DOE/ER-0715

ENERGY MATERIALS COORDINATING COMMITTEE (EMaCC)

Fiscal Year 1996

August 1997

Annual Technical Report

U.S. Department of Energy
Office of Energy Research
Office of Basic Energy Sciences
Division of Materials Sciences
Germantown, MD 20874-1290

DISCLAIMER

DISCLAIMER

Portions of this document may be illegible electronic image products. Images are produced from the best available original document.

Dedication

The FY 1996 Energy Materials Coordinating Committee report is dedicated to the memory of Dr. Cynthia Carter, who died of cancer on December 22, 1996.

Her colleagues at the Department of Energy knew her as a special person who touched many lives, an internationally recognized fencer, a loving and supportive mother to three sons, a dedicated scientist and a very brave and courageous person. She served as EMaCC chair during 1994-1995.

One of the loves of her life was fencing, which she pursued very seriously during much of her life. Cynthia was very successful and was highly ranked nationally in her age group. In many competitions she also fenced in the open division and was still a formidable opponent. She could defeat women in their twenties and thirties, while Cynthia was in her mid-fifties. She was an outstanding athlete.

TABLE OF CONTENTS

TABLE OF CONTENTS (continued)

TABLE OF CONTENTS (continued)

INTRODUCTION

The DOE Energy Materials Coordinating Committee (EMaCC) serves primarily to enhance coordination among the Department's materials programs and to further effective use of materials expertise within the Department. These functions are accomplished through the exchange of budgetary and planning information among program managers and through technical meetings/workshops on selected topics involving both DOE and major contractors. In addition, EMaCC assists in obtaining materials-related inputs for both intra- and interagency compilations.

Six topical subcommittees have been established to focus on materials areas of particular importance to the Department; the subcommittees and their respective chairmen are:

Electrochemical Technologies - Richard Kelley, ER-132, (301) 903-6051
Metals and Intermetallics - Fred Glaser, FE-72, (301) 903-2786
Radioactive Waste Containers - Helen Farrell, ER-131, (301) 903-5998
Semiconductors - Jerry Smith, ER-132, (301) 903-4269
Structural Ceramics - Charles Sorrell, EE-232, (202) 586-1514
Superconductivity - James Daley, EE-142, (202) 586-1165

Membership in the EMaCC is open to any Department organizational unit; participants are appointed by Division or Office Directors. The current active membership is listed on pages 3-5.

Five meetings were scheduled for 1997. The dates, themes and speakers are as follows:

January 7

Subcommittee on Environmental Issues (10:05-11:25, Room E-401)
Helen Farrell and Gordon Roesler

Interactions among DOE offices were discussed in the context of the role of materials in enhancing environmental technology and sustainability. While some such interactions currently exist, many others require more focus. These gaps represent opportunities to enhance intra-agency communications and synergism.

The Environmental Management Science Program (EMSP) is a new research funding mechanism within DOE. Operated as a partnership between ER and EM, the purpose as stated in Congressional language is to "stimulate the required basic research, development and demonstration efforts to seek new and innovative cleanup methods to replace current conventional approaches which are often costly and ineffective." Obviously, some of the issues in waste management, environmental restoration, and nuclear materials stabilization are materials issues. The materials research currently being conducted under the EMSP was discussed, along with the contents of the FY 1997 EMSP Request for Applications. The RFA has been extensively coordinated within EM and ER, and emphasizes certain critical areas for materials research to support EM missions.

March 25

Subcommittee on Superconductivity (Room 6A-092, Forrestal, DC)
Chris Platt and Jim Daley

The EERE Superconductivity program has seen many exciting successes in the past year. The new Coated Conductor Initiative based on key lab inventions, the world records set in the SPI, R&D100 awards and participation by new key industries mark a strong DOE push to carry this technology to maturity.

Coordination activities through the Council on Environment Quality on materials/energy use and flow, and through MatTec were discussed.

The DOE Power Electronics Program, interactions with other agencies, and related materials issues were described.

May 20 **Subcommittee on Structural Ceramics (10:00-11:20, Room E-301)**
Brian Volintine (for Charlie Sorrell) and Bill Wiffen

An overview was presented of the materials R&D in the Office of Fusion Energy Sciences, including materials development, evaluation and qualification programs to meet the wide range of needs of fusion program experiments, major devices and future power generating systems. These range from the supports for high loads; conductors and stabilizers for high field magnets; components of systems to generate, transmit, launch and shield radio frequency power; specialized materials to interact with neutrons for the generation of tritium, conversion and transfer of energy; to the structural components in the high neutron flux zones of the device; and to the components that interact directly with the fusion plasma. The most intensive element of the fusion materials program is the Advanced Materials activity focused on the development of the structural materials for the first wall and blanket region of fusion power systems. Materials for this application must meet all of the usual requirements of a long service, high temperature unprecedented neutron flux—and do so without producing very long lived radioisotopes and thus unacceptable waste management burdens. These are referred to as low activation structural materials. They include ferritic steels, vanadium alloys and SiC composites. The Program collaborates with BES, NE and NRC in the area of radiation effects, with DoD and NASA in the area of composites, as well as with Japan, Russia and European Union.

A brief presentation was made on the Structural Ceramics Program in OIT. Three projects were discussed: (1) CVD Coating of BN on Oxide Fibers (SNL, DuPont Lanxide); (2) Microwave Joining of SiC (FM Technologies, LANL, Coors Ceramics and Stone & Webster); and (3) Improved Refractories for the Glass Industry (ORNL, University of Missouri at Rolla and various industrial participants, e.g., Owens Corning, PPG). It was noted that BES/MS has been instrumental in providing the knowledge base for development of structural ceramic materials for industrial applications.

The calendar of DOE materials events was reviewed and the R&D Integration Meeting was discussed, with an emphasis on new opportunities for integration of ER R&D activities with those of the end-use sectors.

July 10 **Subcommittee on Electrochemical Technologies**
Richard Kelley, Forrestal

September 9 **Subcommittee on Semiconductors**
Jerry Smith, Germantown

The EMaCC reports to the Director of the Office of Energy Research in his or her capacity as overseer of the technical programs of the Department. This annual technical report is mandated by the EMaCC terms of reference. This report summarizes EMaCC activities for FY 1996 and describes the materials research programs of various offices and divisions within the Department.

The Chairman of EMaCC for FY 1996 was Dr. Debbie Haught. The compilation of this report was performed by Dr. JoAnn Milliken, EMaCC Executive Secretary for FY 1997, with the assistance of FM Technologies, Inc.

