound horizontal out-of-balance force on the centrifuge. We conducted all centrifuge tests at 0.83 cycles per second. Ground motion was too small to be measured using triple-axis accelerometers.

The analytic approach compared the phase error of portions of the scene containing different amounts of seismic vibration. We used the phase-gradient autofocus algorithm to compute the phase error. No ground vibration was detectable in the LRS315-S data.

The results of this project include a data collection effort and an analysis of the data.

We collected the data with the airborne multisensor pod system (AMPS) in the spotlight radar mode, which we flew over the site in a P-3 aircraft. We selected a site near the large sled-track facility and brought in a large vibra-seiz truck to excite the earth in the vertical axis at 30, 15, and 9 Hz. Waves propagated radially from the truck with wavelengths of 40, 80, and 133 feet. We measured vibration amplitude using three-axis accelerometers. Ground motion exceeded 0.001 inch over a large

surface area. We distributed 40 coffee and soup cans over the northern half of the field in an effort to increase contrast over natural cover.

We collected additional data at the LCF, where excitation was provided by operation at 0.83 Hz at the maximum allowable out-of-balance force of 100,000 pounds. The resulting ground-vibration amplitude was less than .001 inch; this was too small to be measured using available instrumentation, although measurable motion did occur in the metal centrifuge building structure. The reason for the unexpectedly low response of the ground at this site is believed to be the size and depth of the rigid centrifuge foundation.

We based the analytic plan on being able to measure radar phase error between the aircraft platform and the vibrating earth. We planned to analyze the time-series consisting of these phase errors for the presence of energy in excess of background at the seismic excitation frequency. At this time, only the higher-amplitude sled track data have been analyzed. We found that the data contained insufficient image contrast to permit the phase-gradient autofocus algorithm to accurately compute phase error. We detected no ground vibration. We do not know if it would have been possible to detect the ground vibration if image contrast were higher.

3535.070

Development of Laser-Cutting/-Welding Depth Control Using Laser Spectroscopy and Open Architecture Control of a Robotic System

R. G. McKee

The research effort undertaken in this project centers in the development of real-time sensor-based control of a precision automation platform capable of delivering noncontact manufacturing processes such as welding, cutting, and plasma spraying.

The research and development project incorporates a PaR 6-degree-of-freedom (DOF) gantry robot and a 2-kW Nd:YAG laser. The research goal is the development of a precise robotic system and a suite of sensors that we can use to control automated laser welding and cutting processes in real time. The integration of the sensors onto the precision robotic platform will allow real-time information generated at the manufacturing process to be used for process control via path or process parameter modification.

We broke the project into four task areas. The task areas were interdependent, which directed a parallel research effort. We identified the task areas as follows:

- (1) automated delivery platform development,*
- (2) sensor identification and development,*
- (3) integration of sensors onto automated platform, and*
- (4) research into noncontact manufacturing process control.*

The thrust for FY97 was the research and development of the automated delivery platform and the identification of sensors. We directed staff efforts to bringing the automated platform into a state that would support sensor development. This effort included hardware modifications and the development of software for controlling the platform. In a parallel effort, staff identified the first two sensors to be developed in the project: noncontact capacitive sensing and laser-induced breakdown spectroscopy (LIBS). Sandia staff were assigned the capacitive sensing development task and, in collaboration with Los Alamos National Laboratory's (LANL's) Nuclear Materials Technology (NMT) Division, are developing the LIBS sensor. As we made progress on the robotic platform, we integrated the sensors on it.

(1) Automated delivery platform development. We made substantial progress in this task. The software team researched and developed methods to extract process information from a computer-aided design (CAD) model of a generic part that would be processed on the robotic platform. We then used the

information to generate path plans and to check for collisions between the robotic system and the part. The software developed for the PaR robotic system also verified the path and associated information generated via a graphical user interface (GUI).

The team reviewed the capabilities of the current configuration of the robotic system. We determined that the 27–30-msec closed-loop feedback response for path modification was not fast enough for the noncontact processes. We established a goal of 10 msec and generated designs for this goal. We ordered hardware modifications and wrote software upgrades to support the effort. We built four new controller boards and installed them into the PaR controller module. The effort resulted in decreasing the closed-loop feedback time to 12 msec. The design allowed for net communication between the sensors at the process and the path modification controller. Testing of the upgrade continued into the last month of the fiscal year.

We installed the 2-kW Nd:YAG laser systems, tested them in the lab, and installed the fiber-optic system on the PaR robotic platform.

(2) *Sensor identification and development.* The original proposal stated that the research would center on LIBS and noncontact capacitive sensing. After looking at these and other candidates, we decided that the original selection best supported laser cutting and welding. We reviewed the capacitive sensing process and decided that a full three-dimensional version of the technology would support the research and development effort. We designed, built, and tested the sensor and its associated electronics on the robotic platform.

The LIBS sensor development work is being carried out in collaboration with LANL. LANL is currently working the design and expects to have the sensor available soon. The availability of the LIBS sensor will enhance the noncontact

processing capability for welding control and is required for cutting control of clad materials. The delivery timeframe of the LANL LIBS sensor meets the original schedule established in the proposal.

(3) *Integration of sensors onto automated platform.* We directed the development effort in the final month of FY97 at integrating the developed technologies onto the PaR robotic platform. We tested the PaR upgrade using a standard sensor input and determined the feedback time to be 12 msec. We tested the software system using a right cylinder of 18-inch diameter as the generic CAD part. We placed a number of line features that simulated a laser cut or weld on the cylinder. We positioned the features so the cuts produced a horizontal cut through the cylinder and an off-axis cut that produced an ellipse. We submitted the CAD model to the software module where the features were extracted, paths were generated and checked to ensure that they were collision-free, and then downloaded to the PaR robotic controller. We then successfully executed the paths on the robotic platform. After we proved the software control system functional, we put the capacitive sensor on the robotic platform for testing and characterization. We successfully installed, calibrated, and demonstrated the capacitive sensor.

3535.090

Aerosol Stand-off Detection Test-Bed

R. P. Toth

This project supports the development of technologies for biologic defense. The application we selected is naval port and airfield defense. The objective is to provide early warning and indication of a biological warfare (BW) attack by means of a stand-off sensor. Furthermore, this

sensor is directed toward detection of encapsulated microorganisms.

This project idea exploration is to develop a test-bed for a novel method of detection based on RF interrogation of the BW cloud. In some sense, it resembles a meteorological radar. The test-bed, when complete, will aid in estimation of sensitivity and range for such a sensor.

(1) *Selected an RF transmission system for controlled studies of aerosol detection.* We accomplished this by comparing anechoic chamber, tapered chamber, waveguide, and transverse electric/magnetic (TEM) cell for cost, aerosol production compatibility, reproducibility of propagation parameters, and suitability for estimation of system performance in the free-space, bistatic configuration in which we ultimately intend to operate. The anechoic chamber was an early choice because it provided a good simulation of free-space propagation. We developed plans for its use with arrays of monopole doublets. We ultimately rejected the chamber option because of schedule conflicts and concerns of downtime to dry the absorber material. We rejected waveguide because only TM or TE modes were available. We rejected the tapered chamber on the grounds of cost and modifications needed for bistatic operation. The final choice was a TEM cell.

(2) *Designed an aerosol generation system for use in the TEM cell.* We selected and ordered nozzles for 1-micron droplets, along with an argon pressure system.

(3) *Fit the TEM cell with nozzles and pressure distribution lines.* We accomplished this within the materials available.

(4) *Designed and selected RF, bistatic instrumentation to characterize the aerosol.* We completed the design and tested existing vector (phase-coherent) receivers. We encountered delivery problems with the TEM cell, part of the pressure system, and the oscillator.

Cryogenic EOS Capabilities on Pulsed-Radiation Sources (Z pinch)

D. L. Hanson, R. R. Johnston

Experimental cryogenic capabilities are essential for the study of inertial confinement fusion (ICF) high-gain target and weapons effects issues involving dynamic material response at low temperatures. The goal of this project is to develop a general-purpose cryogenic target system for precision equation-of-state (EOS) and shock physics measurements at liquid helium (LHe) temperatures on the Z-accelerator Z-pinch pulsed-radiation source. Activity during the first phase of this project focused on development of a conceptual design for the cryogenic target system based on consideration of physics, operational and safety issues, design and fabrication of principal system components, construction and instrumentation of a cryogenic test facility for off-line thermal and optical testing at LHe temperatures, initial thermal testing of a cryogenic target assembly, and the design of a cryogenic system interface to the Z-pulsed-radiation source (Z PRS) facility.

The prediction and analysis of ICF high-gain targets and other weapons physics issues requires models of dynamic materials response that can accurately describe thermodynamic properties and high-rate mechanical phenomena over an extensive range of pressures and temperatures. For ICF materials, these capabilities are needed at cryogenic temperatures since most ICF designs are based on performance of cryogenic multishell capsules. The goal of this project is to develop a general-purpose cryogenic target system for

precision EOS and shock physics studies on the Z-accelerator PRS at LHe temperatures.

During the first phase of this project, we accomplished the following: (1) developed a conceptual design for the cryogenic target system, (2) designed and fabricated major system components, (3) constructed and instrumented a cryogenic test facility for off-line thermal testing at LHe temperatures, (4) performed initial thermal testing of a cryogenic target assembly, and (5) designed a cryogenic system interface to the Z PRS facility.

We developed a detailed conceptual design for a cryogenic target system that will meet the safety and operational requirements for Z hohlraum experiments. We used LHe cooling and active temperature feedback control to maintain samples at a fixed temperature. We designed variations of the cryogenic sample holder to (1) condense cryogenic liquid samples from the gas phase (specifically liquid deuterium and hydrogen at about 20° K), (2) cool solid samples, such as polycarbonate and metallic ablaters for ICF studies, to a specified temperature in the range of 6°–30° K, and (3) condense solid layers from the gas phase onto a substrate. Each target assembly includes the capability to use various shock diagnostics, such as VISAR (Velocity Interferometer System for Any Reflector) interferometry for particle velocity measurements and optical fibers for shock velocity measurements.

We assembled a cryogenic test facility to evaluate and refine cryogenic target system designs. We installed a thermal model of the complete Z-pinch experiment. We instrumented the test assembly with an array of silicon diode temperature sensors, a LHe-level sensor,

and vacuum pressure gauges. Fabrication of gas-handling and temperature-control systems is almost complete. In initial thermal testing, we cooled the cryogenic sample holder, connected to the cryostat through a cold-finger, to a steady state of about 5° K in 20 minutes. The thermal gradient between the cryostat and the sample holder was only about 0.5° K, suggesting that a much longer connecting link can be tolerated when attempting to cool the sample holder to 20° K for liquid deuterium. Under those conditions, we can connect the sample holder to the cryostat through a high-conductivity copper cable, with the cryostat protected from destruction behind a debris shield. Based on this thermal testing, we designed an improved cryostat with extensive thermal insulation to allow more efficient use of LHe for temperature control over extended periods. The 1-c-m-long thermal break between the cryogenic sample holder at 5° K and the primary hohlraum assembly, which must be maintained near room temperature to prevent dimensional changes in the wire-array support structure, worked effectively.

Publications

Other

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Synchronized RF Sources for IW Applications

R. P. Toth

One of the critical needs for information warfare (IW) is the ability to mount a precision attack. In this context, precision implies the ability to attack a specific target located at a particular point in space without damaging nearby objects that might be equally vulnerable. An approach to this problem is to array a set of short-pulse transmitters in the vicinity of the target and to time their pulses such that they add coherently at the target but nowhere else (or at most at a small number of other isolated points). The basic transmitter technology exists. The objective of this proposal is to add the one piece of technology required to implement this concept, namely synchronization. Generally one wants to generate one or two cycles of RF, the number of cycles and the wavelength determining the size of the irradiated spot. This is done with spark-gap-switched Hertzian oscillators. To get a highest possible intensity at the spot, it is necessary to control the transmitters' timing to about 5% of their period. That has been done in the laboratory with very robust triggering of the spark-gap switch, much more robust triggering than one might expect to be practical in the field. This project addresses the problem of applying light-triggered semiconductor switch technology to create a more viable trigger system.

The initial objective of this project was to demonstrate that high-power Hertzian oscillator could be synchronized using high-power semiconductor switching. Synchronization requires that

the one standard deviation time jitter between an external trigger source and the output of the oscillator be no larger than 5% of the period corresponding of the oscillator's center frequency (or about 250 ps for the 200-MHz case that we studied). High power implies that the oscillator is operating at the air corona level (about 200 kV). Driving an optimal dipole antenna, a single oscillator radiates about 300 MW average power corresponding to 500 MW effective radiated power (ERP). For ten such units, properly arrayed and synchronized, the ERP is 50 GW, which is a very interesting level for a variety of applications. The concept we identified was to switch oscillators with trigatron-type spark gaps. At the start of this project, we demonstrated that the 200-MHz synchronization could be achieved with this design using a complex trigger system suitable for laboratory applications. The objective of the project was to demonstrate that this trigger could be replaced with a subcircuit placed on each oscillator using a high-gain photoconductive GaAs switch as its timing element. This type of GaAs device easily can switch up to 100 kV with subnanosecond precision, but semiconductor switches tend to be fragile. In practice this project was to demonstrate the compatibility of semiconductor switches for this application. The advantages accruing to the use of this technology include the ability to build smaller, lighter systems and to steer the beam from the array on a pulse-to-pulse basis. The scope of work was to demonstrate the feasibility of the concept to the greatest extent possible without actually building and testing the final hardware.

A number of issues needed to be resolved before we constructed the final configuration. To minimize the require-

ments on the GaAs switch, we wanted to minimize the voltage required to achieve synchronization. To achieve synchronization, the trigger voltage risetime must be on the order of the jitter allowed, but it is critical to know precisely how long a risetime can be tolerated, as this has substantial system implications. We built several trigatron switches and triggered them with two waveforms with different risetimes to bracket the triggering requirements. We developed what appears to be an optimal trigatron geometry. We were able to settle on a 30-kV trigger voltage. The full answer of the risetime requirement can not be given yet because the requirements may depend on the gas-switching medium used in the trigatron. For example, we achieved suitable synchronization with 1-ns risetime trigger pulses using a 20% SF₆-80% N₂ gas mix. However, the switching energy losses were large. Using H₂, the losses were reduced substantially, but we were not able to get the synchronization required with 1-ns risetime trigger pulses. We believe that we can achieve better synchronization with 200-ps risetime pulses but were not able to complete this demonstration. We modeled circuits that can achieve the 1-ns risetime and are convenient for use with the Hertzian oscillator. There is more work to be done before we have a suitable 200-ps risetime configuration. In summary, using the 20% SF₆-80% N₂ gas mix, we have all the data to design a GaAs-based trigger system for 200-kV oscillators.

Investigation of Analysis Techniques for Swarm Behavior

B. L. Spletzer, R. J. Pryor

Predicting the behavior of large swarms of intelligent agents, whether human or machine, is a difficult computational problem. The problems of both predicting the actions of swarms and developing rules so that a swarm exhibits desired behavior are of great interest in such diverse areas as robotics, site security, and economic modeling. Recent work with the Aspen economics model shows that evolutionary learning methods could be applied to swarms. Also, it appears that the techniques of classical mechanics used for analyzing continua may also apply to behavior of large swarms.