Dr. Yok Chen
Office of Energy Research
Chairman of EMaCC, FY 1997

MEMBERSHIP LIST
DEPARTMENT OF ENERGY
ENERGY MATERIALS COORDINATING COMMITTEE

ORGANIZATION	REPRESENTATIVE	PHONE NO.
ENERGY EFFICIENCY AND RENEWABLE ENERGY		
Building Technology, State and Community Programs		
Building Systems	Arun Vohra, EE-41	202/586-2193
Industrial Technologies		
Industrial Energy Efficiency	Scott Richlen, EE-221	202/586-2078
Waste Materials Management	Kurt D. Sisson EE-222	202/586-6750
Materials Processing	Matthew McMonigle, EE-234	202/586-2082
Advanced Industrial Materials	Charles Sorrell, EE-232	202/586-1514
Separations	Brian Volintine, EE-233	202/586-1739
Transportation Technologies		
Automotive Propulsion System Materials	Debbie Haught, EE-34	202/586-2211
Automotive Lightweight Vehicle Materials	Toni Maréchaux, EE-34	202/586-8501
Advanced Battery Systems	Albert Landgrebe, EE-32	202/586-1483
Fuel Cell Systems	JoAnn Milliken, EE-32	202/586-2480
Heavy Vehicle Propulsion System Materials	Robert Schulz, EE-34	202/586-8051
High Strength Weight Reduction Materials	Sidney Diamond, EE-34	202/586-8032
Utility Technologies		
Wind/Hydro/Ocean Technologies	William Richards, EE-121	202/586-5410
Geothermal Technology	Raymond LaSala, EE-122	202/586-4198
Photovoltaic Technology	Richard King, EE-131	202/586-1693
Advanced Utility Concepts	James Daley, EE-142	202/586-1165
	Christine Platt, EE-142	202/586-8943
	Chris Kang, EE-142	202/586-4563

ORGANIZATION	REPRESENTATIVE	PHONE NO.
ENERGY RESEARCH		
Basic Energy Sciences		
Materials Sciences	Iran L. Thomas, ER-10	301/903-3081
	Robert J. Gottschall, ER-13	301/903-3427
Metallurgy and Ceramics	Alan Dragoo, ER-131	301/903-4895
	Yok Chen, ER-131	301/903-3428
	Helen Kerch, ER-131	301/903-3428
	John Mundy, ER-131	301/903-4271
	Tim Fitzsimmons, ER-131	301/903-9830
	Helen Farrell, ER-131	301/903-5998
Solid State Physics and Materials Chemistry	W. Oosterhuis, ER-132	301/903-3426
	Jerry Smith, ER-132	301/903-3426
	Richard Kelley, ER-132	301/903-3426
	Manfred Leiser, ER-132	301/903-3426
Chemical Sciences	Robert S. Marianelli, ER-14	301/903-5808
Engineering and Geosciences	Paula Davidson, ER-15	301/903-5822
Advanced Energy Projects	Walter M. Polansky, ER-32	301/903-5995
Safety and Health	Albert Evans, ER-13	301/903-3427
	Michael Teresinski, ER-13	301/903-5155
Laboratory Management		
Laboratory Technology Transfer	Ted Vojnovich, ER-80	202/586-2343
Fusion Energy		
Fusion Technologies	F. W. (Bill) Wiffen, ER-543	301/903-4963
ENVIRONMENTAL RESTORATION AND WASTE MANAGEMENT		
Waste Operations		
Waste Management Projects	Doug Tonkay, EM-34	301/903-7212
Science and Technology		
Research and Development	Gordon M. Roesler, EM-13	202/586-0231

ORGANIZATION	REPRESENTATIVE	PHONE NO.
NUCLEAR ENERGY, SCIENCE AND TECHNOLOGY		
Space and National Security Programs		
Defense Energy Projects	John W. Warren, NE-52	301/903-6491
Radioisotope Power Systems	William Barnett, NE-53	301/903-3097
Naval Reactors	David I. Curtis, NE-60	703/603-5561
Nuclear Safety Self-Assessment		
Nuclear Quality Assurance	John Dowicki, NE-50	301/903-7729
CIVILIAN RADIOACTIVE WASTE MANAGEMENT		
Analysis and Verification	Alan Berusch, RW-37	202/586-9362
DEFENSE PROGRAMS		
Research and Advanced Technology		
Research and Technology Development	Bharat Agrawal, DP-16	301/903-2057
Inertial Confinement Fusion	Carl B. Hilland, DP-18	301/903-3687
FOSSIL ENERGY		
Advanced Research	Fred M. Glaser	301/903-2786

ORGANIZATION OF THE REPORT

The FY 1996 budget summary for DOE Materials Activities is presented on pages 7-9. The distribution of these funds between DOE laboratories, private industry, academia and other organizations is presented in tabular form on page 10.

Following the budget summary is a set of detailed program descriptions for the FY 1996 DOE Materials activities. These descriptions are presented according to the organizational structure of the Department. A mission statement, a budget summary listing the project titles and FY 1996 funding, and detailed project summaries are presented for each Assistant Secretary office and the Office of Energy Research. The project summaries also provide DOE, laboratory, academic and industrial contacts for each project, as appropriate.

FY 1996 BUDGET SUMMARY FOR DOE MATERIALS ACTIVITIES

(These numbers represent materials-related activities only. They do not include those portions of program budgets which are not materials related.)

	FY 1996
OFFICE OF BUILDING TECHNOLOGY, STATE AND COMMUNITY PROGRAMS	$ 725,000
Office of Building Systems	725,000
OFFICE OF INDUSTRIAL TECHNOLOGIES	$26,395,000
Office of Industrial Crosscut Technologies	26,395,000
Advanced Industrial Materials Program	8,898,000
Advanced Turbine Systems Program	8,400,000
Heat Exchanger Program	358,000
Continuous Fiber Ceramic Composites (CFCC) Program	7,884,000
Solar Industrial Program	855,000
OFFICE OF TRANSPORTATION TECHNOLOGIES	$30,554,000
Transportation Materials Technology	18,985,000
Automotive Materials Technology	14,832,000
Propulsion Systems Materials	3,432,000
Lightweight Vehicle Materials	11,400,000
Advanced Battery Materials	2,753,000
Fuel Cell Materials	1,400,000
Heavy Vehicle Materials Technology	11,569,000
Propulsion Systems Materials	9,080,000
High Strength Weight Reduction Materials	2,489,000
OFFICE OF UTILITY TECHNOLOGIES	$34,790,000
Office of Solar Energy Conversion	16,200,000
Photovoltaic Energy Technology Division	16,200,000
Office of Geothermal Technologies	590,000
Office of Energy Management	18,000,000
Advanced Utility Concepts Division	18,000,000
High Temperature Superconductivity for Electric Systems	18,000,000

FY 1996 BUDGET SUMMARY FOR DOE MATERIALS ACTIVITIES (continued)

	FY 1996
OFFICE OF ENERGY RESEARCH	$417,462,697
Office of Basic Energy Sciences	343,943,766
Division of Materials Sciences	332,060,000
Division of Chemical Sciences	5,300,000
Division of Engineering and Geosciences	6,583,766
Engineering Sciences Research	3,946,973
Geosciences Research	2,636,793
Office of Computational and Technology Research	56,309,931
Division of Advanced Energy Projects and Technology Research	56,309,931
Laboratory Technology Research (LTR) Program	4,897,000
Advanced Energy Projects	8,034,851
Small Business Innovation Research Program	40,399,742
Small Business Technology Transfer Program	2,978,338
Office of Fusion Energy Sciences	17,209,000
OFFICE OF ENVIRONMENTAL MANAGEMENT	$ 40,091,517
Office of Waste Management	2,579,000
High Level Waste Division	2,579,000
Office of Science and Technology	37,512,517
Office of Technology Development	37,512,517
Office of Science and Risk Policy	14,449,517
Office of Technology Systems	23,063,000
OFFICE OF NUCLEAR ENERGY, SCIENCE AND TECHNOLOGY	$ 51,830,000
Office of Engineering and Technology Development	1,830,000
Space and National Security Programs	1,830,000
Office of Naval Reactors	50,000,000[1]
OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT	$ 9,600,000

[1]*This excludes $45 million for the cost of irradiation testing in the Advanced Test Reactor (ATR).*

FY 1996 BUDGET SUMMARY FOR DOE MATERIALS ACTIVITIES (continued)

	FY 1996
OFFICE OF DEFENSE PROGRAMS	$108,694,000
The Weapons Research Development and Test Program	108,694,000
Sandia National Laboratories	64,697,000
Lawrence Livermore National Laboratory	16,970,000
Los Alamos National Laboratory	27,027,000
OFFICE OF FOSSIL ENERGY	$ 6,713,000
Office of Advanced Research	6,713,000
Fossil Energy AR&TD Materials Program	6,713,000
TOTAL	**$726,855,214**

The distribution of these funds between DOE laboratories, private industry, academia and other organizations is listed below.