This research will investigate the feasibility of applying these two different techniques to the behavior of swarms. With regard to evolutionary learning methods, Sandia will test different genetic programming learning strategies. The experience

gained this way will provide a foundation for solving swarm behavior problems. The work toward a continuum analysis approach will strive to develop the underlying theory and appropriate analogies needed to apply classical analysis to swarm behavior.

Sandia's work this year on developing a behavior for intelligent agents using genetic programming focused on two areas: (1) incorporating agent learning from previous learning sessions, and, (2) coevolving the problem difficulty with the level of agent learning.

Learning is usually done in several sessions. Incorporating what was learned from previous sessions is therefore a necessary part of the solution procedure to find an acceptable behavior. The issue was to not introduce previous learning too fast, which would tend to make the agents focus on possibly unproductive regions of the solution space. We found a gradual introduction through gene splicing (crossover) to be the most optimum strategy. The second area deals with evolving the problem difficulty with the current level of learning. Learning

occurs most quickly when the difficulty of the problem gradually increases. Starting a learning session with the most difficult problems will most likely not lead to a solution. Starting with easy problems and working toward harder ones is best. This work is ongoing, but we have gained a qualitative understanding of the learning levels.

We completed a multi-action behavior for the agent that can navigate around walls and be used on any number of agents. A single-action behavior is now under development. We also completed a viewer that we can use to analyze the results of a simulation.

The continuum and statistical mechanics approach concentrated on developing the underlying theory of this revolutionary approach to understanding behavior. We developed several geometric analogies directly from existing continua. In addition, initial work on the first nongeometric analogy has begun. This idea exploration work has been very useful in providing direction and a basic understanding of the nature of these analogies.

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R&D 100 Award, <i>R&D Magazine</i> : Aztec Library of Equation Solvers	3504.020	Modeling Complex Turbulent Chemically Reacting Flows on Massively Parallel Supercomputers
Best Presentation in Session, IEEE Conference on Computer Vision & Pattern Recognition, June 1997	3504.080	Sensing and Compressing 3-D Models
R&D 100 Award, <i>R&D Magazine</i> : Nonvolatile Field-Effect Transistor Device	3506.230	A Novel Nondestructive Silicon-on-Insulator Nonvolatile Memory
Lockheed-Martin NOVA Award for Technical Excellence: Inventions and Advances in IMEMS Technology	3506.280	Vacuum Encapsulation of MEMS Structures
R&D 100 Award, <i>R&D Magazine</i> : Filmetrics F-30 Optical Probe	3506.310	Agile Dry Etching of Compound Semiconductors for Science-Based Manufacturing Using <i>In Situ</i> Process Control
Sandia President's Quality Award (Special Recognition): Cleaning for Adhesive Bonding	3510.590	Investigation of the Impact of Cleaning on the Adhesive Bond and the Process Implications
Sandia President's Quality Award (Special Recognition): Laser Wire Deposition	3510.620	Laser Wire Deposition for Fully Dense Net Shapes
<i>Discover Magazine</i> Award for Technological Innovation in Sight: Developing Room-Temperature Gamma Radiation Detector	3515.170	Development of a Portable X-Ray and Gamma-Ray Detector Instrument and Imaging Camera for Use in Radioactive and Hazardous Material Management
Lockheed Martin NOVA Awards: ARM Program Set UAV Endurance Record and Established Dominance of Clouds in Global-Warming Physics	3519.070	Environmental Monitoring: Civilian Space Application and Global Climate Change
R&D 100 Award, <i>R&D Magazine</i> : GEO SEIS™ Mini-Hole Seismic Surface Initiation System	3523.090	A New Concept for Very Low-Energy Detonators and Torches
E. O. Lawrence Award: Fundamental Work in Signal Processing and its Applications to National Security	3525.040	Image Formation Algorithms for Spotlight Mode Synthetic Aperture Radar
Sandia President's Quality Award (Turquoise Award): Explosive-Detecting Personnel Portal	3536.020	Molecular Concentrator

Appendix C: Awards/Recognition List

Awards/Recognition	Project Number	Project Title
R&D 100 Award, <i>R&D Magazine</i> : Biocavity Laser	3539.220	Biocavity Laser Microscopy/Spectroscopy of Cells
BES Materials Science Award: Nanoclusters	3539.270	Tailorable, Visible, Room- Temperature Light Emission from Si, Ge, and Si-Ge Nanoclusters
Joseph F. Engelberger Robotics Award by the Robotics Industries Association: Leadership in establishing one of the world's premiere centers of robotics		58 LDRD contributing projects from FY95 through FY97

Legend

		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***

* 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

*** Hypotheses Status
 6 - Hypothesis Proved
 7 - Hypothesis Remains Unchanged
 8 - Hypothesis Modified
 9 - Hypothesis Redefined
 10 - Hypothesis Disproved
 11 - Project Terminated

Appendix D: 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***
Sol-Gel Preservation of Mankind's Cultural Heritage in Objects Constructed of Stone	3502.010	2	1	1				1	1		2		95%	1	8
Physico-Chemical Stability of Solid Surfaces	3502.020	4						1	1				100%	1	5
Catalytic Membrane Sensors	3502.030	5		1	1			2	1	11			95%	1	7
Photonic Bandgap Structures as a Gateway to Nano-Photonics	3502.040	2		1									100%	1	6
Wide-Bandgap Compound Semiconductors to Enable Novel Semiconductor Devices	3502.050	11											100%	1	3
Synthesis and Modeling of Field-Structured Anisotropic Composites	3502.060	5			3				1				100%	1	6
Model Determination and Validation for Reactive Wetting Processes	3502.070	4											90%	1	6
Ultra-Hard Multilayer Coatings	3502.080	19											100%	1	7
Scanning Probe-Based Processes for Nanometer-Scale Device Fabrication	3502.090		2					1	1				50%	3	7
Molecular-Scale Lubricants for Micromachine Applications	3502.110	2											90%	2	7
Surface-Micromachined Flexural Plate Wave Device Integrated on Silicon	3502.120	5							2	2			90%	2	7
Molecular Imprinting in Aerogels for Remote Sensing of Chemical Weapons and Pesticides	3502.130	2	1	1				2	3				40%	3	8
Smart Interface Bonding Alloys (SIBA): Tailoring Thin-Film Mechanical Properties	3502.140	6											90%	1	7
Understanding and Control of Energy Transfer Mechanisms in Optical Ceramics	3502.150	3							1				90%	2	6
Integrated Thin-Film Structures for IR Imaging	3502.160	1	6	1	1			4	2				85%	2	6
Recognizing Atoms in Atomically Engineered Nanostructures: An Interdisciplinary Approach	3502.170									5			100%	1	7
Modeling Electrodeposition for Metal Microdevice Fabrication	3502.180	1		1									95%	1	6
The Initiation and Propagation of Nanoscale Cracks at an Adhesive/Solid Interface	3502.190		3										80%	2	6
Monolithic Structures for Nanoseparation	3502.210							2					100%	1	7
Fundamental Aspects of Micromachine Reliability	3502.220	2							1				90%	1	6
Enabling Science and Technology for Cold-Spray Direct Fabrication	3502.230	1	1	1									100%	1	7
Atomic-Level Studies of Surfactant-Directed Materials Growth	3502.240	14	26						1		2		90%	2	7
Intelligent Polymers for Nanodevice Performance Control	3502.250	1											80%	2	7
Freeforming of Ceramics and Composites from Colloidal Slurries	3502.260	1	10	1				2	1				100%	1	7
Quantum Dot Arrays	3502.270												100%	1	6
Laser-Assisted Arc Welding for Aluminum Alloys	3502.280		1	1									80%	4	7
System Studies in Electrochemical Processing	3502.290		1					2					90%	1	8

Appendix D: 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***
Parallel Quantum Chemistry for Material Aging and Synthesis	3504.010	1											100%	1	7
Modeling Complex Turbulent Chemically Reacting Flows on Massively Parallel Supercomputers	3504.020	3	4				1		1	1			80%	2	7
Scalability of Cryptographic Algorithms and Protocols	3504.030	5						1					100%	2	6
Computer-Designed Molecular Memory and Switching Elements	3504.040	14	16	1				4					95%	1	6
Automated Geometric Model Builder Using Range Image Sensor Data	3504.050	1											100%	1	7
A Massively Parallel Sparse Eigensolver for Structural Dynamics Finite Element	3504.060	1	1					1	1				100%	1	7
Density Functional Theory for Classical Fluids at Complex Interfaces	3504.070	3	4										70%	2	7
Sensing and Compressing 3-D Models	3504.080	3			1			2			1		20%	4	9
Gradient-Driven Diffusion of Multi-Atom Molecules Through Macromolecules and Membranes	3504.090	4							1	1			100%	1	7
An Easier Way? An Attempt to Tightly Couple Complete Grid Generation with the Flow Solver for Discretized Governing Equations	3504.110	1											70%	3	6
Fast and Easy Parallel I/O for Efficient Scientific Computing	3504.120				2					1			100%	1	7
Novel Load-Balancing for Scalable, Parallel Electromagnetic and Plasma Physics Simulation Software	3504.130							1					75%	2	6
Parallel Computational Chemistry Using Constraints	3504.140		3										100%	1	7
Accurate Numerical Methods for Wave Propagation	3504.150												70%	11	11
Massively Parallel Ab Initio Validation for ASCI Materials Aging	3504.160												100%	1	7
Dynamically Coupled, Massively Parallel Simulation of Grain Growth and Aging/Degradation	3504.170	18							2				100%	1	7
An Investigation of Wavelet Bases for Multiscale, Grid-Based Simulation	3504.180	1	6						1	1			100%	1	7
Integrated Quantum/Classical Modeling of Hydrogenic Materials	3504.190	1	2										90%	1	7
The Next Generation of Teraflop Density Functional Electronic Structure Codes	3504.210												70%	2	7
Methodology for Characterizing Modeling and Discretization Uncertainties in Computational Simulation	3504.220												70%	3	7
A Critical Evaluation of Algorithms for Global Optimization	3504.230	6	6				1	1					100%	1	7
Dynamic Simulation of Mechanical Systems with Intermittent Contacts	3504.240	1											100%	1	7
High-Speed Modulation of Vertical-Cavity Surface-Emitting Lasers	3506.010	12						1					90%	1	6
Micromachined Inertial Sensors (Accelerometer, Gyroscope)	3506.020		1	1									95%	2	7
Red-to-Blue-Wavelength Photonic Devices	3506.030	8											75%	2	6

Appendix D: 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***
Double Electron Layer Tunneling Transistor	3506.040	13	3	2	1			2	1				70%	2	6
Subwavelength Diffractive Optics	3506.050	1	2										60%	3	6
Vehicle Exhaust-Gas Chemical Sensors Using Acoustic-Wave Resonators	3506.060	9	1					3	1				90%	2	6
GaAs PIC Development for High-Performance Communications	3506.070	3						2					90%	2	6
Application-Specific Tester-on-a-Resident-Chip (TORCH)	3506.080		1					2					80%	2	6
Ultra-Low-Power Microwave CHFET Integrated Circuit Development	3506.090		2										100%	1	9
Wafer Fusion for Integration of Semiconductor Materials and Devices	3506.110	1						1					100%	1	7
Highly Parallel, Low-Power, Photonic Interconnects for Inter-Board Signal Distribution	3506.120												90%	2	7
Achromatic Nonlinear Optics for Sensing and Process Control	3506.130	4	1	2	1				1				90%	2	6
Virtual Reactor for the Semiconductor Manufacturing Plant of the Future	3506.140		1										100%	1	7
Integrated Separation and Optical Detection for Novel On-Chip Chemical Analysis	3506.150		3										50%	3	8
Selective Oxidation Technology and Its Applications Toward Electronic and Optoelectronic Devices	3506.160	23		1		1		2					100%	1	7
High-G Accelerometer for Earth-Penetrator Weapons Applications	3506.170		2										100%	1	6
Agile Prototyping of Microelectromechanical Systems (MEMS)	3506.180		3								1		100%	1	6
Advanced Concepts for High-Power VCSELs and VCSEL Arrays	3506.190	8	2	1	1						1		100%	1	7
Midwave-Infrared (2-6 μm) Emitter-Based Chemical Sensor Systems	3506.210	1											90%	2	7
Microelectronic Biosensors	3506.220	2							2	1			88%	2	7
A Novel Nondestructive Silicon-on-Insulator Nonvolatile Memory	3506.230	4	2	3							1		100%	1	8
Integration of Optoelectronics and MEMS by Free-Space Microoptics	3506.240			1				1					75%	3	7
Advanced Laser Structures for Short-Pulsed Power in Active Optical Sensor Systems	3506.250	2		2				1					90%	2	7
Metal Micro-Heat-Pipe Substrates for High-Power-Density Electronics	3506.260	2		2	2	1							100%	1	6
Integration of Microsensor Technology into a Miniature Robotic Vehicle	3506.270												90%	2	7
Vacuum Encapsulation of MEMS Structures	3506.280		1		1						1		100%	1	7
Massively Parallel Sensor Arrays for Volatile Organic Detection	3506.290							1					100%	1	7
Agile Dry Etching of Compound Semiconductors for Science-Based Manufacturing Using In Situ Process Control	3506.310												100%	1	7

Appendix D: 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***
Precision-Formed Micromagnets	3506.320												100%	1	6
Time-Resolved Ion-Beam-Induced Charge-Collection (TRIBICC) Imaging	3506.330												100%	1	7
Composite-Resonator Surface-Emitting Lasers	3506.340												100%	1	7
Role of Defects in III-Nitride-Based Electronics	3506.350	6						1	1	1			90%	2	7
Ultra-Low-Power Sensors for Microtelemetry Systems	3506.360							1	1				100%	2	7
Double Quantum-Well Long-Wavelength Optoelectronic Devices	3506.370	2						1					70%	2	7
The Development of Integrated Chemical Microsensors in GaAs	3506.380		1	1						1			100%	1	7
Systems Studies in Compound Semiconductor Processing (U)	3506.390												90%	1	6
Unexplored Penetrator Regime Against Super-Hard Underground Facilities	3508.010							1					90%	2	7
Optimization of Computationally Challenging Problems in Engineering Sciences	3508.030	8	5				1		1				100%	1	6
Using Higher-Order Gradients to Modeling Localization Phenomena	3508.040	1	5						1				85%	2	6
Investigation of Nonequilibrium Microscopic Hydrodynamic Phenomena	3508.050	2						2					95%	2	9
Enhanced Vapor-Phase Diffusion in Porous Media	3508.060	6	1					2					100%	1	7
Numerical and Experimental Investigation of Vortical Flow-Flame Interaction	3508.070		3						2				80%	2	7
Temporal and Spatial Resolution of Fluid Flows	3508.080												75%	2	6
Characterization of Fluid Transport in Microscale Structures	3508.090	1		1						1			90%	2	6
Stress Evaluation and Model Validation Using Laser Ultrasonics	3508.110	2											100%	1	6
Altered Simulation Properties for Tetrahedral Finite Elements for Use in Engineering Simulation	3508.120	3	2										100%	1	6
Development, Implementation, and Experimental Validation of the Lattice Boltzmann Method for Modeling Three-Dimensional Complex Flows	3508.130	1	10						2				100%	1	8
Joint Task: Capturing Recrystallization of Metals with a Multiscale Material Model	3508.140	1	4					1	2				80%	2	7
Nondeterministic Modeling in Engineering Science	3508.150												85%	2	7
Lagrangian Modeling of Radiative Transport	3508.160	1						1					100%	1	7
VIEWES—Virtual Interactive Environment Work Space	3510.410	3	3	1	2			1					90%	1	6
Distributed Object and Intelligent Agents in a Wide-Area Network Test-Bed	3510.420	5						1					50%	4	7
Solid Variant Geometry Modeling	3510.430												50%	4	9
Rapid Prototyping/Rapid Manufacturing via Freeform Fabrication of Polymer-Matrix Composites	3510.440	1		1	1			1					90%	2	7
Solid Model Design Simplification	3510.450		1										80%	1	6
Laser-Spray Fabrication for Net-Shape Rapid Product Realization	3510.460	2	6	3				1	1	1			100%	1	7