OFFICE	DOE LABORATORIES	PRIVATE INDUSTRY	ACADEMIA	OTHER	TOTAL
Office of Building Technology, State and Community Programs	$725,000	$0	$0	$0	$725,000
Office of Industrial Technologies	$12,533,000	$12,997,000	$635,000	$230,000	$26,395,000
Office of Transportation Technologies	$17,476,000	$10,477,000	$2,601,000	$0	$30,554,000
Office of Utility Technologies	$21,340,000	$8,810,000	$4,640,000	$0	$34,790,000
Office of Energy Research	$330,680,850	$46,268,080	$40,414,038	$99,729	$417,462,697
Office of Environmental Management	$26,330,251	$750,000	$12,522,266	$489,000	$40,091,517
Office of Nuclear Energy, Science and Technology	$51,830,000	$0	$0	$0	$51,830,000
Office of Civilian Radioactive Waste Management	$9,600,000	$0	$0	$0	$9,600,000
Office of Defense Programs	$108,194,000	$500,000	$0	$0	$108,694,000
Office of Fossil Energy	$4,786,000	$826,000	$1,101,000	$0	$6,713,000
TOTALS	$583,495,101	$80,628,080	$61,913,304	$818,729	$726,855,214

OFFICE OF ENERGY EFFICIENCY AND RENEWABLE ENERGY

The Office of Energy Efficiency and Renewable Energy seeks to develop the technology needed for the Nation to use its existing energy supplies more efficiently, and for it to adopt, on a large scale, renewable energy sources. Toward this end, the Office conducts long-term, high-risk, high-payoff R&D that will lay the groundwork for private sector action.

A number of materials R&D projects are being conducted within the Energy Efficiency and Renewable Energy program. The breadth of this work is considerable, with projects focusing on coatings and films, ceramics, solid electrolytes, elastomers and polymers, corrosion, materials characterization, transformation, superconductivity and other research areas. The level of funding indicated refers only to the component of actual materials research.

The Office of Energy Efficiency and Renewable Energy conducts materials research in the following offices and divisions:

	FY 1996
OFFICE OF BUILDING TECHNOLOGY, STATE AND COMMUNITY PROGRAMS	$ 725,000
Office of Building Systems	725,000
OFFICE OF INDUSTRIAL TECHNOLOGIES	$26,395,000
Office of Industrial Crosscut Technologies	26,395,000
Advanced Industrial Materials Program	8,898,000
Advanced Turbine Systems Program	8,400,000
Heat Exchanger Program	358,000
Continuous Fiber Ceramic Composites (CFCC) Program	7,884,000
Solar Industrial Program	855,000
OFFICE OF TRANSPORTATION TECHNOLOGIES	$30,554,000
Transportation Materials Technology	18,985,000
Automotive Materials Technology	14,832,000
Propulsion Systems Materials	3,432,000
Lightweight Vehicle Materials	11,400,000
Advanced Battery Materials	2,753,000
Fuel Cell Materials	1,400,000
Heavy Vehicle Materials Technology	11,569,000
Propulsion Systems Materials	9,080,000
High Strength Weight Reduction Materials	2,489,000
OFFICE OF UTILITY TECHNOLOGIES	$34,790,000
Office of Solar Energy Conversion	16,200,000
Photovoltaic Energy Technology Division	16,200,000
Office of Geothermal Technologies	590,000
Office of Energy Management	18,000,000
Advanced Utility Concepts Division	18,000,000
High Temperature Superconductivity for Electric Systems	18,000,000

OFFICE OF BUILDING TECHNOLOGY, STATE AND COMMUNITY PROGRAMS

	FY 1996
Office of Building Technology, State and Community Programs - Grand Total	$725,000
Office of Building Systems	$725,000
Materials Properties, Behavior, Characterization or Testing	$725,000
Development of Non-HCFC Foam Insulations	100,000
Evacuated Powder Panel Insulation	275,000
Gas-Filled Reflective Insulation Panel	50,000
Accelerated Lifetime Test Procedure Development	200,000
Standardized Procedures for Measuring Solar Reflectivity on Horizontal Surfaces	100,000

OFFICE OF BUILDING TECHNOLOGY, STATE AND COMMUNITY PROGRAMS

OFFICE OF BUILDING SYSTEMS

The goal of this Office is to provide a scientific and technical basis (including model standards) for reducing the use of energy in residential and commercial buildings by 35 percent by the year 2000 from that used in 1975, while maintaining existing levels of human comfort, heaxlth and safety. The Division's primary objectives are to support research that advances the scientific and technical options for increased energy efficiency in buildings, to promote the substitution of abundant fuels for scarce fuels in buildings, and to promulgate standards for increased efficiency of energy use. To accomplish a portion of this, the Building Materials program seeks to: (1) develop new and improve existing insulating materials; (2) develop and verify analytical models that are useful to building designers and researchers for predicting the thermal performance characteristics of materials; (3) develop methods for measuring the thermal performance characteristics; and (4) provide technical assistance and advice to industry and the public. The DOE contact is Arun Vohra, (202) 586-2193.

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

1. **DEVELOPMENT OF NON-HCFC FOAM INSULATIONS**
   $100,000
   DOE Contact: Arun Vohra, (202) 586-2193
   ORNL Contact: Ken Wilkes, (423) 574-5931

This project is for the development of foam insulations that use alternative blowing agents as drop-in replacements for the CFC blowing agents that were previously used in the manufacture of foam insulation products and for the HCFC blowing agents that are currently being used. Prototype foam insulation boards and refrigerator panels were sent to ORNL for testing and evaluation. Tests are being conducted to determine thermal properties and aging characteristics.

Keywords: CFC, Foam Insulation, Insulation Sheathing, Roofs, HCFC, Refrigerators

2. **EVACUATED POWDER PANEL INSULATION**
   $275,000
   DOE Contact: Arun Vohra, (202) 586-2193
   ORNL Contact: Ken Wilkes, (423) 574-5931

This project is for the development of an advanced technology super insulation concept. A layer of powder is encapsulated in a vacuum barrier and a soft vacuum is drawn on the powder filler. Current technology produces R-30 and R-40 per inch panels. More efficient and/or less expensive fillers and longer life encapsulating materials are being developed. Initial applications are to the walls and doors of refrigerators/freezers. Other applications, including building envelopes, are being developed.

Keywords: Insulation, Vacuum, Heat Transfer, Refrigerators

3. **GAS-FILLED REFLECTIVE INSULATION PANEL**
   $50,000
   DOE Contact: Arun Vohra, (202) 586-2193
   LBL Contact: Dariush Arasteh, (510) 486-6844

This project is for the development of a super insulation concept that utilizes layers of reflective films enclosed in a flexible film panel which is filled with low conductivity gases. Procedures to mass produce the baffle material are being investigated. Prototypes and design advice are being provided to potential manufacturers interested in specific applications.

Keywords: Insulation, Reflective Films, Low Conductivity Gases

4. **ACCELERATED LIFETIME TEST PROCEDURE DEVELOPMENT**
   $200,000
   DOE Contact: Arun Vohra, (202) 586-2193
   ORNL Contact: Ken Wilkes, (423) 574-5931

This joint project with the Appliance Research Consortium is for the development of an ASTM standard test procedure for measuring the thermal resistance and aging characteristics of insulating materials with R-values in excess of 20 per inch. The procedure requires the development of a specialized measurement configuration, the modelling of the test specimen within the test configuration, and the conduction of round robins with industry partners.

Keywords: Thermal Resistance, Test Procedures

5. **STANDARDIZED PROCEDURES FOR MEASURING SOLAR REFLECTIVITY ON HORIZONTAL SURFACES**
$100,000
DOE Contact: Mark Decot, (202) 586-6501
LBL Contact: Hashem Akbari, (510) 486-4287

The reflectivity of exterior building materials used for pavement and roofing has been demonstrated to affect heating and cooling costs in buildings where they are applied. The reflectivity of these surfaces also has an effect on ambient air temperature that has an additional indirect effect on heating and cooling costs in buildings. This research on procedures for measuring reflectivity is being conducted in cooperation with ASTM, the Lawrence Berkeley Laboratory and the Urban Heat Island Research Program.

Keywords: Solar, Reflectivity, Building Materials

OFFICE OF INDUSTRIAL TECHNOLOGIES

	FY 1996
Office of Industrial Technologies - Grand Total	$26,395,000
Office of Industrial Crosscut Technologies	$26,395,000
Advanced Industrial Materials Program	$ 8,898,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 4,560,000
Intermetallic Alloy Development and Technology Transfer of Intermetallic Alloys	1,050,000
Synthesis and Design of $MoSi_2$ Intermetallic Materials	700,000
Development of Weldable, Corrosion Resistant Iron-Aluminide Alloys	250,000
Composites and Coatings Through Reactive Metal Infiltration	360,000
Microwave Processing of Continuous Ceramic Oxide Filaments	400,000
Conducting Polymers: Synthesis and Industrial Applications	300,000
Microwave Assisted Chemical Vapor Infiltration	200,000
Surface Treatment of Materials by Induction Hardening	50,000
Chemical Vapor Deposition Ceramic Synthesis	400,000
Gel Casting Technology	150,000
Uniform Droplet Spray Forming	500,000
Composites and Blends from Biobased Materials	200,000
Materials Properties, Behavior, Characterization or Testing	$ 1,000,000
Materials for Recovery Boilers	1,000,000
Materials Structure and Composition	$ 2,088,000
Metallic and Intermetallic Bonded Ceramic Composites	230,000
Advanced Metallic and Intermetallic Materials	1,353,000
Processing of Polymers in a Magnetic Field	300,000
Microwave Joining of SiC	205,000
Device or Component Fabrication, Behavior or Testing	$ 1,250,000
Advanced Microwave Processing Concepts	250,000
Selective Inorganic Thin Films	350,000
Chemical Vapor Infiltration of TiB_2 Composites	100,000
Metals Processing Laboratory User (MPLUS) Center	350,000
Development of Improved Refractories	200,000
Advanced Turbine Systems Program	$ 8,400,000
Device or Component Fabrication, Behavior or Testing	$ 8,400,000
Ceramic Components for Stationary Gas Turbines in Cogeneration Service	5,000,000
Long-Term Testing of Ceramic Components for Stationary Gas Turbines	400,000
ATS Materials Base Technology Support	3,000,000

OFFICE OF INDUSTRIAL TECHNOLOGIES (continued)

	FY 1996
Office of Industrial Processes (continued)	
Heat Exchanger Program	$ 358,000
Materials Properties, Behavior, Characterization or Testing	$ 120,000
Advanced Heat Exchanger Material Technology Development	120,000
Device or Component Fabrication, Behavior or Testing	$ 238,000
HiPHES System for Energy Production	0
HiPHES System for Ethylene Production	238,000
Continuous Fiber Ceramic Composites (CFCC) Program	$7,884,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$5,584,000
CFCC Program - Industry Tasks	5,584,000
Materials Properties, Behavior, Characterization or Testing	$2,300,000
Continuous Fiber Ceramic Composites (CFCC) Supporting Technologies	2,300,000
Solar Materials Research Program	$ 855,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 855,000
Photocatalysts Based on Titanium Dioxide	280,000
Solar Materials Processing	575,000

OFFICE OF INDUSTRIAL TECHNOLOGIES

Through the Industries of the Future strategy, the DOE Office of Industrial Technologies (DOE-OIT) is stimulating the development and use of industrial technologies that increase energy efficiency and lower the costs of environmental protection and regulatory compliance. The Industries of the Future strategy is concentrating on seven industries—petroleum refining, chemicals, pulp and paper, steel, aluminum, foundries and glass—which are vital to the U.S. economy; and which at the same time, account for 88 percent of energy consumed in manufacturing and more than 90 percent of the wastes generated. Research in support of the Industries of the Future is being conducted in partnership with industry, according to R&D priorities established by industry participants. Materials research addresses the need for industrial processes to run at increased temperatures with longer service lives, reduced downtime, and lower capital costs.

OFFICE OF INDUSTRIAL CROSSCUT TECHNOLOGIES

ADVANCED INDUSTRIAL MATERIALS PROGRAM

New or improved materials can save significant energy and improve productivity by enabling systems to operate at higher temperatures, last longer, and reduce capital costs. The Advanced Industrial Materials program is a crosscutting program with emphasis on industrial needs of the "Industries of the Future" initiative and of crosscutting industries including carbon products, forging, heat treating, and welding. Efforts in FY 1996 were focused on partnerships between industry and the National Laboratories for commercialization of new materials and processes. The program manager is Charles A. Sorrell, (202) 586-1514.

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

6. **INTERMETALLIC ALLOY DEVELOPMENT AND TECHNOLOGY TRANSFER OF INTERMETALLIC ALLOYS**
   $1,050,000
   DOE Contact: Charles A. Sorrell, (202) 586-1414
   ORNL Contacts: M. L. Santella, (423) 574-4805 and V. K. Sikka, (423) 574-5112

The objective of this project is to develop and apply the excellent oxidation and carburization resistance and higher strength of intermetallic alloys including nickel aluminides to Industries of the Future related manufacturing application. Progress in bringing technologies to development and commercialization in FY 1996 included the following: (1) the case compositions were licensed to United Defense LP for commercial production; (2) the Exo-Melt process for air melting Ni_3Al based alloys was transferred to industry; (3) castings of the cast alloy IC-221M were installed in various commercial environments including rolls for heat treating steel furnaces at Bethlehem Corp., heat treating fixtures at GM Saginaw; (4) the base metal composition was developed to enable welding of fully restrained materials up to 1" in thickness; (5) weld design procedures were developed to enable butt weld in rings of large diameter tubes and to enable dissimilar metal weld between a ring of Ni_3Al and Alloy 800 H; (6) strong efforts continued on technology transfer efforts.