Appendix D: 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***
Carbon Coatings for Improved Spryttron-Tube Performance and Reliability	3510.470	1											100%	1	6
Low-Cost Pd-Catalyzed Metallization Technology for Rapid Prototyping of Electronic Substrates and Devices	3510.480	2	3		1			3					90%	2	3
Smart Cutting Tools for Precision Manufacturing	3510.490	5		1				1					100%	1	6
Solution Synthesis and Processing of PZT Materials for Neutron-Generator Applications	3510.510		3					1					100%	1	7
Development of an Immersive Environment to Aid in Automatic Mesh Generation	3510.520	1											90%	2	3
Effect of Composition and Processing Conditions on the Reliability of Cermet/Alumina Components	3510.530	3		1									80%	2	7
Ultra-Precise Assembly of Microelectromechanical Systems (MEMS)	3510.540		2										100%	1	7
Self-Tuning Process-Monitoring System for Process-Based Product Validation	3510.550												95%	1	6
Process Optimization for Electron Beam Joining of Ceramic and Glass Components	3510.560		1										100%	1	6
Finite-Element Meshing Approached as a Global Minimization Process	3510.570							2					50%	3	7
Application of Parallel Mechanism Technology to Manufacturing	3510.580		1	2	6			2	1	2	1		95%	1	6
Investigation of the Impact of Cleaning on the Adhesive Bond and the Process Implications	3510.590							2	1		1		100%	1	6
Standard Cells for Microelectromechanical Systems (MEMS)	3510.610		1					2					100%	1	6
Laser Wire Deposition for Fully Dense Net Shapes	3510.620								1	1	1		100%	2	6
High-Throughput Dry Processes for Large-Area Devices	3510.630	1				1							100%	1	7
Assuring High Reliability and Production Readiness in Low-Volume Manufacturing	3510.640							1					90%	2	7
Advanced Control Methods for Improved Grinding Processes	3510.650												50%	3	7
Automatic Generation of Multimedia Documentation for Assembly Operations	3511.010		1				1						80%	2	7
Distributed Life-Cycle Models in Enterprise Simulations to Answer System Questions	3511.020		1										100%	1	7
Chain Models for Life-Cycle Systems Engineering	3511.030												90%	11	11
Immersive CAD	3511.040							2					100%	1	7
Automatic Planning of Life-Cycle Assembly Processes	3511.050	4					1						100%	1	9
Automatic Generation of Foolproof Manufacturing Plans	3511.060		1										95%	1	7
Design of a Highly Secure Smartcard	3512.110		5	4		2							90%	1	5
Object-Oriented Parallel Discrete Event Simulation System—An Enabling Foundation for Rapid Development of High-Performance, Large-Scale Simulations	3512.120	2					1						100%	1	5
Biometric Identity Verification for Remote User Authentication and Access Control Applications	3512.130							1					60%	3	8

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		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***
“Robustness-Agile” Asynchronous Transfer Mode (ATM) Encryption and Associated Use Control	3512.140	2	3	1							1		95%	2	6
Agent-Based Remediation of the Mosaic Classification Problem	3512.150						1						80%	3	6
Content-Based Search of Geometric Databases	3512.160												90%	2	7
Integrated Service Provisioning in an “IPv6 over ATM” Research Network	3512.170	3	1										90%	2	7
Virtual Desktop Engineering with Integrated Multimedia Data	3512.180												100%	1	7
Mission Surety for Large-Scale Real-Time Information Systems	3512.190	5			1		1	2	1	1	3		100%	1	7
Integrated and Robust Security Infrastructure	3512.210												80%	11	11
Scaled ATM End-to-End Encryption	3512.220		6	5			1				1		95%	2	7
Network Surety Modeling for Wireless ATM Networks (and Other Distributed Computing Systems)	3512.230	1	1					1					90%	2	7
Superconductive Gravity Gradiometers for Underground Target Recognition	3516.020												50%	5	7
Moving Mass Trim Control for Precision-Strike Warheads	3516.030	1			1								100%	1	6
Micro-Holographic Tagging	3516.040	4	2	3	1				1	1			100%	1	6
Electrokinetic Immunoaffinity Chemical Sensors	3516.050								1				97%	1	7
Information-Efficient Spectral Imaging System (ISIS)	3516.060		1	1				3					100%	1	6
Imaging of Moving Targets Using Simultaneous Synthetic Aperture Radar (SAR) and Moving Target Indicator (MTI) Radar	3516.070												95%	2	7
Sampling and Sensing Systems for High-Priority Analytes	3516.080		2						1				100%	1	7
Automated Vegetation Height Measurement for Automatic Terrain Mapping	3516.090												100%	1	6
Development of Inexpensive Metal Macrocyclic Complexes for Direct Oxidation of Methanol in Fuel Cells	3518.020	1		1									100%	1	6
Designed Molecular Recognition Materials for Chiral Sensors, Separations, and Catalytic Materials	3518.030	6	1	1				2	1				100%	1	6
Real-Time 3-D and Heterogeneous Data Fusion	3518.040		1										100%	2	6
Rapid Screening of Complex Chemical Samples via Capillary Array Analysis	3518.050		1					1	1	1			100%	1	7
Designed Synthesis of Controlled Degradative Materials	3518.060								1				90%	2	7
Mechanistic Models for Radionuclide Desorption from Soils	3518.070	1	2								1		100%	1	6
Reliability Degradation Due to Stockpile Aging	3520.210		1										100%	1	6
Integrated Approach to Develop Microelectromechanical Systems (MEMS)	3520.220	2							1				75%	1	6
Precursors to Failure of Oxides and Metal Lines in CMOS Technology	3520.230												100%	1	8
An Extensible Object-Oriented Framework for Risk & Reliability Analysis	3520.240												95%	2	7

Appendix D: 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***
Risk-Based Characterization of Network Vulnerability	3520.250	1											90%	11	11
Enhancing Risk Analysis Using New Mathematical Structures	3520.260	2	1		1			4					78%	11	11
Science on the Microdomain	3522.010		1						1	2			100%	1	6
Autonomous MicroChem Laboratory (μChemLab)	3522.020	7	1	4	1			1	3	3			100%	1	7
Cooperative, Distributed Sensing and Action Using Microminiature, Intelligent Agents	3522.030												100%	1	7
Development of Innovative Combustion Processes for a Direct-Injection Diesel Engine	3524.110		3										90%	1	6
Hydrogen Production for Fuel Cells by Selective Dehydrogenation of Alkanes in Catalytic Membrane Reactors	3524.120	1						2	2				80%	2	8
Hybrid Vehicle Engine Development	3524.130	1	1					2					100%	1	6
A 700-kV, Short-Pulse, Repetitive Accelerator for Industrial Applications	3524.140	1	9										70%	2	7
High-Power Ion Beam (HPIB) Modification of One- and Two-Layer Metal Surfaces	3524.150	1	1	1				2	1				90%	2	6
Advanced 3-D Electromagnetic and Particle-in-Cell Modeling	3524.160		3										90%	2	6
Electromagnetic Impulse Radar for Detection of Underground Structures	3524.170		2										95%	1	6
Computational Methods for Predicting the Response of Critical As-Built Infrastructure to Dynamic Loads (Architectural Surety)	3530.030	1											90%	1	6
An Advanced Unmanned Vehicle for Remote Applications	3530.040												95%	2	7
Cosmic Rate of Expansion from the Ambient Temperature's Observed Relaxation (CREATOR)	3530.050							3	1				25%	5	7
Productivity Enhancements for Analysts	3530.070		1										95%	1	6
Web Vulnerability Demonstration	3530.080												100%	2	6
System of Labs Direct Fabrication Technology	3531.020		3	1				1					90%	2	6
Cold-Cathodes for Sensors and Vacuum Microelectronics	3531.030	8	3										80%	2	7
In Situ Optical Photoreflectance During MOCVD	3531.040												100%	2	8
Novel Thermoelectrics for Next-Generation Power Sources	3531.050												50%	4	7
Micromachined Contact Fuses for Earth-Penetrator Applications	3531.060		2										100%	1	7
Advanced Stress-Sensing Assembly Test Chip Design	3531.070												75%	3	7
Cat's-Eye Modulator Fabricated in GaAs	3531.080												100%	1	6
Interfacial Charge Removal for MOVPE-Grown pHEMTs by In Situ Cleaning	3531.090	2											100%	1	6
Infrared Quantum-Well Intersubband Photodetector Development	3531.110												90%	2	7
Advanced Quantum-Well Structures for Improved Modulator Performance	3531.120												80%	2	6

Appendix D: 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***
High-Temperature Stereolithography Female Molds for Small-Lot Composite Manufacturing	3531.130												100%	1	6
Chemical Feedstocks for the Future: Oxidative Dehydrogenation	3532.010		1					1					100%	1	8
Global Approaches to Infrastructural Analysis (GAIA)	3532.030		1										100%	1	7
Modeling the Atmospheric Entry Physics and Terminal Explosions of the Anomalous October 3, 1996, Bolide Swarm	3532.040	1						1					90%	2	9
Advanced Subterranean Warfare (ASW) for Deep Underground Structures	3532.050		1										95%	1	6
Dispersive Measurements of Velocity in Heterogeneous Materials	3532.060												100%	2	7
Policy and Resource Allocations in Risk Management	3533.020	1			1								100%	1	7
Ceramic Membranes for Electrically Driven Ionic Separations	3533.030			1				3	1				100%	2	7
Developing On-Line Process-Monitoring Capabilities	3533.040												100%	1	7
SAM Telemetry for Measurements While Drilling	3533.050			3	1								90%	3	8
Dynamic Simulation Models and Geographic Information Systems	3533.060	2						1					80%	3	7
Design-for-Manufacturability Applied to Photovoltaic Modules	3533.070	1		1									100%	1	7
Applicability of a Metalloprotein Toxic Heavy-Metal Detector to DOE Production and Waste	3533.080		1					1					70%	3	7
Enhancing Energy Security Through New Routes to Petrochemical Feedstocks	3533.090		2										80%	2	8
Cathodic Protection of Zero-Valent Iron-Reactive Barriers	3533.110		1	1					1				70%	2	7
Consequence-Based Rationale for an Infrastructure Assurance Program	3533.120		2										100%	2	6
Modeling Interdependence in the U.S. Infrastructure	3533.130												90%	1	7
Surety of North American Electric Power Transmission Network	3533.140		1										80%	11	11
Protective Coatings for Concrete	3533.150								1				60%	3	7
Low-Cost Cadmium Zinc Telluride Radiation Detectors Based on Electron-Transport-Only Designs	3534.020	1		1				2					100%	1	6
LIGA Micromachining	3534.030							1		1			75%	3	7
Chemistry and Physics of Microfluids	3534.040									1			85%	2	7
Combinatorial Peptides for Chemical Sensing	3534.050												25%	4	8
Pulser in a Chip	3535.020	1	2						0.3				100%	1	6
Ultra-High-Pressure EOS Studies on Metals and ICF Ablators Using PBFA-Z	3535.030	1	1						1	4			95%	1	6
Flocking Small Smart Machines	3535.040												95%	2	7
Development of Explosive-Event Scale Model Testing Capability at Sandia	3535.050	1									1		95%	2	6
Application of SAR Vibrometry to Distributed Seismic Sources	3535.060												50%	3	7

Appendix D: 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***
Development of Laser-Cutting/-Welding Depth Control Using Laser Spectroscopy and Open Architecture Control of a Robotic System	3535.070												80%	11	11
Cryogenic EOS Capabilities on Pulsed-Radiation Sources (Z-pinch)	3535.080		2										70%	3	7
Aerosol Stand-off Detection Test-Bed	3535.090												75%	2	7
Investigation of Analysis Techniques for Swarm Behavior	3535.110												80%	2	7
Synchronized RF Sources for IW Applications	3535.120												100%	1	7
		371	247	65	31	5	9	108	61	44	19	0			

†Identification of new non-LDRD-funded projects is now completed in the fiscal year following the annual report.