Keywords: Nickel Aluminides, Processing, Steel, Metalcasting, Aluminum, Heat Treating, Welding

7. **SYNTHESIS AND DESIGN OF $MoSi_2$ INTERMETALLIC MATERIALS**
   $700,000
   DOE Contact: Charles A. Sorrell, (202) 586-1514
   LANL Contacts: J. J. Petrovic, (505) 667-0125 and Richard Castro, (505) 667-5191

The objective of this project is to develop $MoSi_2$-based composites that will combine good room temperature fracture toughness with excellent oxidation resistance and high-temperature strength for industrial applications. Activities in FY 1996 included the development of $MoSi_2$-based materials and components for fiberglass melting and processing applications, and development and characterization of $MoSi_2$-Si_3N_4 and $MoSi_2$-SiC composites, plasma spraying of $MoSi_2$-based materials and joining of $MoSi_2$ materials to metals.

Keywords: Composites, Intermetallics, Molydisilicides

8. **DEVELOPMENT OF WELDABLE, CORROSION RESISTANT IRON-ALUMINIDE ALLOYS**
   $250,000
   DOE Contact: Charles A. Sorrell, (202) 586-1514
   ORNL Contact: P. J. Maziasz, (423) 574-5082

The objectives of this project are to develop FeAl alloys with improved weldability and mechanical and corrosion properties for use in structural applications; and to develop the potential for weldable FeAl alloys for use in weld-overlay cladding applications. Several developments were made in FY 1996. Cast FeAl alloys tested in carburizing atmosphere simulating industrial ethylene pyrolysis or steam reformer environments showed excellent corrosion resistance. Ductile and weldable FeAl was also successfully produced by the extrusion processing of powders. FeAl weld overlays were made on several types of steels and additional development is focusing on elimination of cold cracking. FeAl components are being tested in several industrial environments including for use as grate bars and in carburizing atmospheres.

Keywords: Iron Aluminides, Coatings, Claddings, Thermophysical Properties

9. **COMPOSITES AND COATINGS THROUGH REACTIVE METAL INFILTRATION**
   $360,000
   DOE Contact: Charles A. Sorrell, (202) 586-1514
   SNL Contact: R. E. Loehman, (505) 844-2222

Ceramic-metal composites have advantages as engineering materials because of their high stiffness-to-weight ratios, good fracture toughness, and because their electrical and thermal properties can be varied through control of their composition and microstructure. Reactive metal infiltration is a promising new route to synthesize and process a wide range of ceramic and metal-matrix composites to near-net-shape with control of both composition and microstructure. In FY 1996 significant improvements were made in the fracture toughness of composites. Composites prepared by heating Al with porous mullite had a fracture toughness of 10.5 Mpam$^{1/2}$. The Mo-Si-Al system was investigated and a process for making composites was developed and materials prepared for property measurements.

Keywords: Metal Matrix Composites, Reactive Metal Infiltration, Ceramics

10. **MICROWAVE PROCESSING OF CONTINUOUS CERAMIC OXIDE FILAMENTS**
    $400,000
    DOE Contact: Charles A. Sorrell, (202) 586-1514
    LANL Contacts: G. J. Vogt and J. D. Katz, (505) 665-1424

The objective of this research is to develop economic microwave processing technology for the complete manufacturing of continuous ceramic oxide filament tows from extruded solution-based gels with greater energy efficiency than conventional thermal processing. The approach is to use volumetric microwave absorption to heat ceramic oxide tows in order to drive the process drying, prefiring, and sintering in the preparation of continuous tows from solution-based gels. Microwave heating of filament tows was successfully controlled by pulse modulation of a magnetron source and by active feedback control of the pulse rate and frequency through an optical feedback sensor. Current efforts are focused on developing microwave techniques for drying, organic burnout, and sintering of sol-gel filament tows.

Keywords: Microwave Processing, Filaments

11. **CONDUCTING POLYMERS: SYNTHESIS AND INDUSTRIAL APPLICATIONS**
    $300,000
    DOE Contact: Charles A. Sorrell, (202) 586-1514
    LANL Contact: S. Gottesfeld, (505) 667-0853

The process of separating pure components out of a mixture of gases is of great industrial importance. Current gas separation technologies have major shortcomings, including poor energy efficiency and the generation of secondary pollution. The objective of this project is to develop superior membranes for gas separation using doped polyaniline polymers. Because these materials are electrical conductors, membrane properties can be changed following synthesis, and even during use, to control the process flow. A key portion of this project is fabrication of integrally skinned, asymmetric membranes of polyaniline using highly refined solution chemistry. In FY 1996, membranes consisting of a dense very thin "skin" (2 um thick, or less) on top of a porous (e.g., 40 mm thick) base layer, were developed with permeant throughput enhancement 50 to 80 times that of uniformly dense membranes and the selectivity of pair gas separations was maintained within a factor of 2.

Keywords: Electrically Conducting Polymers, Gas Separation, Capacitors

12. **MICROWAVE ASSISTED CHEMICAL VAPOR INFILTRATION**
    $200,000
    DOE Contact: Charles A. Sorrell, (202) 586-1514
    LANL Contact: D. J. Devlin, (505) 667-9914

The use of microwave heating of ceramic fiber preforms is being explored as a means of developing an improved rapid process for the fabrication of composites by chemical vapor infiltration. The volumetric and preferential heating of certain materials by microwaves provides a means of establishing inverted thermal gradients in a preform. The result is the ability to rapidly infiltrate the preform developing the matrix from the inside-out. A successful microwave/RF assisted infiltration process would eliminate may limitations encountered in conventional approaches. Work has been initiated with an industrial partner to further develop a microwave driven densification process for the manufacture of carbon-carbon composites. Research with another industrial partner is being conducted to develop membranes with controlled porosity for the separation of oleofins from hydrogen streams. The development of the required pore structure entails the closing of the pores of a suitable substrate by vapor deposition techniques.

Keywords: Microwave Processing, Chemical Vapor Infiltration, Ceramics, Composites

13. **SURFACE TREATMENT OF MATERIALS BY INDUCTION HARDENING**
$50,000
DOE Contact: Charles A. Sorrell, (202) 586-1514
SNL Contact: B. Damkroger, (505) 584-8116

Induction hardening is widely used in the industrial sector to case harden components to provide increased strength and wear behavior. It is an energy efficient process that can directly impact manufacturing of materials. The goal of this project was to develop induction hardening processes and to bring together an industrial team such that the technology could be used across a broader range of processes. In FY 1996, the feasibility of applying recently developed induction hardening technology to materials and industries beyond current applications was explored. Experiments were performed to characterize the variability of materials/process interactions and their role in process control.

Keywords: Induction, Hardening, Heat Treating, Metals, Alloys, Control, Processes

14. **CHEMICAL VAPOR DEPOSITION CERAMIC SYNTHESIS**
$400,000
DOE Contact: Charles A. Sorrell, (202) 586-1514
SNL - Livermore Contact: M. D. Allendorf, (415) 294-2895

Comprehensive models, including detailed gas-phase and surface chemistry coupled with reactor fluid mechanics, are required to optimize and scale-up chemical vapor deposition (CVD) processes. The objective of this project is to use the unique diagnostic and modeling capabilities at the Sandia National Laboratories - California to understand and develop new techniques for chemical vapor deposition (CVD). A research reactor, originally constructed with DOE-OIT funding, is being used to determine identities and amounts of gaseous phase species present during CVD. Research efforts are focused on development of CVD processes for oxide fiber-preforms and plate glass surfaces for the improvement of properties. In FY 1996 efforts focused on the CVD of Boron Nitride. A verified model was developed to predict the deposition of BN layers on ceramic fiber preforms. The gas phase and surface processes occurring during deposition were characterized and the results are being incorporated in the model.