Pg #	Title	Case Number	Science of Complex Systems	Modeling & Simulation of Complex Systems	High-Performance Computing	Nuclear Weapons Predictive Capability (Classified)	Safety Assessments & Engineering	Use Control & Verification	Nonproliferation & Security	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	Other
10	Sol-Gel Preservation of Mankind's Cultural Heritage in Objects Constructed of Stone	3502010000	•	•												•				
9	Physico-Chemical Stability of Solid Surfaces	3502020000			•		•							•		•				
11	Catalytic Membrane Sensors	3502030000															•			•
12	Photonic Bandgap Structures as a Gateway to Nano-Photonics	3502040000			•			•	•			•		•		•				
12	Wide-Bandgap Compound Semiconductors to Enable Novel Semiconductor Devices	3502050000	•	•	•				•			•		•						
14	Synthesis and Modeling of Field-Structured Anisotropic Composites	3502060000														•				
15	Model Determination and Validation for Reactive Wetting Processes	3502070000												•						
16	Ultra-Hard Multilayer Coatings	3502080000			•					•				•		•				
16	Scanning Probe-Based Processes for Nanometer-Scale Device Fabrication	3502090000												•						
18	Molecular-Scale Lubricants for Micromachine Applications	3502110000												•		•				
18	Surface-Micromachined Flexural Plate Wave Device Integrated on Silicon	3502120000							•		•			•						
19	Molecular Imprinting in Aerogels for Remote Sensing of Chemical Weapons and Pesticides	3502130000		•			•	•	•					•			•	•		

Pg #	Title	Case Number	Science of Complex Systems	Modeling & Simulation of Complex Systems	High-Performance Computing	Nuclear Weapons Predictive Capability (Classified)	Safety Assessments & Engineering	Use Control & Verification	Nonproliferation & Security	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	Other
20	Smart Interface Bonding Alloys (SIBA): Tailoring Thin-Film Mechanical Properties	3502140000	•													•				
21	Understanding and Control of Energy Transfer Mechanisms in Optical Ceramics	3502150000						•				•		•						
22	Integrated Thin-Film Structures for IR Imaging	3502160000							•					•						
23	Recognizing Atoms in Atomically Engineered Nanostructures: An Interdisciplinary Approach	3502170000												•		•				
24	Modeling Electrodeposition for Metal Microdevice Fabrication	3502180000		•										•		•				
24	The Initiation and Propagation of Nanoscale Cracks at an Adhesive/Solid Interface	3502190000	•	•	•	•								•		•				
25	Monolithic Structures for Nanoseparation	3502210000	•	•		•	•	•	•	•	•				•	•	•	•	•	
26	Fundamental Aspects of Micromachine Reliability	3502220000														•			•	
27	Enabling Science and Technology for Cold-Spray Direct Fabrication	3502230000		•								•		•		•	•	•		•
28	Atomic-Level Studies of Surfactant-Directed Materials Growth	3502240000												•		•				
30	Intelligent Polymers for Nanodevice Performance Control	3502250000						•								•				
32	Freeforming of Ceramics and Composites from Colloidal Slurries	3502260000	•	•												•	•			

Pg #	Title	Case Number	Science of Complex Systems	Modeling & Simulation of Complex Systems	High-Performance Computing	Nuclear Weapons Predictive Capability (Classified)	Safety Assessments & Engineering	Use Control & Verification	Nonproliferation & Security	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	Other
31	Quantum Dot Arrays	3502270000														•				
33	Laser-Assisted Arc Welding for Aluminum Alloys	3502280000										•				•	•			
34	System Studies in Electrochemical Processing	3502290000														•				
37	Parallel Quantum Chemistry for Material Aging and Synthesis	3504010000				•					•					•				
38	Modeling Complex Turbulent Chemically Reacting Flows on Massively Parallel Supercomputers	3504020000	•	•	•				•					•		•		•		
39	Scalability of Cryptographic Algorithms and Protocols	3504030000			•			•	•											
40	Computer-Designed Molecular Memory and Switching Elements	3504040000	•	•										•		•				
43	Automated Geometric Model Builder Using Range Image Sensor Data	3504050000		•	•				•			•							•	
42	A Massively Parallel Sparse Eigensolver for Structural Dynamics Finite Element	3504060000	•	•	•	•			•								•		•	
44	Density Functional Theory for Classical Fluids at Complex Interfaces	3504070000	•	•												•				
45	Sensing and Compressing 3-D Models	3504080000	•	•	•				•										•	
45	Gradient-Driven Diffusion of Multi-Atom Molecules Through Macromolecules and Membranes	3504090000		•	•						•					•	•	•		

Pg #	Title	Case Number	Science of Complex Systems	Modeling & Simulation of Complex Systems	High-Performance Computing	Nuclear Weapons Predictive Capability (Classified)	Safety Assessments & Engineering	Use Control & Verification	Nonproliferation & Security	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	Other
46	An Easier Way? An Attempt to Tightly Couple Complete Grid Generation with the Flow Solver for Discretized Governing Equations	3504110000		•	•															
46	Fast and Easy Parallel I/O for Efficient Scientific Computing	3504120000		•	•															
47	Novel Load-Balancing for Scalable, Parallel Electromagnetic and Plasma Physics Simulation Software	3504130000		•	•	•						•	•	•						
48	Parallel Computational Chemistry Using Constraints	3504140000		•	•											•				
49	Accurate Numerical Methods for Wave Propagation	3504150000		•	•				•											
49	Massively Parallel Ab Initio Validation for ASCI Materials Aging	3504160000			•	•										•				
50	Dynamically Coupled, Massively Parallel Simulation of Grain Growth and Aging/Degradation	3504170000	•	•										•		•	•			
52	An Investigation of Wavelet Bases for Multiscale, Grid-Based Simulation	3504180000	•	•	•	•	•													
53	Integrated Quantum/Classical Modeling of Hydrogenic Materials	3504190000	•	•	•											•				
54	The Next Generation of Teraflop Density Functional Electronic Structure Codes	3504210000		•	•															
54	Methodology for Characterizing Modeling and Discretization Uncertainties in Computational Simulation	3504220000	•	•	•			•	•								•		•	

Pg #	Title	Case Number	Science of Complex Systems	Modeling & Simulation of Complex Systems	High-Performance Computing	Nuclear Weapons Predictive Capability (Classified)	Safety Assessments & Engineering	Use Control & Verification	Nonproliferation & Security	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	Other
55	A Critical Evaluation of Algorithms for Global Optimization	3504230000	•	•	•		•		•							•	•		•	
56	Dynamic Simulation of Mechanical Systems with Intermitent Contacts	3504240000	•	•			•										•		•	
59	High-Speed Modulation of Vertical-Cavity Surface-Emitting Lasers	3506010000			•			•	•			•		•				•	•	
60	Micromachined Inertial Sensors (Accelerometer, Gyroscope)	3506020000					•			•				•		•			•	
60	Red-to-Blue-Wavelength Photonic Devices	3506030000	•	•					•			•		•						
62	Double Electron Layer Tunneling Transistor	3506040000							•					•						
64	Subwavelength Diffractive Optics	3506050000			•			•		•		•		•		•		•	•	
64	Vehicle Exhaust-Gas Chemical Sensors Using Acoustic-Wave Resonators	3506060000								•				•		•				
66	GaAs PIC Development for High-Performance Communications	3506070000			•		•	•						•						
67	Application-Specific Tester-on-a-Resident-Chip (TORCH)	3506080000					•			•				•					•	•
68	Ultra-Low-Power Microwave CHFET Integrated Circuit Development	3506090000							•					•						
68	Wafer Fusion for Integration of Semiconductor Materials and Devices	3506110000			•			•	•		•	•		•						

Pg #	Title	Case Number	Science of Complex Systems	Modeling & Simulation of Complex Systems	High-Performance Computing	Nuclear Weapons Predictive Capability (Classified)	Safety Assessments & Engineering	Use Control & Verification	Nonproliferation & Security	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	Other
69	Highly Parallel, Low-Power, Photonic Interconnects for Inter-Board Signal Distribution	3506120000			•		•				•		•							
70	Achromatic Nonlinear Optics for Sensing and Process Control	3506130000						•			•									
71	Virtual Reactor for the Semiconductor Manufacturing Plant of the Future	3506140000											•		•	•				
72	Integrated Separation and Optical Detection for Novel On-Chip Chemical Analysis	3506150000						•			•		•							
74	Selective Oxidation Technology and Its Applications Toward Electronic and Optoelectronic Devices	3506160000			•		•	•			•		•							
73	High-G Accelerometer for Earth-Penetrator Weapons Applications	3506170000							•				•							
76	Agile Prototyping of Microelectromechanical Systems (MEMS)	3506180000					•	•				•	•					•		
76	Advanced Concepts for High-Power VCSELs and VCSEL Arrays	3506190000			•		•	•			•		•							
78	Midwave-Infrared (2-6 μm) Emitter-Based Chemical Sensor Systems	3506210000			•		•	•			•		•							
78	Microelectronic Biosensors	3506220000						•					•							
80	A Novel Nondestructive Silicon-on-Insulator Nonvolatile Memory	3506230000			•								•							
81	Integration of Optoelectronics and MEMS by Free-Space Microoptics	3506240000			•		•	•			•		•							

Pg #	Title	Case Number	Science of Complex Systems	Modeling & Simulation of Complex Systems	High-Performance Computing	Nuclear Weapons Predictive Capability (Classified)	Safety Assessments & Engineering	Use Control & Verification	Nonproliferation & Security	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	Other
82	Advanced Laser Structures for Short-Pulsed Power in Active Optical Sensor Systems	3506250000						•				•		•						
82	Metal Micro-Heat-Pipe Substrates for High-Power-Density Electronics	3506260000												•						
83	Integration of Microsensor Technology into a Miniature Robotic Vehicle	3506270000	•						•					•					•	
84	Vacuum Encapsulation of MEMS Structures	3506280000						•	•	•				•		•			•	
85	Massively Parallel Sensor Arrays for Volatile Organic Detection	3506290000							•					•						
86	Agile Dry Etching of Compound Semiconductors for Science-Based Manufacturing Using In Situ Process Control	3506310000												•			•			
86	Precision-Formed Micromagnets	3506320000	•					•						•		•				
87	Time-Resolved Ion-Beam-Induced Charge-Collection (TRIBICC) Imaging	3506330000												•						
88	Composite-Resonator Surface-Emitting Lasers	3506340000										•		•						
88	Role of Defects in III-Nitride-Based Electronics	3506350000										•		•						
90	Ultra-Low-Power Sensors for Microtelemetry Systems	3506360000						•	•					•					•	
90	Double Quantum-Well Long-Wavelength Optoelectronic Devices	3506370000			•			•	•			•		•						

Appendix E: DOE Critical Technologies

Pg #	Title	Case Number	Science of Complex Systems	Modeling & Simulation of Complex Systems	High-Performance Computing	Nuclear Weapons Predictive Capability (Classified)	Safety Assessments & Engineering	Use Control & Verification	Nonproliferation & Security	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	Other
92	The Development of Integrated Chemical Microsensors in GaAs	3506380000							•					•					•	
92	Systems Studies in Compound Semiconductor Processing (U)	3506390000												•						
96	Unexplored Penetrator Regime Against Super-Hard Underground Facilities	3508010000		•		•								•		•				
96	Optimization of Computationally Challenging Problems in Engineering Sciences	3508030000		•	•	•	•							•		•	•	•	•	•
95	Using Higher-Order Gradients to Modeling Localization Phenomena	3508040000	•	•	•	•	•			•					•	•	•	•		
98	Investigation of Nonesilibrium Microscopic Hydrodynamic Phenomena	3508050000		•	•									•						
99	Enhanced Vapor-Phase Diffusion in Porous Media	3508060000	•	•																
100	Numerical and Experimental Investigation of Vortical Flow-Flame Interaction	3508070000		•	•															
101	Temporal and Spatial Resolution of Fluid Flows	3508080000	•	•	•		•													
101	Characterization of Fluid Transport in Microscale Structures	3508090000							•										•	
102	Stress Evaluation and Model Validation Using Laser Ultrasonics	3508110000	•	•		•	•			•	•	•		•	•		•	•		
103	Altered Simulation Properties for Tetrahedral Finite Elements for Use in Engineering Simulation	3508120000		•	•	•	•	•	•								•			

Pg #	Title	Case Number	Science of Complex Systems	Modeling & Simulation of Complex Systems	High-Performance Computing	Nuclear Weapons Predictive Capability (Classified)	Safety Assessments & Engineering	Use Control & Verification	Nonproliferation & Security	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	Other
104	Development, Implementation, and Experimental Validation of the Lattice Boltzmann Method for Modeling Three-Dimensional Complex Flows	3508130000	•	•	•		•		•							•				
106	Joint Task: Capturing Recrystallization of Metals with a Multiscale Material Model	3508140000	•	•	•	•	•			•					•	•	•			
105	Nondeterministic Modeling in Engineering Science	3508150000	•	•	•			•	•								•		•	
107	Lagrangian Modeling of Radiative Transport	3508160000	•	•	•		•													
111	VIEWS—Virtual Interactive Environment Work Space	3510410000		•	•	•											•			
112	Distributed Object and Intelligent Agents in a Wide-Area Network Test-Bed	3510420000															•			•
112	Solid Variant Geometry Modeling	3510430000															•		•	
113	Rapid Prototyping/Rapid Manufacturing via Freeform Fabrication of Polymer-Matrix Composites	3510440000														•	•		•	
114	Solid Model Design Simplification	3510450000		•	•														•	
114	Laser-Spray Fabrication for Net-Shape Rapid Product Realization	3510460000	•	•	•		•				•					•	•	•	•	
116	Carbon Coatings for Improved Spryttron-Tube Performance and Reliability	3510470000		•							•					•	•			

Pg #	Title	Case Number	Science of Complex Systems	Modeling & Simulation of Complex Systems	High-Performance Computing	Nuclear Weapons Predictive Capability (Classified)	Safety Assessments & Engineering	Use Control & Verification	Nonproliferation & Security	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	Other
116	Low-Cost Pd-Catalyzed Metallization Technology for Rapid Prototyping of Electronic Substrates and Devices	3510480000		•									•	•			•	•	•	
118	Smart Cutting Tools for Precision Manufacturing	3510490000	•	•					•					•			•	•	•	
118	Solution Synthesis and Processing of PZT Materials for Neutron-Generator Applications	3510510000		•										•						
120	Development of an Immersive Environment to Aid in Automatic Mesh Generation	3510520000		•	•	•	•									•	•			
121	Effect of Composition and Processing Conditions on the Reliability of Cermet/Alumina Components	3510530000														•				
122	Ultra-Precise Assembly of Microelectromechanical Systems (MEMS)	3510540000												•			•		•	
122	Self-Tuning Process-Monitoring System for Process-Based Product Validation	3510550000															•		•	
124	Process Optimization for Electron Beam Joining of Ceramic and Glass Components	3510560000		•									•				•	•	•	•
124	Finite-Element Meshing Approached as a Global Minimization Process	3510570000	•	•	•	•	•										•	•	•	•
125	Application of Parallel Mechanism Technology to Manufacturing	3510580000	•	•													•	•	•	•
126	Investigation of the Impact of Cleaning on the Adhesive Bond and the Process Implications	3510590000	•	•														•	•	
126	Standard Cells for Microelectromechanical Systems (MEMS)	3510610000						•												

Appendix E: DOE Critical Technologies

Pg #	Title	Case Number	Science of Complex Systems	Modeling & Simulation of Complex Systems	High-Performance Computing	Nuclear Weapons Predictive Capability (Classified)	Safety Assessments & Engineering	Use Control & Verification	Nonproliferation & Security	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	Other
127	Laser Wire Deposition for Fully Dense Net Shapes	3510620000		•												•	•	•		
128	High-Throughput Dry Processes for Large-Area Devices	3510630000		•										•				•		
129	Assuring High Reliability and Production Readiness in Low-Volume Manufacturing	3510640000		•			•										•			
130	Advanced Control Methods for Improved Grinding Processes	3510650000	•	•													•			
133	Automatic Generation of Multimedia Documentation for Assembly Operations	3511010000		•													•			
134	Distributed Life-Cycle Models in Enterprise Simulations to Answer System Questions	3511020000	•	•	•															
134	Chain Models for Life-Cycle Systems Engineering	3511030000	•	•																
135	Immersive CAD	3511040000	•	•	•														•	
136	Automatic Planning of Life-Cycle Assembly Processes	3511050000		•													•	•	•	
137	Automatic Generation of Foolproof Manufacturing Plans	3511060000		•			•										•		•	
141	Design of a Highly Secure Smartcard	3512110000						•												•