Keywords: Chemical Vapor Deposition, Gas-Phase Chemistry, Modeling

15. **GEL CASTING TECHNOLOGY**
$150,000
DOE Contact: Charles A. Sorrell, (202) 586-1514
ORNL Contact: M. A. Janney, (423) 576-5183

Gelcasting is an advanced powder forming process. It can be used to form ceramic or metal powders into simple or complex, near net shapes. The sol-gel process is being developed in order to produce aluminum oxide tubes for use in high-intensity industrial lighting, and H13 steel dies. For the lighting application the sol-gel process will produce identical materials at lower temperatures and in far less time than do conventional methods which involve prolonged high temperature sintering with sintering aids. In FY 1996, tubes which meet lighting specifications for transparency have been fabricated in a variety of sizes and shapes. A method for preparing H13 steel powder into complex shapes was also developed. The green parts were arc machinable into complex shapes similar to those used as, for example, die casting dies.

Keywords: Sol-Gel, Aluminum Oxide, Lighting Tubes, H13 Steel, Dies

16. **UNIFORM DROPLET SPRAY FORMING**
$500,000
DOE Contact: Charles A. Sorrell, (202) 586-1514
ORNL Contact: Craig A. Blue, (423) 574-4351 and Vinod Sikka, (423) 574-5123

The purpose of this project is to adapt the process to higher melting materials, e.g., intermetallic alloys, stainless, steel, superalloys; to provide superior metal powders for the powder metallurgy industry and to develop methods for spray coating or casting of high temperature materials, including aluminide intermetallics. Spray forming of metallic systems is being investigated. Participants in this research include Oak Ridge National Laboratory, Massachusetts Institute of Technology, Northeastern University and powder metal companies. In FY 1996 the intermediate temperature system was completed with the capacity of forming up to 8 Kg of materials at temperatures up to 1250°C. Both aluminum and bronze spherical powders were successfully produced. A high temperature system capable of spraying materials up to 1650°C was also partially assembled. Production of new alloys and laminar materials will be explored in the future.

Keywords: Powder, Near Net Shape Forming, Aluminum, Alloys, Steel, Intermetallics

17. **COMPOSITES AND BLENDS FROM BIOBASED MATERIALS**
$200,000
DOE Contact: Charles A. Sorrell, (202) 586-1514
NREL Contacts: S. S. Kelley and S. S. Shojaie, (303) 384-6123

The goals of this project are to develop polymer membranes for gas and vapor separation applications, and to develop novel ester materials. In FY 1996 the separations work is being performed under an agreement with a chemical company. Work included the determination of effects of several processing variables including initial composition, effect of chemical, mechanical and transport properties. Sol gel techniques were also applied to the development of crosslinked ester materials.

Keywords: Membranes, Polymers, Sol Gel, Chemicals

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

18. **MATERIALS FOR RECOVERY BOILERS**
$1,000,000
DOE Contact: Charles A. Sorrell, (202) 586-1514
ORNL Contact: James R. Kaiser, (423) 574-4453

The purpose of this project is to determine the cause of failure of composite tubes used in Kraft Black Liquor recovery boilers during pulp and paper making, and to develop new materials to eliminate failures. The project consists of three efforts: (1) obtaining operating data and failure analyses from pulp and paper companies, boiler manufacturers and composite tube manufacturers, (2) determining residual stresses in new and used composite tubes and microstructural characteristics of tubes as related to stresses and failure mechanisms, and (3) developing new materials and/or fabrication methods for improvements in boiler efficiency, service life, and safety. Participants include Oak Ridge National Laboratory, Institute of Paper Science and Technology, and 11 industrial collaborators. In FY 1996 a model of recovery boiler floor tubes was developed, experimental through thickness measurements were made on as produced and exposed tubes, new and failed tubes were characterized, and mechanical and corrosion testing of current and alternate materials were performed.

Keywords: Recovery Boilers, Composite Tubes, Pulp and Paper

MATERIALS STRUCTURE AND COMPOSITION

19. **METALLIC AND INTERMETALLIC BONDED CERAMIC COMPOSITES**
$230,000
DOE Contact: Charles A. Sorrell, (202) 586-1514
ORNL Contacts: P. F. Becker, (423) 574-5197 and T. N. Tiegs, (423) 574-5173

To improve the reliability of ceramic components, new approaches to increasing the fracture toughness of ceramics over an extended temperature range are needed. One method is the incorporation of ductile phases into ceramic matrix alloys for local plastic deformation during crack bridging processes. The objective of this program is to develop ceramic composites with high fracture toughness for intermediate temperature use in wear, tribological and engine applications. In FY 1996 TiC based composites with Ni_3Al binder have been developed with high oxidation resistance, high fracture strength (<1Gpa) that are retained up to 900°C. The acidic corrosion resistance of these materials is also promising. The microstructural features yielding optimal toughening have been identified and composites have been fabricated with properties comparable to, or better than, commercial ceramic composites at a lower raw material cost.

Keywords: Ceramics, Composites, Nickel Aluminide

20. **ADVANCED METALLIC AND INTERMETALLIC MATERIALS**
$1,353,000
DOE Contact: Charles A. Sorrell, (202) 586-1514
ORNL Contact: P. Angelini, (423) 574-4565 and C. T. Liu, (423) 574-4459

The goals of this project are to develop new and improved materials. Many metallic and ordered intermetallic alloys possess unique properties and have the potential to be developed as new materials for energy related applications. In FY 1996 grain size was identified as the key microstructural parameter controlling room temperature tensile properties of TiAl alloys with lamellar structures. The mechanical properties of TiAl alloys with ultra-fine lamellar structure produced by hot extrusion are superior to other advanced TiAl alloys. Efforts were also made in the development of alloys for the glass industry and modeling glass forming operations. Metalcasting efforts focused on partnering with industry in developing a massively parallel version of a software package. This effort will enable much more rapid turnaround time in analyzing various casting processes including sand and centrifugal.

Keywords: Intermetallics, Ordered Alloys, TiAl, Ni_3Al, Metalcasting, Glass

21. **PROCESSING OF POLYMERS IN A MAGNETIC FIELD**
$300,000
DOE Contact: Charles A. Sorrell, (202) 586-1514
LANL Contact: Elliot P. Douglas, (505) 665-4828

The purpose of this project is to demonstrate the utility of magnetic fields, to beneficially modify or control the physical, optical and electrical properties of materials through the application of magnetic fields during polymerization processing and solidification. Researchers at Los Alamos National Laboratory, in collaboration with an industrial partner, have demonstrated that using high (10-20 Tesla) magnetic fields to orient liquid crystal polymers during processing can lead to substantial improvements in mechanical properties. In FY 1996 work focused on the development of liquid crystalline thermoset in a magnetic field over the range of 0-18 Tesla. Curing was performed with specimens of sufficient size to permit mechanical property measurements to be made. Orientation in magnetic fields leads to an increase in the modulus of almost three times that of the unoriented material. The coefficient of thermal expansion and X-ray diffraction show a high degree of anisotropy indicating significant chain alignment by the use of a magnetic field. A kinetic model was used to predict qualitative trends in the orientation kinetics.