Pg #	Title	Case Number	Science of Complex Systems	Modeling & Simulation of Complex Systems	High-Performance Computing	Nuclear Weapons Predictive Capability (Classified)	Safety Assessments & Engineering	Use Control & Verification	Nonproliferation & Security	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	Other
142	Object-Oriented Parallel Discrete Event Simulation System—An Enabling Foundation for Rapid Development of High-Performance, Large-Scale Simulations	3512120000	•	•	•				•						•				•	
143	Biometric Identity Verification for Remote User Authentication and Access Control Applications	3512130000						•												
144	“Robustness-Agile” Asynchronous Transfer Mode (ATM) Encryption and Associated Use Control	3512140000			•			•									•			
145	Agent-Based Remediation of the Mosaic Classification Problem	3512150000	•		•			•											•	
146	Content-Based Search of Geometric Databases	3512160000		•	•												•	•	•	
147	Integrated Service Provisioning in an “IPv6 over ATM” Research Network	3512170000			•															
148	Virtual Desktop Engineering with Integrated Multimedia Data	3512180000		•	•			•									•		•	
148	Mission Surety for Large-Scale Real-Time Information Systems	3512190000	•	•					•											
149	Integrated and Robust Security Infrastructure	3512210000	•	•				•	•											
150	Scaled ATM End-to-End Encryption	3512220000						•	•											
151	Network Surety Modeling for Wireless ATM Networks (and Other Distributed Computing Systems)	3512230000		•	•															•

Appendix E: DOE Critical Technologies

Pg #	Title	Case Number	Science of Complex Systems	Modeling & Simulation of Complex Systems	High-Performance Computing	Nuclear Weapons Predictive Capability (Classified)	Safety Assessments & Engineering	Use Control & Verification	Nonproliferation & Security	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	Other
155	Superconductive Gravity Gradiometers for Underground Target Recognition	3516020000																		
155	Moving Mass Trim Control for Precision-Strike Warheads	3516030000																		
156	Micro-Holographic Tagging	3516040000																		
157	Electrokinetic Immunoaffinity Chemical Sensors	3516050000																		
158	Information-Efficient Spectral Imaging System (ISIS)	3516060000																		
158	Imaging of Moving Targets Using Simultaneous Synthetic Aperture Radar (SAR) and Moving Target Indicator (MTI) Radar	3516070000																		
159	Sampling and Sensing Systems for High-Priority Analytes	3516080000																		
160	Automated Vegetation Height Measurement for Automatic Terrain Mapping	3516090000																		
163	Development of Inexpensive Metal Macrocyclic Complexes for Direct Oxidation of Methanol in Fuel Cells	3518020000																		
164	Designed Molecular Recognition Materials for Chiral Sensors, Separations and Catalytic Materials	3518030000																		
165	Real-Time 3-D and Heterogeneous Data Fusion	3518040000																		

Pg #	Title	Case Number	Science of Complex Systems	Modeling & Simulation of Complex Systems	High-Performance Computing	Nuclear Weapons Predictive Capability (Classified)	Safety Assessments & Engineering	Use Control & Verification	Nonproliferation & Security	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	Other
166	Rapid Screening of Complex Chemical Samples via Capillary Array Analysis	3518050000						•										•		
166	Designed Synthesis of Controlled Degradative Materials	3518060000					•									•				
168	Mechanistic Models for Radionuclide Desorption from Soils	3518070000	•	•																
171	Reliability Degradation Due to Stockpile Aging	3520210000	•	•	•	•								•		•				
172	Integrated Approach to Develop Microelectromechanical System (MEMS)	3520220000												•				•		
173	Precursors to Failure of Oxides and Metal Lines in CMOS Technology	3520230000												•						
174	An Extensible Object-Oriented Framework for Risk & Reliability Analysis	3520240000		•			•													
175	Risk-Based Characterization of Network Vulnerability	3520250000		•															•	
176	Enhancing Risk Analysis Using New Mathematical Structures	3520260000		•			•												•	
179	Science on the Microdomain	3522010000	•					•	•										•	
180	Autonomous MicroChem Laboratory (μ ChemLab)	3522020000	•	•		•		•	•		•			•		•	•			
181	Cooperative, Distributed Sensing and Action Using Microminiature, Intelligent Agents	3522030000	•	•				•											•	

Pg #	Title	Case Number	Science of Complex Systems	Modeling & Simulation of Complex Systems	High-Performance Computing	Nuclear Weapons Predictive Capability (Classified)	Safety Assessments & Engineering	Use Control & Verification	Nonproliferation & Security	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	Other
185	Development of Innovative Combustion Processes for a Direct-Injection Diesel Engine	3524110000																		•
186	Hydrogen Production for Fuel Cells by Selective Dehydrogenation of Alkanes in Catalytic Membrane Reactors	3524120000														•				
186	Hybrid Vehicle Engine Development	3524130000																		•
188	A 700-kV, Short-Pulse, Repetitive Accelerator for Industrial Applications	3524140000					•		•			•	•	•		•				
187	High-Power Ion Beam (HPIB) Modification of One- and Two-Layer Metal Surfaces	3524150000		•							•		•			•	•	•		
189	Advanced 3-D Electromagnetic and Particle-in-Cell Modeling	3524160000	•	•	•	•							•	•						
190	Electromagnetic Impulse Radar for Detection of Underground Structures	3524170000							•			•	•	•						
193	Computational Methods for Predicting the Response of Critical As-Built Infrastructure to Dynamic Loads (Architectural Surety)	3530030000		•	•											•				
194	An Advanced Unmanned Vehicle for Remote Applications	3530040000							•			•							•	
194	Cosmic Rate of Expansion from the Ambient Temperature's Observed Relaxation (CREATOR)	3530050000																		
195	Productivity Enhancements for Analysts	3530070000							•											•
196	Web Vulnerability Demonstration	3530080000	•					•												

Pg #	Title	Case Number	Science of Complex Systems	Modeling & Simulation of Complex Systems	High-Performance Computing	Nuclear Weapons Predictive Capability (Classified)	Safety Assessments & Engineering	Use Control & Verification	Nonproliferation & Security	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	Other
196	System of Labs Direct Fabrication Technology	3531020000	•	•								•				•	•	•	•	
198	Cold-Cathodes for Sensors and Vacuum Microelectronics	3531030000	•											•						
197	In Situ Optical Photoreflexance During MOCVD	3531040000												•		•				
200	Novel Thermoelectrics for Next-Generation Power Sources	3531050000	•													•				
199	Micromachined Contact Fuses for Earth-Penetrator Applications	3531060000						•		•				•						
201	Advanced Stress-Sensing Assembly Test Chip Design	3531070000		•						•				•						
202	Cat's-Eye Modulator Fabricated in GaAs	3531080000												•						
202	Interfacial Charge Removal for MOVPE-Grown pHEMTs by In Situ Cleaning	3531090000												•			•			
203	Infrared Quantum-Well Intersubband Photodetector Development	3531110000												•						
204	Advanced Quantum-Well Structures for Improved Modulator Performance	3531120000							•					•						
204	High-Temperature Stereolithography Female Molds for Small-Lot Composite Manufacturing	3531130000														•	•	•	•	
206	Chemical Feedstocks for the Future: Oxidative Dehydrogenation	3532010000														•			•	

Pg #	Title	Case Number	Science of Complex Systems	Modeling & Simulation of Complex Systems	High-Performance Computing	Nuclear Weapons Predictive Capability (Classified)	Safety Assessments & Engineering	Use Control & Verification	Nonproliferation & Security	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	Other
207	Global Approaches to Infrastructural Analysis (GAIA)	3532030000	•	•	•															
205	Modeling the Atmospheric Entry Physics and Terminal Explosions of the Anomalous October 3, 1996, Bolide Swarm	3532040000			•				•											
208	Advanced Subterranean Warfare (ASW) for Deep Underground Structures	3532050000	•	•					•											
208	Dispersive Measurements of Velocity in Heterogeneous Materials	3532060000		•	•											•				
210	Policy and Resource Allocations in Risk Management	3533020000																		
209	Ceramic Membranes for Electrically Driven Ionic Separations	3533030000														•				
210	Developing On-Line Process-Monitoring Capabilities	3533040000							•							•	•	•		
210	SAM Telemetry for Measurements While Drilling	3533050000								•										•
212	Dynamic Simulation Models and Geographic Information Systems	3533060000		•					•											
212	Design-for-Manufacturability Applied to Photovoltaic Modules	3533070000												•			•	•		
211	Applicability of a Metalloprotein Toxic Heavy-Metal Detector to DOE Production and Waste	3533080000																•		
213	Enhancing Energy Security Through New Routes to Petrochemical Feedstocks	3533090000														•				•

Pg #	Title	Case Number	Science of Complex Systems	Modeling & Simulation of Complex Systems	High-Performance Computing	Nuclear Weapons Predictive Capability (Classified)	Safety Assessments & Engineering	Use Control & Verification	Nonproliferation & Security	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	Other
214	Cathodic Protection of Zero-Valent Iron-Reactive Barriers	3533110000																		•
216	Consequence-Based Rationale for an Infrastructure Assurance Program	3533120000	•	•																•
215	Modeling Interdependence in the U.S. Infrastructure	3533130000		•	•															
216	Surety of North American Electric Power Transmission Network	3533140000	•	•	•		•													•
218	Protective Coatings for Concrete	3533150000	•	•			•									•				
218	Low-Cost Cadmium Zinc Telluride Radiation Detectors Based on Electron-Transport-Only Designs	3534020000						•	•					•	•	•				
219	LIGA Micromachining	3534030000		•												•				
220	Chemistry and Physics of Microfluids	3534040000						•						•					•	
220	Combinatorial Peptides for Chemical Sensing	3534050000							•							•				
220	Pulser in a Chip	3535020000						•			•	•	•	•						
222	Ultra-High-Pressure EOS Studies on Metals and ICF Ablators Using PBFA-Z	3535030000		•	•					•	•		•							
222	Flocking Small Smart Machines	3535040000						•	•										•	

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223	Development of Explosive-Event Scale Model Testing Capability at Sandia	3535050000		•						•										
224	Application of SAR Vibrometry to Distributed Seismic Sources	3535060000							•											
224	Development of Laser-Cutting/-Welding Depth Control Using Laser Spectroscopy and Open Architecture Control of a Robotic System	3535070000										•				•	•	•	•	
226	Cryogenic EOS Capabilities on Pulsed-Radiation Sources (Z-pinch)	3535080000		•	•					•		•	•							
225	Aerosol Stand-off Detection Test-Bed	3535090000																		•
228	Investigation of Analysis Techniques for Swarm Behavior	3535110000	•	•				•	•										•	
227	Synchronized RF Sources for IW Applications	3535120000							•			•	•	•						

Pg #	Title	Case Number	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 and Technical Information	Defense Programs	Department of Defense (DoD)	Other Federal Agencies*	Other (Industry, Consortia)**
10	Sol-Gel Preservation of Mankind's Cultural Heritage in Objects Constructed of Stone	3502010000	•			•			•	•	•		•	•	•	•	•	Other Federal Agencies* Other (Industry, Consortia)** Metropolitan Museum of Art (NYC), Getty Conservation Institute (LA), DOC
9	Physico-Chemical Stability of Solid Surfaces	3502020000									•			•			•	
11	Catalytic Membrane Sensors	3502030000										•		•				
12	Photonic Bandgap Structures as a Gateway to Nano-Photonics	3502040000							•			•		•	•			
12	Wide-Bandgap Compound Semiconductors to Enable Novel Semiconductor Devices	3502050000	•									•		•				
14	Synthesis and Modeling of Field-Structured Anisotropic Composites	3502060000												•	•			
15	Model Determination and Validation for Reactive Wetting Processes	3502070000												•	•			
16	Ultra-Hard Multilayer Coatings	3502080000	•						•	•			•	•	•		•	
16	Scanning Probe-Based Processes for Nanometer-Scale Device Fabrication	3502090000							•	•				•				
18	Molecular-Scale Lubricants for Micromachine Applications	3502110000							•					•				
18	Surface-Micromachined Flexural Plate Wave Device Integrated on Silicon	3502120000	•			•	•					•		•	•			
19	Molecular Imprinting in Aerogels for Remote Sensing of Chemical Weapons and Pesticides	3502130000	•			•	•		•			•			•			
20	Smart Interface Bonding Alloys (SIBA): Tailoring Thin-Film Mechanical Properties	3502140000	•											•				
21	Understanding and Control of Energy Transfer Mechanisms in Optical Ceramics	3502150000				•				•	•	•		•	•			
22	Integrated Thin-Film Structures for IR Imaging	3502160000							•					•	•			

Appendix F: Major National Programs

Pg #	Title	Case Number	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 and Technical Information	Defense Programs	Department of Defense (DoD)	Other Federal Agencies*	Other (Industry, Consortia)**	Other Federal Agencies* Other (Industry, Consortia)**
23	Recognizing Atoms in Atomically Engineered Nanostructures: An Interdisciplinary Approach	3502170000																	
24	Modeling Electrodeposition for Metal Microdevice Fabrication	3502180000																*NASA	
24	The Initiation and Propagation of Nanoscale Cracks at an Adhesive/Solid Interface	3502190000																**Industry	
25	Monolithic Structures for Nanoseparation	3502210000																*EPA, NIH, **auto, steel, glass, chemical, etc.	
26	Fundamental Aspects of Micromachine Reliability	3502220000																	
27	Enabling Science and Technology for Cold-Spray Direct Fabrication	3502230000																*DOC, **U.S. car industry, other U.S. industries	
28	Atomic-Level Studies of Surfactant-Directed Materials Growth	3502240000																	
30	Intelligent Polymers for Nanodevice Performance Control	3502250000																	
32	Freeforming of Ceramics and Composites from Colloidal Slurries	3502260000																	
31	Quantum Dot Arrays	3502270000																	
33	Laser-Assisted Arc Welding for Aluminum Alloys	3502280000																**Industry	
34	System Studies in Electrochemical Processing	3502290000																	
37	Parallel Quantum Chemistry for Material Aging and Synthesis	3504010000																	
38	Modeling Complex Turbulent Chemically Reacting Flows on Massively Parallel Supercomputers	3504020000																	
39	Scalability of Cryptographic Algorithms and Protocols	3504030000																	

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40	Computer-Designed Molecular Memory and Switching Elements	3504040000								•	•			•					
43	Automated Geometric Model Builder Using Range Image Sensor Data	3504050000								•	•	•		•	•				
42	A Massively Parallel Sparse Eigensolver for Structural Dynamics Finite Element	3504060000	•	•	•		•				•		•	•	•	•			
44	Density Functional Theory for Classical Fluids at Complex Interfaces	3504070000					•				•					•			
45	Sensing and Compressing 3-D Models	3504080000	•				•					•		•	•				
45	Gradient-Driven Diffusion of Multi-Atom Molecules Through Macromolecules and Membranes	3504090000		•	•		•	•	•		•			•					
46	An Easier Way? An Attempt to Tightly Couple Complete Grid Generation with the Flow Solver for Discretized Governing Equations	3504110000												•	•				
46	Fast and Easy Parallel I/O for Efficient Scientific Computing	3504120000									•	•		•	•				
47	Novel Load-Balancing for Scalable, Parallel Electromagnetic and Plasma Physics Simulation Software	3504130000								•	•	•		•	•		•	**Microelectronics	
48	Parallel Computational Chemistry Using Constraints	3504140000										•		•	•				
49	Accurate Numerical Methods for Wave Propagation	3504150000					•				•			•					
49	Massively Parallel Ab Initio Validation for ASCI Materials Aging	3504160000												•	•				
50	Dynamically Coupled, Massively Parallel Simulation of Grain Growth and Aging/Degradation	3504170000									•	•		•					

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52	An Investigation of Wavelet Bases for Multiscale, Grid-Based Simulation	3504180000																	
53	Integrated Quantum/Classical Modeling of Hydrogenic Materials	3504190000																	
54	The Next Generation of TeraFlop Density Functional Electronic Structure Codes	3504210000																	
54	Methodology for Characterizing Modeling and Discretization Uncertainties in Computational Simulation	3504220000																	
55	A Critical Evaluation of Algorithms for Global Optimization	3504230000																	
56	Dynamic Simulation of Mechanical Systems with Intermittent Contacts	3504240000																	
59	High-Speed Modulation of Vertical-Cavity Surface-Emitting Lasers	3506010000																	**Optoelectronics
60	Micromachined Inertial Sensors (Accelerometer, Gyroscope)	3506020000																	
60	Red-to-Blue-Wavelength Photonic Devices	3506030000																	**Optoelectronics
62	Double Electron Layer Tunneling Transistor	3506040000																	
64	Subwavelength Diffractive Optics	3506050000																	**Optoelectronics
64	Vehicle Exhaust-Gas Chemical Sensors Using Acoustic-Wave Resonators	3506060000																	*DOT, EPA, **USCAR, Industry
66	GaAs PIC Development for High-Performance Communications	3506070000																	**Communication, Sensing and Control Industries
67	Application-Specific Tester-on-a-Resident-Chip (TORCH)	3506080000																	**Electronics/Microelectronics

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68	Ultra-Low-Power Microwave CHFET Integrated Circuit Development	3506090000	•					•			•	•			•	•			
68	Wafer Fusion for Integration of Semiconductor Materials and Devices	3506110000							•		•				•	•			
69	Highly Parallel, Low-Power, Photonic Interconnects for Inter-Board Signal Distribution	3506120000									•					•	•		*NSA, CIA
70	Achromatic Nonlinear Optics for Sensing and Process Control	3506130000									•	•			•				
71	Virtual Reactor for the Semiconductor Manufacturing Plant of the Future	3506140000									•				•	•			
72	Integrated Separation and Optical Detection for Novel On-Chip Chemical Analysis	3506150000					•				•				•	•			
74	Selective Oxidation Technology and Its Applications Toward Electronic and Optoelectronic Devices	3506160000							•		•				•	•			
73	High-G Accelerometer for Earth-Penetrator Weapons Applications	3506170000													•	•	•		**Auto Airbag Actuator
76	Agile Prototyping of Microelectromechanical Systems (MEMS)	3506180000							•						•	•	•		**Aerospace
76	Advanced Concepts for High-Power VCSELs and VCSEL Arrays	3506190000							•		•				•	•			
78	Midwave-Infrared (2-6 μ m) Emitter-Based Chemical Sensor Systems	3506210000							•		•				•	•			
78	Microelectronic Biosensors	3506220000				•					•				•				
80	A Novel Nondestructive Silicon-on-Insulator Nonvolatile Memory	3506230000									•				•	•	•	•	*DOE, **Industry
81	Integration of Optoelectronics and MEMS by Free-Space Microoptics	3506240000							•		•				•				

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82	Advanced Laser Structures for Short-Pulsed Power in Active Optical Sensor Systems	3506250000							●		●			●	●	●		*3-letter	
82	Metal Micro-Heat-Pipe Substrates for High-Power-Density Electronics	3506260000									●			●	●		●	**Electronics Manufacturers	
83	Integration of Microsensor Technology into a Miniature Robotic Vehicle	3506270000									●					●			
84	Vacuum Encapsulation of MEMS Structures	3506280000				●					●			●	●		●	**Analog Devices Inc., Rockwell International, Texas Instruments	
85	Massively Parallel Sensor Arrays for Volatile Organic Detection	3506290000				●					●			●					
86	Agile Dry Etching of Compound Semiconductors for Science-Based Manufacturing Using In Situ Process Control	3506310000							●		●			●					
86	Precision-Formed Micromagnets	3506320000							●	●	●			●	●				
87	Time-Resolved Ion-Beam-Induced Charge-Collection (TRIBICC) Imaging	3506330000							●					●	●	●	●	*NSA, Air Force, NASA, **IC industries	
88	Composite-Resonator Surface-Emitting Lasers	3506340000									●			●	●				
88	Role of Defects in III-Nitride-Based Electronics	3506350000									●			●	●				
90	Ultra-Low-Power Sensors for Microtelemetry Systems	3506360000	●		●	●					●			●	●				
90	Double Quantum-Well Long-Wavelength Optoelectronic Devices	3506370000							●		●			●	●				
92	The Development of Integrated Chemical Microsensors in GaAs	3506380000									●			●		●		*Environmental Protection Agency	
92	Systems Studies in Compound Semiconductor Processing (U)	3506390000									●								

Appendix F: Major National Programs

Pg #	Title	Case Number	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 and Technical Information	Defense Programs	Department of Defense (DoD)	Other Federal Agencies*	Other (Industry, Consortia)**
96	Unexplored Penetrator Regime Against Super-Hard Underground Facilities	3508010000																
96	Optimization of Computationally Challenging Problems in Engineering Sciences	3508030000																**Goodyear & Sematech, CRADAs, CRMPC consortium
95	Using Higher-Order Gradients to Modeling Localization Phenomena	3508040000																**NCMS, USCAR
98	Investigation of Nonequilibrium Microscopic Hydrodynamic Phenomena	3508050000																
99	Enhanced Vapor-Phase Diffusion in Porous Media	3508060000																
100	Numerical and Experimental Investigation of Vortical Flow-Flame Interaction	3508070000																
101	Temporal and Spatial Resolution of Fluid Flows	3508080000																*DOT (FAA), DOI (MMS), DOA (USFS), **Insurance
101	Characterization of Fluid Transport in Microscale Structures	3508090000																
102	Stress Evaluation and Model Validation Using Laser Ultrasonics	3508110000																*NRC, EPA, **auto, glass, steel, energy, chemical
103	Altered Simulation Properties for Tetrahedral Finite Elements for Use in Engineering Simulation	3508120000																**Auto, aerospace
104	Development, Implementation, and Experimental Validation of the Lattice Boltzmann Method for Modeling Three-Dimensional Complex Flows	3508130000																*NASA
106	Joint Task: Capturing Recrystallization of Metals with a Multiscale Material Model	3508140000																**NCMS, USCAR, aluminum & steel suppliers
105	Nondeterministic Modeling in Engineering Science	3508150000																
107	Lagrangian Modeling of Radiative Transport	3508160000																*FAA, NASA, **Insurance

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111	VIEWS—Virtual Interactive Environment Work Space	3510410000									•				•				
112	Distributed Object and Intelligent Agents in a Wide-Area Network Test-Bed	3510420000													•	•		•	**Academia
112	Solid Variant Geometry Modeling	3510430000													•	•			
113	Rapid Prototyping/Rapid Manufacturing via Freeform Fabrication of Polymer-Matrix Composites	3510440000													•	•			
114	Solid Model Design Simplification	3510450000											•	•	•			•	**Goodyear, CRADA
114	Laser-Spray Fabrication for Net-Shape Rapid Product Realization	3510460000	•	•		•				•					•			•	**LENS Consortium
116	Carbon Coatings for Improved Sprytren-Tube Performance and Reliability	3510470000											•	•	•				
116	Low-Cost Pd-Catalyzed Metallization Technology for Rapid Prototyping of Electronic Substrates and Devices	3510480000								•					•	•		•	**Industry
118	Smart Cutting Tools for Precision Manufacturing	3510490000	•				•				•				•	•		•	**Machine Tool Industry
118	Solution Synthesis and Processing of PZT Materials for Neutron-Generator Applications	3510510000													•				
120	Development of an Immersive Environment to Aid in Automatic Mesh Generation	3510520000									•	•			•	•		•	**Meshing Consortia
121	Effect of Composition and Processing Conditions on the Reliability of Cermet/Alumina Components	3510530000								•		•		•	•	•	•	•	*DOL, **AACC MCI, Inc. (a subdivision of the Association of American Ceramic Component Manufacturers)
122	Ultra-Precise Assembly of Microelectromechanical Systems (MEMS)	3510540000																•	**Industry

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122	Self-Tuning Process-Monitoring System for Process-Based Product Validation	3510550000													•				
124	Process Optimization for Electron Beam Joining of Ceramic and Glass Components	3510560000	•												•	•		•	**Structural Ceramics
124	Finite-Element Meshing Approached as a Global Minimization Process	3510570000	•	•			•	•	•		•				•				
125	Application of Parallel Mechanism Technology to Manufacturing	3510580000							•					•	•	•	•	•	*NIST, **Hexpod Users Group
126	Investigation of the Impact of Cleaning on the Adhesive Bond and the Process Implications	3510590000	•			•			•						•	•		•	**NCMS, Sematech, Industry
126	Standard Cells for Microelectromechanical Systems (MEMS)	3510610000							•						•	•		•	**Aerospace
127	Laser Wire Deposition for Fully Dense Net Shapes	3510620000							•				•	•	•				
128	High-Throughput Dry Processes for Large-Area Devices	3510630000			•						•				•			•	**Semiconductor Industry
129	Assuring High Reliability and Production Readiness in Low-Volume Manufacturing	3510640000									•	•			•	•			
130	Advanced Control Methods for Improved Grinding Processes	3510650000							•		•				•			•	
133	Automatic Generation of Multimedia Documentation for Assembly Operations	3511010000										•			•	•		•	**Consortia
134	Distributed Life-Cycle Models in Enterprise Simulations to Answer System Questions	3511020000										•			•	•			
134	Chain Models for Life-Cycle Systems Engineering	3511030000														•		•	**Industry
135	Immersive CAD	3511040000									•				•	•			
136	Automatic Planning of Life-Cycle Assembly Processes	3511050000													•	•		•	**Consortia

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137	Automatic Generation of Foolproof Manufacturing Plans	3511060000																	**Industry
141	Design of a Highly Secure Smartcard	3512110000	•			•			•	•	•	•		•	•	•	•	•	*Dept. of Treasury, Dept. of Commerce, Dept. of Agric., HHS, VA, National Financial Infrastructure Components
142	Object-Oriented Parallel Discrete Event Simulation System—An Enabling Foundation for Rapid Development of High-Performance, Large-Scale Simulations	3512120000							•	•	•	•	•	•	•	•			
143	Biometric Identity Verification for Remote User Authentication and Access Control Applications	3512130000									•				•	•			
144	"Robustness-Agile" Asynchronous Transfer Mode (ATM) Encryption and Associated Use Control	3512140000									•				•	•	•	•	*DOE, Treas, **ATM Forum, FORE Systems
145	Agent-Based Remediation of the Mosaic Classification Problem	3512150000							•	•	•	•		•	•				
146	Content-Based Search of Geometric Databases	3512160000				•			•	•	•	•			•			•	**Industry
147	Integrated Service Provisioning in an "IPv6 over ATM" Research Network	3512170000							•	•					•			•	**Communications and Networking
148	Virtual Desktop Engineering with Integrated Multimedia Data	3512180000												•					
148	Mission Surety for Large-Scale Real-Time Information Systems	3512190000		•							•	•		•	•	•			
149	Integrated and Robust Security Infrastructure	3512210000									•								
150	Scaled ATM End-to-End Encryption	3512220000									•				•				
151	Network Surety Modeling for Wireless ATM Networks (and Other Distributed Computing Systems)	3512230000							•	•					•	•		•	**Telecom Standards

Pg #	Title	Case Number	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 and Technical Information	Defense Programs	Department of Defense (DoD)	Other Federal Agencies*	Other (Industry, Consortia)**	Other Federal Agencies* Other (Industry, Consortia)**
155	Superconductive Gravity Gradiometers for Underground Target Recognition	3516020000	•								•	•	•	•	•	•	•	•	*NASA, **petroleum & mineral exploration
155	Moving Mass Trim Control for Precision-Strike Warheads	3516030000									•				•	•			
156	Micro-Holographic Tagging	3516040000									•				•				
157	Electrokinetic Immunoaffinity Chemical Sensors	3516050000	•				•				•					•			
158	Information-Efficient Spectral Imaging System (ISIS)	3516060000	•		•		•	•			•				•	•			
158	Imaging of Moving Targets Using Simultaneous Synthetic Aperture Radar (SAR) and Moving Target Indicator (MTI) Radar	3516070000									•	•				•			
159	Sampling and Sensing Systems for High-Priority Analytes	3516080000	•			•	•		•	•	•				•	•	•		*CIA, FBI
160	Automated Vegetation Height Measurement for Automatic Terrain Mapping	3516090000									•					•	•		*NIMA, DOE-NN, Army Tec
163	Development of Inexpensive Metal Macrocyclic Complexes for Direct Oxidation of Methanol in Fuel Cells	3518020000	•	•	•	•	•	•		•	•				•	•			
164	Designed Molecular Recognition Materials for Chiral Sensors, Separations, and Catalytic Materials	3518030000														•	•		**Chemical and Pharmaceutical
165	Real-Time 3-D and Heterogeneous Data Fusion	3518040000	•				•		•		•					•			
166	Rapid Screening of Complex Chemical Samples via Capillary Array Analysis	3518050000	•				•										•		*USEPA
166	Designed Synthesis of Controlled Degradative Materials	3518060000									•					•			

Pg #	Title	Case Number	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 and Technical Information	Defense Programs	Department of Defense (DoD)	Other Federal Agencies*	Other (Industry, Consortia)**
168	Mechanistic Models for Radionuclide Desorption from Soils	3518070000	•				•											Other Federal Agencies* Other (Industry, Consortia)**
171	Reliability Degradation Due to Stockpile Aging	3520210000																**Industry
172	Integrated Approach to Develop Microelectromechanical Systems (MEMS)	3520220000									•					•		
173	Precursors to Failure of Oxides and Metal Lines in CMOS Technology	3520230000										•				•		
174	An Extensible Object-Oriented Framework for Risk & Reliability Analysis	3520240000									•	•				•		**Industry
175	Risk-Based Characterization of Network Vulnerability	3520250000									•					•	•	*CIA, **Telecommunications
176	Enhancing Risk Analysis Using New Mathematical Structures	3520260000											•			•		*FAA, NASA
179	Science on the Microdomain	3522010000	•				•				•				•	•		
180	Autonomous MicroChem Laboratory (μ ChemLab)	3522020000	•	•	•	•	•	•	•	•	•	•	•	•	•	•	•	*NIJ, EPA, Veterans, DARPA, NIH **Industry, Universities
181	Cooperative, Distributed Sensing and Action Using Microminiature, Intelligent Agents	3522030000	•				•				•				•			
185	Development of Innovative Combustion Processes for a Direct-Injection Diesel Engine	3524110000		•							•						•	**Diesel Engine Manufacturers
186	Hydrogen Production for Fuel Cells by Selective Dehydrogenation of Alkanes in Catalytic Membrane Reactors	3524120000		•				•			•				•	•		
186	Hybrid Vehicle Engine Development	3524130000		•	•			•			•				•			
188	A 700-kV, Short-Pulse, Repetitive Accelerator for Industrial Applications	3524140000	•					•			•				•			