Keywords: Organic Polymers, Magnetic Processing, Mechanical Properties

22. **MICROWAVE JOINING OF SiC**
$205,000
DOE Contact: Charles A. Sorrell, (202) 586-1514
LANL Contact: Joel D. Katz, (505) 665-1424
FM Technologies, Inc. Contact: R. Silberglitt, (703) 425-5111
George Mason University Contact: W. Murray Black, (703) 993-4069

The objective of this project is to develop and optimize a joining method that can be applied to large scale fabrication of components such as radiant burner tubes and high temperature, high pressure heat exchangers. Microwave joining of both reaction bonded silicon carbide and sintered silicon carbide has been demonstrated for tubes up to 5 cm in diameter. Joints are leak tight at service temperature, and have adequate mechanical strength for desired applications. In FY 1996 a new multimode applicator, approximately 16" in diameter and 16" long, was designed, fabricated and tested. It is capable of evacuating and backfilling to establish environment required for producing SiC or other interlayers from chemical reactions *in situ*. The applicator was used to join commercial SiC/SiC composite plates using commercial polymer precursor to form a SiC interlayer *in situ*. Collaborative work with an industrial partner has been initiated to demonstrate scale-up of the joining technique for a high temperature reactor in the petroleum refining industry.

Keywords: Microwave Processing, Microwave Joining, SiC

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

23. **ADVANCED MICROWAVE PROCESSING CONCEPTS**
$250,000
DOE Contact: Charles A. Sorrell, (202) 586-1514
ORNL Contacts: R. J. Lauf and A. D. McMillan, (423) 574-5176

The purpose of this project is to explore the feasibility of several advanced microwave processing concepts to develop new energy-efficient materials and processes. A variable frequency microwave furnace was developed by Oak Ridge National Laboratory and commercialized by Lambda Technologies. Current emphasis is on determining the curing behavior of thermosetting resins and polymer-matrix composites under microwave heating conditions. In FY 1996 (1) two patents on the variable frequency microwave source were issued, one of which was licensed to Lambda Technologies, Inc., (2) the use of microwave curing of adhesives for joining metals, metal to polymer, and metal to ceramic materials was performed. An epoxy-based adhesive and a commercially available sheet adhesive are being examined. The results show that the curing times are reduced by a factor of three as compared to conventional processing.

Keywords: Microwave Processing, Polymers, Composites, Variable Frequency

24. **SELECTIVE INORGANIC THIN FILMS**
$350,000
DOE Contact: Charles A. Sorrell, (202) 586-1514
SNL Contact: Mark Phillips, (505) 844-8969

The purpose of this research is to develop a new class of inorganic membranes for light gas separation and use this technology to improve on separation efficiencies currently available with polymer membranes, particularly for light alkanes. The approach is to nucleate and crystallize zeothlitic phases from sol-gel derived amorphous coatings, using porous filters and gas membranes as supports for these films. Current efforts have focused on controlling porosity in several oxide film compositions. These films have been deposited on quartz acoustic plate mode devices. Zeolite films and composite films of zeolites embedded in amorphous matrices have also been synthesized. Future efforts include utilizing nonaluminosilicate molecular sieves as membranes as well as exploring other sources of nutrient for zeolitic film crystallization.

Keywords: Coatings, Sol-Gel Processing

25. **CHEMICAL VAPOR INFILTRATION OF TiB_2 COMPOSITES**
$100,000
DOE Contact: Charles A. Sorrell, (202) 586-1514
ORNL Contact: T. Besmann, (423) 574-6852

This project is designed to develop a Hall-Heroult aluminum smelting cathode with substantially improved properties. The carbon cathodes in current use require significant anode-to-cathode spacing in order to prevent shorting, causing significant electrode inefficiencies. A fiber reinforced-TiB_2 matrix composite would have the requisite wettability, strength, strain-to-failure, cost, and lifetime to solve this problem. The approach is to fabricate a cathode material through chemical vapor infiltration (CVI). In FY 1996 bench testing of a section of a 8"x8" disc provided to Alcoa Technical Center revealed excellent electrical, wetting and aluminum production capability. However, issues related to delamination arose. Efforts to increase the intermellar strength of the composites were begun.

Keywords: Chemical Vapor Infiltration, Composites, Hall-Heroult Cell

26. **METALS PROCESSING LABORATORY USER (MPLUS) CENTER**
$350,000
DOE Contact: Charles A. Sorrell, (202) 586-1514
ORNL Contacts: M. Mackiewicz-Ludtka, (423) 576-4552 and H. W. Hayden, (423) 574-6936

The Metals Processing Laboratory User (MPLUS) Center was officially designated as a DOE User Facility in February 1996. Its primary purpose is to assist U.S. industry and academia in improving energy efficiency and enhancing U.S. competitiveness. MPLUS is designed to provide U.S. Industries with access to processing issues that limit the development and implementation of emerging materials and materials processing technologies. MPLUS includes the following primary user centers: Metals Processing, Metal Joining, Metals Characterization and Metals Process Modeling. As of September 1996, a total of 31 MPLUS proposals were received from 27 companies and universities representing 17 states; and 12 had already utilized the MPLUS. Projects crosscut all of the seven industries in the "Industries of the Future" initiative; other crosscutting industries including forging, heat treating, and welding; and crosscutting programs.

Keywords: Industry, User Center, Metals, Materials, Processing, Joining, Properties, Characterization, Modeling, Process

27. **DEVELOPMENT OF IMPROVED REFRACTORIES**
$200,000
DOE Contact: Charles A. Sorrell, (202) 586-1514
ORNL Contact: A. A. Wereszczak, (423) 574-7601

Refractories are critical for various industrial processes. For example, glass melting furnaces are fabricated with various types of refractories which enable the furnaces to be operated at very high temperatures, steel or aluminum smelting and melting vessels are lined with refractories, etc. The goal of this project is to develop improved refractories and to determine critical mechanical and thermophysical properties. In FY 1996, work was focused on determining high temperature creep and corrosion behavior of refractories for use in oxifuel fired glass making furnaces. Two high temperature (up to 3300°F) creep testing stations were dedicated to this project. Partners in this activity include the Oak Ridge National Laboratory, Alfred University's Center for Glass

Research (CGR), Satellite Center at the University of Missouri-Rolla, and an industrial technical team representing glass and refractories manufacturers.

Keywords: Refractories, Glass, Furnace, Oxy-fuel, High Temperature, Mechanical, Thermophysical, Properties, Corrosion

ADVANCED TURBINE SYSTEMS PROGRAM

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

28. **CERAMIC COMPONENTS FOR STATIONARY GAS TURBINES IN COGENERATION SERVICE**
$5,000,000
DOE Contact: P. Hoffman, (202) 586-6074
Solar Contact: M. Van Roode, (619) 544-5549

The performance of stationary gas turbines is limited by the temperature and strength capabilities of the metallic structural materials in the engine hot section. Because of their superior high temperature strength and durability uncooled ceramics can be used in the engine hot section at increased turbine inlet temperatures. An existing gas turbine engine will be retrofitted with first stage ceramic blades, first stage ceramic nozzles and ceramic combustor liners. This project will design and test these components for a stationary 3.5MW gas turbine for cogeneration service. The three components are the combustor, first stage rotor, and first stage nozzle. The project will culminate in a 4000 hour field demonstration of the engine.