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187	High-Power Ion Beam (HPIB) Modification of One- and Two-Layer Metal Surfaces	3524150000							•		•			•	•				
189	Advanced 3-D Electromagnetic and Particle-in-Cell Modeling	3524160000		•						•				•	•		•	**Microelectronics, microwave devices	
190	Electromagnetic Impulse Radar for Detection of Underground Structures	3524170000					•				•			•	•				
193	Computational Methods for Predicting the Response of Critical As-Built Infrastructure to Dynamic Loads (Architectural Surety)	3530030000													•	•	•	*GSA, FEMA, **ASCE, AIA (Professional Societies), Civil Engineering, Architecture	
194	An Advanced Unmanned Vehicle for Remote Applications	3530040000					•				•				•				
194	Cosmic Rate of Expansion from the Ambient Temperature's Observed Relaxation (CREATOR)	3530050000																*NASA	
195	Productivity Enhancements for Analysts	3530070000									•		•						
196	Web Vulnerability Demonstration	3530080000									•				•				
196	System of Labs Direct Fabrication Technology	3531020000															•		
198	Cold-Cathodes for Sensors and Vacuum Microelectronics	3531030000									•						•	**Field-Emission Flat-Panel Device Technology, Motorola	
197	In Situ Optical Photorefectance During MOCVD	3531040000							•	•	•				•				
200	Novel Thermoelectrics for Next-Generation Power Sources	3531050000		•						•									
199	Micromachined Contact Fuses for Earth-Penetrator Applications	3531060000									•				•				
201	Advanced Stress-Sensing Assembly Test Chip Design	3531070000									•		•	•	•	•	•	**Sematech	

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202	Cat's-Eye Modulator Fabricated in GaAs	3531080000									•								
202	Interfacial Charge Removal for MOVPE-Grown pHEMTs by In Situ Cleaning	3531090000							•		•								
203	Infrared Quantum-Well Intersubband Photodetector Development	3531110000									•				•				
204	Advanced Quantum-Well Structures for Improved Modulator Performance	3531120000									•				•				
204	High-Temperature Stereolithography Female Molds for Small-Lot Composite Manufacturing	3531130000									•				•	•	•	**Industry	
206	Chemical Feedstocks for the Future: Oxidative Dehydrogenation	3532010000	•				•		•	•									
207	Global Approaches to Infrastructural Analysis (GAIA)	3532030000	•	•	•		•		•		•	•	•						
205	Modeling the Atmospheric Entry Physics and Terminal Explosions of the Anomalous October 3, 1996, Bolide Swarm	3532040000							•		•			•		•			
208	Advanced Subterranean Warfare (ASW) for Deep Underground Structures	3532050000									•				•				
208	Dispersive Measurements of Velocity in Heterogeneous Materials	3532060000		•					•		•			•		•	•	*NASA	
210	Policy and Resource Allocations in Risk Management	3533020000	•				•		•	•						•	•	*EPA	
209	Ceramic Membranes for Electrically Driven Ionic Separations	3533030000	•				•		•										
210	Developing On-Line Process-Monitoring Capabilities	3533040000			•	•			•										
210	SAM Telemetry for Measurements While Drilling	3533050000	•				•			•									

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212	Dynamic Simulation Models and Geographic Information Systems	3533060000	•	•	•					•	•	•					•	•	•
212	Design-for-Manufacturability Applied to Photovoltaic Modules	3533070000			•				•	•	•								
211	Applicability of a Metalloprotein Toxic Heavy-Metal Detector to DOE Production and Waste	3533080000	•			•													
213	Enhancing Energy Security Through New Routes to Petrochemical Feedstocks	3533090000		•			•		•	•	•							•	•
214	Cathodic Protection of Zero-Valent Iron-Reactive Barriers	3533110000					•												
216	Consequence-Based Rationale for an Infrastructure Assurance Program	3533120000														•	•	•	•
215	Modeling Interdependence in the U.S. Infrastructure	3533130000									•								
216	Surety of North American Electric Power Transmission Network	3533140000			•		•		•	•	•	•					•	•	•
218	Protective Coatings for Concrete	3533150000	•							•								•	•
218	Low-Cost Cadmium Zinc Telluride Radiation Detectors Based on Electron-Transport-Only Designs	3534020000	•			•	•		•	•	•	•	•			•	•	•	•
219	LIGA Micromachining	3534030000								•	•	•		•					
220	Chemistry and Physics of Microfluids	3534040000	•							•	•	•		•					
220	Combinatorial Peptides for Chemical Sensing	3534050000										•				•			
220	Pulsar in a Chip	3535020000								•						•			
222	Ultra-High-Pressure EOS Studies on Metals and ICF Ablators Using PBFA-Z	3535030000										•				•			

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222	Flocking Small Smart Machines	3535040000	•				•		•			•				•			
223	Development of Explosive-Event Scale Model Testing Capability at Sandia	3535050000										•				•			
224	Application of SAR Vibrometry to Distributed Seismic Sources	3535060000										•				•			
224	Development of Laser-Cutting/-Welding Depth Control Using Laser Spectroscopy and Open Architecture Control of a Robotic System	3535070000	•							•									
226	Cryogenic EOS Capabilities on Pulsed-Radiation Sources (Z - pinch)	3535080000														•			
225	Aerosol Stand-off Detection Test-Bed	3535090000										•				•	•		*FBI, DOS
228	Investigation of Analysis Techniques for Swarm Behavior	3535110000	•				•		•			•				•	•		*DARPA, FBI, CIA
227	Synchronized RF Sources for IW Applications	3535120000										•				•			

Pg#	Title	Case Number	Aeronautics	Applied Molecular Biology	Ceramics	Composites	Computer Simulation & 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	Materials Synthesis & Processing	Medical Technology	Micro- and Nano-Fabrication	Microelectronics and Optoelectronics	Photonic Materials	Pollution Min., Remediation, and Waste Mgmt.	Sensors & 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)
10	Sol-Gel Preservation of Mankind's Cultural Heritage in Objects Constructed of Stone	3502010000			●	●	●		●	●						●		●	●		●							●
9	Physico-Chemical Stability of Solid Surfaces	3502020000	●																									
11	Catalytic Membrane Sensors	3502030000																●						●				
12	Photonic Bandgap Structures as a Gateway to Nano-Photonics	3502040000							●										●									
12	Wide-Bandgap Compound Semiconductors to Enable Novel Semiconductor Devices	3502050000					●	●	●	●	●					●			●	●	●	●					●	
14	Synthesis and Modeling of Field-Structured Anisotropic Composites	3502060000				●	●											●										
15	Model Determination and Validation for Reactive Wetting Processes	3502070000	●		●	●	●		●							●			●									●
16	Ultra-Hard Multilayer Coatings	3502080000						●	●	●	●					●		●	●	●		●					●	
16	Scanning Probe-Based Processes for Nanometer-Scale Device Fabrication	3502090000							●							●		●	●	●								●
18	Molecular-Scale Lubricants for Micromachine Applications	3502110000														●		●	●	●		●					●	
18	Surface-Micromachined Flexural Plate Wave Device Integrated on Silicon	3502120000			●				●							●		●	●	●		●						●
19	Molecular Imprinting in Aerogels for Remote Sensing of Chemical Weapons and Pesticides	3502130000		●		●				●						●		●	●	●		●					●	
20	Smart Interface Bonding Alloys (SIBA): Tailoring Thin-Film Mechanical Properties	3502140000			●	●	●											●				●						●
21	Understanding and Control of Energy Transfer Mechanisms in Optical Ceramics	3502150000			●	●	●	●	●		●					●		●	●	●	●	●	●					●

Pg#	Title	Case Number	Aeronautics	Applied Molecular Biology	Ceramics	Composites	Computer Simulation & 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	Materials Synthesis & Processing	Medical Technology	Micro- and Nano-Fabrication	Microelectronics and Optoelectronics	Photonic Materials	Pollution Min., Remediation, and Waste Mgmt.	Sensors & 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)
22	Integrated Thin-Film Structures for IR Imaging	3502160000			●			●	●			●				●			●			●				●	●	●
23	Recognizing Atoms in Atomically Engineered Nanostructures: An Interdisciplinary Approach	3502170000						●			●					●			●				●					●
24	Modeling Electrodeposition for Metal Microdevice Fabrication	3502180000						●					●			●			●								●	●
24	The Initiation and Propagation of Nanoscale Cracks at an Adhesive/Solid Interface	3502190000				●						●				●			●								●	●
25	Monolithic Structures for Nanoseparation	3502210000	●						●							●		●									●	●
26	Fundamental Aspects of Micromachine Reliability	3502220000																●									●	●
27	Enabling Science and Technology for Cold-Spray Direct Fabrication	3502230000	●			●			●			●				●					●						●	●
28	Atomic-Level Studies of Surfactant-Directed Materials Growth	3502240000						●										●									●	●
30	Intelligent Polymers for Nanodevice Performance Control	3502250000														●											●	●
32	Freeforming of Ceramics and Composites from Colloidal Slurries	3502260000			●	●			●							●											●	●
31	Quantum Dot Arrays	3502270000							●							●		●		●								●
33	Laser-Assisted Arc Welding for Aluminum Alloys	3502280000	●						●	●						●											●	●
34	System Studies in Electrochemical Processing	3502290000							●				●			●										●		
37	Parallel Quantum Chemistry for Material Aging and Synthesis	3504010000			●	●						●				●											●	

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38	Modeling Complex Turbulent Chemically Reacting Flows on Massively Parallel Supercomputers	3504020000	●				●	●	●			●			●				●			●					●	
39	Scalability of Cryptographic Algorithms and Protocols	3504030000					●	●				●											●				●	
40	Computer-Designed Molecular Memory and Switching Elements	3504040000		●			●	●	●			●	●			●		●	●	●							●	
43	Automated Geometric Model Builder Using Range Image Sensor Data	3504050000					●					●					●										●	
42	A Massively Parallel Sparse Eigensolver for Structural Dynamics Finite Element	3504060000	●			●	●			●	●	●		●					●			●	●	●			●	
44	Density Functional Theory for Classical Fluids at Complex Interfaces	3504070000			●		●									●		●				●						●
45	Sensing and Compressing 3-D Models	3504080000					●										●				●	●	●				●	
45	Gradient-Driven Diffusion of Multi-Atom Molecules Through Macromolecules and Membranes	3504090000		●		●	●		●	●			●	●		●	●	●			●	●	●	●			●	
46	An Easier Way? An Attempt to Tightly Couple Complete Grid Generation with the Flow Solver for Discretized Governing Equations	3504110000	●				●						●										●				●	
46	Fast and Easy Parallel I/O for Efficient Scientific Computing	3504120000					●	●					●										●				●	
47	Novel Load-Balancing for Scalable, Parallel Electromagnetic and Plasma Physics Simulation Software	3504130000					●		●			●							●			●	●				●	
48	Parallel Computational Chemistry Using Constraints	3504140000											●			●											●	
49	Accurate Numerical Methods for Wave Propagation	3504150000					●			●		●											●				●	

Appendix G: Dual-Benefit Areas and Single-Use Categories

Pg#	Title	Case Number	Aeronautics	Applied Molecular Biology	Ceramics	Composites	Computer Simulation & 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	Materials Synthesis & Processing	Medical Technology	Micro- and Nano-Fabrication	Microelectronics and Optoelectronics	Photonic Materials	Pollution Min., Remediation, and Waste Mgmt.	Sensors & 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)
49	Massively Parallel Ab Initio Validation for ASCI Materials Aging	3504160000																										
50	Dynamically Coupled, Massively Parallel Simulation of Grain Growth and Aging/Degradation	3504170000																										
52	An Investigation of Wavelet Bases for Multiscale, Grid-Based Simulation	3504180000																										
53	Integrated Quantum/Classical Modeling of Hydrogenic Materials	3504190000																										
54	The Next Generation of Teraflop Density Functional Electronic Structure Codes	3504210000																										
54	Methodology for Characterizing Modeling and Discretization Uncertainties in Computational Simulation	3504220000																										
55	A Critical Evaluation of Algorithms for Global Optimization	3504230000																										
56	Dynamic Simulation of Mechanical Systems with Intermittent Contacts	3504240000																										
59	High-Speed Modulation of Vertical-Cavity Surface-Emitting Lasers	3506010000																										
60	Micromachined Inertial Sensors (Accelerometer, Gyroscope)	3506020000																										
60	Red-to-Blue-Wavelength Photonic Devices	3506030000																										
62	Double Electron Layer Tunneling Transistor	3506040000																										
64	Subwavelength Diffractive Optics	3506050000																										

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64	Vehicle Exhaust Gas Chemical Sensors Using Acoustic-Wave Resonators	3506060000			●										●	●		●	●	●	●	●		●			●	
66	GaAs PIC Development for High-Performance Communications	3506070000				●			●				●			●		●	●	●		●					●	
67	Application-Specific Tester-on-a-Resident-Chip (TORCH)	3506080000	●					●	●									●	●	●							●	
68	Ultra-Low-Power Microwave CHFET Integrated Circuit Development	3506090000						●	●									●	●	●							●	
68	Wafer Fusion for Integration of Semiconductor Materials and Devices	3506110000						●	●			●						●	●	●		●					●	
69	Highly Parallel, Low-Power, Photonic Interconnects for Inter-Board Signal Distribution	3506120000						●	●			●						●	●	●		●					●	
70	Achromatic Nonlinear Optics for Sensing and Process Control	3506130000					●			●								●	●	●		●					●	
71	Virtual Reactor for the Semiconductor Manufacturing Plant of the Future	3506140000					●		●							●		●	●	●		●					●	
72	Integrated Separation and Optical Detection for Novel On-Chip Chemical Analysis	3506150000		●					●						●		●		●	●		●					●	
74	Selective Oxidation Technology and Its Applications Toward Electronic and Optoelectronic Devices	3506160000						●	●			●						●	●	●		●					●	
73	High-G Accelerometer for Earth-Penetrator Weapons Applications	3506170000																●	●	●		●		●			●	
76	Agile Prototyping of Microelectromechanical Systems (MEMS)	3506180000	●						●		●							●	●	●		●					●	
76	Advanced Concepts for High-Power VCSELs and VCSEL Arrays	3506190000						●	●			●						●	●	●		●					●	
78	Midwave-Infrared (2-6 μ m) Emitter-Based Chemical Sensor Systems	3506210000						●	●			●						●	●	●		●					●	

Appendix G: Dual-Benefit Areas and Single-Use Categories

Pg#	Title	Case Number	Aeronautics	Applied Molecular Biology	Ceramics	Composites	Computer Simulation & 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	Materials Synthesis & Processing	Medical Technology	Micro- and Nano-Fabrication	Microelectronics and Optoelectronics	Photonic Materials	Pollution Min., Remediation, and Waste Mgmt.	Sensors & 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)
78	Microelectronic Biosensors	3506220000																										
80	A Novel Nondestructive Silicon-on-Insulator Nonvolatile Memory	3506230000																										
81	Integration of Optoelectronics and MEMS by Free-Space Microoptics	3506240000																										
82	Advanced Laser Structures for Short-Pulsed Power in Active Optical Sensor Systems	3506250000																										
82	Metal Micro-Heat-Pipe Substrates for High-Power-Density Electronics	3506260000																										
83	Integration of Microsensor Technology into a Miniature Robotic Vehicle	3506270000																										
84	Vacuum Encapsulation of MEMS Structures	3506280000																										
85	Massively Parallel Sensor Arrays for Volatile Organic Detection	3506290000																										
86	Agile Dry Etching of Compound Semiconductors for Science-Based Manufacturing Using In Situ Process Control	3506310000																										
86	Precision-Formed Micromagnets	3506320000																										
87	Time-Resolved Ion-Beam-Induced Charge-Collection (TRIBICC) Imaging	3506330000																										
88	Composite-Resonator Surface-Emitting Lasers	3506340000																										
88	Role of Defects in III-Nitride-Based Electronics	3506350000																										

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90	Ultra-Low-Power Sensors for Microtelemetry Systems	3506360000							•								•	•			•					•	•	
90	Double Quantum-Well Long-Wavelength Optoelectronic Devices	3506370000							•			•								•		•					•	•
92	The Development of Integrated Chemical Microsensors in GaAs	3506380000							•									•		•							•	•
92	Systems Studies in Compound Semiconductor Processing (U)	3506390000							•										•								•	•
96	Unexplored Penetrator Regime Against Super-Hard Underground Facilities	3508010000					•						•							•						•		
96	Optimization of Computationally Challenging Problems in Engineering Sciences	3508030000					•		•				•							•							•	•
95	Using Higher-Order Gradients to Modeling Localization Phenomena	3508040000					•							•													•	•
98	Investigation of Nonequilibrium Microscopic Hydrodynamic Phenomena	3508050000	•				•			•			•						•									•
99	Enhanced Vapor-Phase Diffusion in Porous Media	3508060000					•			•											•							•
100	Numerical and Experimental Investigation of Vortical Flow-Plane Interaction	3508070000					•			•											•						•	•
101	Temporal and Spatial Resolution of Fluid Flows	3508080000																			•						•	•
101	Characterization of Fluid Transport in Microscale Structures	3508090000																•	•		•						•	•
102	Stress Evaluation and Model Validation Using Laser Ultrasonics	3508110000	•				•			•				•					•								•	•
103	Altered Simulation Properties for Tetrahedral Finite Elements for Use in Engineering Simulation	3508120000	•				•																				•	•

Appendix G: Dual-Benefit Areas and Single-Use Categories

Pg#	Title	Case Number	Aeronautics	Applied Molecular Biology	Ceramics	Composites	Computer Simulation & 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	Materials Synthesis & Processing	Medical Technology	Micro- and Nano-Fabrication	Microelectronics and Optoelectronics	Photonic Materials	Pollution Min., Remediation, and Waste Mgmt.	Sensors & 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)
104	Development, Implementation, and Experimental Validation of the Lattice Boltzmann Method for Modeling Three-Dimensional Complex Flows	3508130000																										
106	Joint Task: Capturing Recrystallization of Metals with a Multiscale Material Model	3508140000																										
105	Non deterministic Modeling in Engineering Science	3508150000																										
107	Lagrangian Modeling of Radiative Transport	3508160000																										
111	VIEWS—Virtual Interactive Environment Work Space	3510410000																										
112	Distributed Object and Intelligent Agents in a Wide-Area Network Test-Bed	3510420000																										
112	Solid Variant Geometry Modeling	3510430000																										
113	Rapid Prototyping/Rapid Manufacturing via Freeform Fabrication of Polymer-Matrix Composites	3510440000																										
114	Solid Model Design Simplification	3510450000																										
114	Laser-Spray Fabrication for Net-Shape Rapid Product Realization	3510460000																										
116	Carbon Coatings for Improved Sprytion-Tube Performance and Reliability	3510470000																										
116	Low-Cost Pd-Catalyzed Metallization Technology for Rapid Prototyping of Electronic Substrates and Devices	3510480000																										
118	Smart Cutting Tools for Precision Manufacturing	3510490000																										

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118	Solution Synthesis and Processing of PZT Materials for Neutron-Generator Applications	3510510000			•				•				•			•		•								•		
120	Development of an Immersive Environment to Aid in Automatic Mesh Generation	3510520000					•					•											•				•	
121	Effect of Composition and Processing Conditions on the Reliability of Cermet/Alumina Components	3510530000	•		•	•	•									•										•		
122	Ultra-Precise Assembly of Microelectromechanical Systems (MEMS)	3510540000							•		•							•	•									•
122	Self-Tuning Process Monitoring System for Process-Based Product Validation	3510550000									•				•							•					•	
124	Process Optimization for Electron Beam Joining of Ceramic and Glass Components	3510560000		•	•	•	•		•		•					•			•								•	
124	Finite-Element Meshing Approached as a Global Minimization Process	3510570000	•		•	•	•				•																•	
125	Application of Parallel Mechanism Technology to Manufacturing	3510580000	•								•				•												•	
126	Investigation of the Impact of Cleaning on the Adhesive Bond and the Process Implications	3510590000	•			•			•	•	•					•		•	•		•						•	
126	Standard Cells for Microelectromechanical Systems (MEMS)	3510610000	•						•		•							•	•			•					•	
127	Laser Wire Deposition for Fully Dense Net Shapes	3510620000	•								•				•								•				•	
128	High-Throughput Dry Processes for Large-Area Devices	3510630000							•	•									•								•	
129	Assuring High Reliability and Production Readiness in Low-Volume Manufacturing	3510640000	•								•				•			•	•			•					•	
130	Advanced Control Methods for Improved Grinding Processes	3510650000									•				•	•						•					•	

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133	Automatic Generation of Multimedia Documentation for Assembly Operations	3511010000	•																		•						•	
134	Distributed Life-Cycle Models in Enterprise Simulations to Answer System Questions	3511020000					•						•														•	
134	Chain Models for Life-Cycle Systems Engineering	3511030000	•				•																				•	
135	Immersive CAD	3511040000	•				•				•		•														•	
136	Automatic Planning of Life-Cycle Assembly Processes	3511050000	•				•		•																		•	
137	Automatic Generation of Foolproof Manufacturing Plans	3511060000	•								•						•										•	
141	Design of a Highly Secure Smartcard	3512110000			•											•											•	
142	Object-Oriented Parallel Discrete Event Simulation System—An Enabling Foundation for Rapid Development of High-Performance, Large-Scale Simulations	3512120000		•			•				•		•										•				•	
143	Biometric Identity Verification for Remote User Authentication and Access Control Applications	3512130000																				•	•				•	
144	"Robustness-Agile" Asynchronous Transfer Mode (ATM) Encryption and Associated Use Control	3512140000										•															•	
145	Agent-Based Remediation of the Mosaic Classification Problem	3512150000					•				•		•										•				•	
146	Content-Based Search of Geometric Databases	3512160000					•				•		•										•				•	
147	Integrated Service Provisioning in an "IPv6 over ATM" Research Network	3512170000									•	•	•														•	

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148	Virtual Desktop Engineering with Integrated Multimedia Data	3512180000																										
148	Mission Surety for Large Scale-Real-Time Information Systems	3512190000																										
149	Integrated and Robust Security Infrastructure	3512210000																										
150	Scaled ATM End-to-End Encryption	3512220000																										
151	Network Surety Modeling for Wireless ATM Networks (and Other Distributed Computing Systems)	3512230000																										
155	Superconductive Gravity Gradiometers for Underground Target Recognition	3516020000																										
155	Moving Mass Trim Control for Precision-Strike Warheads	3516030000																										
156	Micro-Holographic Tagging	3516040000																										
157	Electrokinetic Immunoaffinity Chemical Sensors	3516050000																										
158	Information-Efficient Spectral Imaging System (ISIS)	3516060000																										
158	Imaging of Moving Targets Using Simultaneous Synthetic Aperture Radar (SAR) and Moving Target Indicator (MTI) Radar	3516070000																										
159	Sampling and Sensing Systems for High-Priority Analyses	3516080000																										

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160	Automated Vegetation Height Measurement for Automatic Terrain Mapping	3516090000																										
163	Development of Inexpensive Metal Macrocyclic Complexes for Direct Oxidation of Methanol in Fuel Cells	3518020000																										
164	Designed Molecular Recognition Materials for Chiral Sensors, Separations, and Catalytic Materials	3518030000																										
165	Real-Time 3-D and Heterogeneous Data Fusion	3518040000																										
166	Rapid Screening of Complex Chemical Samples via Capillary Array Analysis	3518050000																										
166	Designed Synthesis of Controlled Degradative Materials	3518060000																										
168	Mechanistic Models for Radionuclide Desorption from Soils	3518070000																										
171	Reliability Degradation Due to Stockpile Aging	3520210000																										
172	Integrated Approach to Develop Microelectromechanical Systems (MEMS)	3520220000																										
173	Precursors to Failure of Oxides and Metal Lines in CMOS Technology	3520230000																										
174	An Extensible Object-Oriented Framework for Risk & Reliability Analysis	3520240000																										
175	Risk-Based Characterization of Network Vulnerability	3520250000																										
176	Enhancing Risk Analysis Using New Mathematical Structures	3520260000																										

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179	Science on the Microdomain	3522010000		•			•	•	•	•	•				•	•	•	•	•	•	•	•		•	•	•	•	•
180	Autonomous MicroChem Laboratory (μ ChemLab)	3522020000		•			•	•	•	•	•				•	•	•	•	•	•	•	•		•	•	•	•	•
181	Cooperative, Distributed Sensing and Action Using Microminiature, Intelligent Agents	3522030000					•								•						•	•					•	•
185	Development of Innovative Combustion Processes for a Direct-Injection Diesel Engine	3524110000							•															•				•
186	Hydrogen Production for Fuel Cells by Selective Dehydrogenation of Alkanes in Catalytic Membrane Reactors	3524120000		•					•	•					•	•	•									•	•	•
186	Hybrid Vehicle Engine Development	3524130000							•															•				•
188	A 700-kV, Short-Pulse, Repetitive Accelerator for Industrial Applications	3524140000		•	•			•							•	•	•		•		•	•				•	•	•
187	High-Power Ion Beam (HIPB) Modification of One- and Two-Layer Metal Surfaces	3524150000		•			•	•		•	•			•	•	•			•		•	•				•	•	•
189	Advanced 3-D Electromagnetic and Particle-in-Cell Modeling	3524160000					•	•	•	•					•	•			•		•	•				•	•	•
190	Electromagnetic Impulse Radar for Detection of Underground Structures	3524170000						•											•		•	•				•	•	•
193	Computational Methods for Predicting the Response of Critical As-Built Infrastructure to Dynamic Loads (Architectural Surety)	3530030000				•						•														•	•	•
194	An Advanced Unmanned Vehicle for Remote Applications	3530040000									•										•	•	•				•	•

Appendix G: Dual-Benefit Areas and Single-Use Categories

Pg#	Title	Case Number	Aeronautics	Applied Molecular Biology	Ceramics	Composites	Computer Simulation & 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	Materials Synthesis & Processing	Medical Technology	Micro- and Nano-Fabrication	Microelectronics and Optoelectronics	Photonic Materials	Pollution Min., Remediation, and Waste Mgmt.	Sensors & 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)
194	Cosmic Rate of Expansion from the Ambient Temperature's Observed Relaxation (CREATOR)	3530050000																										
195	Productivity Enhancements for Analysts	3530070000																										
196	Web Vulnerability Demonstration	3530080000																										
196	System of Labs Direct Fabrication Technology	3531020000																										
198	Cold-Cathodes for Sensors and Vacuum Microelectronics	3531030000																										
197	In Situ Optical Photoreflexance During MOCVD	3531040000																										
200	Novel Thermoelectrics for Next-Generation Power Sources	3531050000																										
199	Micromachined Contact Fuses for Earth-Penetrator Applications	3531060000																										
201	Advanced Stress-Sensing Assembly Test Chip Design	3531070000																										
202	Cat's-Eye Modulator Fabricated in GaAs	3531080000																										
202	Interfacial Charge Removal for MOVPE-Grown pHEMTs by In Situ Cleaning	3531090000																										
203	Infrared Quantum-Well Intersubband Photodetector Development	3531110000																										
204	Advanced Quantum-Well Structures for Improved Modulator Performance	3531120000																										

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204	High-Temperature Stereolithography Female Molds for Small-Lot Composite Manufacturing	3531130000	●			●					●					●											●	
206	Chemical Feedstocks for the Future: Oxidative Dehydrogenation	3532010000																									●	●
207	Global Approaches to Infrastructural Analysis (GAIA)	3532030000					●			●		●													●			●
205	Modeling the Atmospheric Entry Physics and Terminal Explosions of the Anomalous October 3, 1996, Bolidé Swarm	3532040000	●				●																			●		
208	Advanced Subterranean Warfare (ASW) for Deep Underground Structures	3532050000					●																		●			
208	Dispersive Measurements of Velocity in Heterogeneous Materials	3532060000			●	●	●			●								●							●			
210	Policy and Resource Allocations in Risk Management	3533020000																								●		
209	Ceramic Membranes for Electrically Driven Ionic Separations	3533030000		●																	●						●	
210	Developing On-Line Process-Monitoring Capabilities	3533040000																			●	●				●		
210	SAM Telemetry for Measurements While Drilling	3533050000								●																	●	
212	Dynamic Simulation Models and Geographic Information Systems	3533060000				●																					●	
212	Design-for-Manufacturability Applied to Photovoltaic Modules	3533070000						●	●																		●	
211	Applicability of a Metalloprotein Toxic Heavy-Metal Detector to DOE Production and Waste	3533080000																			●						●	

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213	Enhancing Energy Security Through New Routes to Petrochemical Feedstocks	3533090000																										
214	Cathodic Protection of Zero-Valent Iron-Reactive Barriers	3533110000																										
216	Consequence-Based Rationale for an Infrastructure Assurance Program	3533120000																										
215	Modeling Interdependence in the U.S. Infrastructure	3533130000																										
216	Surety of North American Electric Power Transmission Network	3533140000																										
218	Protective Coatings for Concrete	3533150000																										
218	Low-Cost Cadmium Zinc Telluride Radiation Detectors Based on Electron-Transport-Only Designs	3534020000																										
219	LIGA Micromachining	3534030000																										
220	Chemistry and Physics of Microfluids	3534040000																										
220	Combinatorial Peptides for Chemical Sensing	3534050000																										
220	Pulser in a Chip	3535020000																										
222	Ultra-High-Pressure EOS Studies on Metals and ICF Ablators Using PBFA-Z	3535030000																										
222	Flocking Small Smart Machines	3535040000																										

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223	Development of Explosive-Event Scale Model Testing Capability at Sandia	3535050000					•															•				•		
224	Application of SAR Vibrometry to Distributed Seismic Sources	3535060000																								•		
224	Development of Laser-Cutting/-Welding Depth Control Using Laser Spectroscopy and Open Architecture Control of a Robotic System	3535070000					•				•				•							•				•		
226	Cryogenic EOS Capabilities on Pulsed-Radiation Sources (Z-pinch)	3535080000					•																			•		
225	Aerosol Stand-off Detection Test-Bed	3535090000																							•			
228	Investigation of Analysis Techniques for Swarm Behavior	3535110000																								•		
227	Synchronized RF Sources for IW Applications	3535120000							•																		•	