Keywords: Structural Ceramics, Cogeneration, Gas Turbines

29. **LONG-TERM TESTING OF CERAMIC COMPONENTS FOR STATIONARY GAS TURBINES**
$400,000
DOE Contact: P. Hoffman, (202) 586-6074
ORNL Contact: M. Ferber, (423) 576-0818

The service life requirements for a land-based Advanced Turbine System (ATS) are significantly longer than for aircraft turbines and will impact the objectives of the respective materials development programs. Land-based gas turbines are generally required to operate for longer periods under steady-state conditions, and creep damage becomes the major consideration. This program performs the characterization tasks of the ATS materials/ manufacturing program. This project will test monolithic ceramics in static and cyclic fatigue for up to 10,000 hours at gas turbine utilization temperatures.

Keywords: Structural Ceramics, Cogeneration, Gas Turbines

30. **ATS MATERIALS BASE TECHNOLOGY SUPPORT**
$3,000,000
DOE Contact: P. Hoffman, (202) 586-6074
ORNL Contact: M. Karnitz, (423) 576-5150

Gas turbine manufacturers have stated a need for a turbine inlet temperature of greater than 2600°F in order to achieve higher efficiencies. New materials developments are necessary to achieve these temperatures for extended operating periods. Advanced casting techniques, metallurgy and coating science will be applied to gas turbines to allow higher operating temperature for increased efficiency while producing fewer emissions. The goals of these projects are improved turbine airfoil castings and reliable, higher performance thermal barrier coatings that will allow for increased turbine inlet temperature.

Keywords: Gas Turbines, Castings, Thermal Barrier Coatings

HEAT EXCHANGER PROGRAM

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

31. **ADVANCED HEAT EXCHANGER MATERIAL TECHNOLOGY DEVELOPMENT**
$120,000
DOE Contact: G. Varga, (202) 586-0082
ORNL Contact: M. Karnitz, (423) 574-5150

This project conducts research to evaluate advanced ceramic materials, fabrication processes and joining techniques. The effects of hot, corrosive environments on candidate ceramic and ceramic composite materials continue to be investigated. Also under investigation is the performance of advanced ceramic materials subjected to the processing environments encountered in steam cracking for ethylene production.

Keywords: Structural Ceramics, Corrosion-Gaseous, Industrial Waste Heat Recovery

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

32. **HiPHES SYSTEM FOR ENERGY PRODUCTION**
$0
DOE Contact: G. Varga, (202) 586-0082
Solar Turbines Contact: B. Harkins, (619) 544-5398

This project is in the second phase of a three-phase effort to develop high pressure heat exchange systems (HiPHES) for recovery of energy from the combustion of hazardous wastes. A multi-tube proof-of-concept test is continuing and high temperature exposure testing to the hazardous waste incinerator environment is continuing.

Keywords: Ceramic Composites, Heat Exchangers

33. **HiPHES SYSTEM FOR ETHYLENE PRODUCTION**
$238,000
DOE Contact: G. Varga, (202) 586-0082
Stone & Webster Engineering Corp. Contact: J. Gondolfe, (713) 368-4379

In this project, advanced ceramics are replacing the alloys conventionally used in ethylene production reactors. Ethylene production technology is mature, with technological advances resulting in gains of much less than 1 percent. Pilot runs on *this* project have demonstrated a 10 percent increase in ethylene production due to an increase in desirable yield and a prolonged run time between decoking cycles.

Keywords: Structured Ceramics, Ethylene, Heat Exchangers

CONTINUOUS FIBER CERAMIC COMPOSITES (CFCC) PROGRAM

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

34. **CFCC PROGRAM - INDUSTRY TASKS**
$5,584,000
DOE Contact: M. Smith, (202) 586-3646

The goal of the CFCC Program is to develop, in U.S. industry, the primary processing methods for the reliable and cost-effective fabrication of continuous fiber ceramic composite components for use in industrial applications. The first phase, completed in 1994, established performance requirements of applications and assessed feasibility of potential processing systems. Phase two, process engineering and component development, is in progress.

Keywords: Ceramic Composites, Continuous Fiber

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

35. **CONTINUOUS FIBER CERAMIC COMPOSITES (CFCC) SUPPORTING TECHNOLOGIES**
$2,300,000
DOE Contact: M. Smith (202) 586-3646
ORNL Contact: M. Karnitz, (423) 574-5150

This project provides basic or generic support to the industry teams conducting CFCC research. Tasks include: composite design, materials characterization, test methods development, database generation, codes and standards, and life prediction.

Keywords: Ceramic Composites, Fiber Architecture, Material Characterization, Test Methods

SOLAR MATERIALS RESEARCH PROGRAM

The objective of solar materials research is to identify and develop viable materials processes that take advantage of the attributes of highly concentrated solar fluxes. Concentrated sunlight from solar furnaces can generate temperatures well over 2000°C. Thin layers of the illuminated surfaces can be driven to very high temperatures in fractions of a second. Concentrated solar energy can be delivered over very large areas, allowing for rapid processing. The result is more efficient use of bulk materials and energy, potentially lower processing costs, and reduced need for strategic materials, all with a technology that does not damage the environment. Also being developed are catalysts for processes that use the sun's energy to destroy hazardous organic chemicals.

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

36. **PHOTOCATALYSTS BASED ON TITANIUM DIOXIDE**
$280,000
DOE Contact: Frank Wilkins, (202) 586-1684
NREL Contact: Daniel M. Blake, (303) 275-3702

The objectives of this work are to develop materials that are more active photocatalysts for the oxidation of organic compounds in air or aqueous phases, determine the characteristics of titanium dioxide and modified forms that influence the activity, and test the catalysts in laboratory and pilot scale reaction systems.

Potential catalysts are prepared inhouse, by NREL subcontractors, or obtained from commercial sources. The ultimate goal is to make photocatalytic oxidation processes for removal of hazardous organic compounds from contaminated air and water a cost-effective option for environmental remediation and process emission control.

Keywords: Photocatalyst, Titanium Dioxide, Oxidation, Remediation

37. **SOLAR MATERIALS PROCESSING**
$575,000
DOE Contact: Frank Wilkins, (202) 586-1684
NREL Contact: Allan Lewandowski, (303) 275-3672

The objective of this work is to develop an alternative method of processing various advanced materials using concentrated sunlight as the energy source. A number of processes have been explored including metalorganic deposition of thin films on ceramics, synthesis, production and processing of advanced ceramic powders, solar assisted chemical vapor deposition of thin films on various substrates, rapid thermal heat treating and cladding, solar production of fullerenes, and other surface modification techniques. The project seeks to explore a wide range of technologies, assess those with commercial potential and develop the most promising technologies in conjunction with industry. Several technologies have demonstrated significant technical success and are now being explored more fully through cooperative research and development agreements.

Keywords: Solar Processing, Advanced Materials, Ceramics, Metallization, Fullerenes, Cladding, Concentrated Sunlight, Solar Furnaces

OFFICE OF TRANSPORTATION TECHNOLOGIES

	FY 1996
Office of Transportation Technologies - Grand Total	$30,554,000
Transportation Materials Technology	$18,985,000
Automotive Materials Technology	$14,832,000
Propulsion Systems Materials	$ 3,432,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 975,000
Gelcasting: Scale-up and Commercialization	650,000
Optimization of Silicon Nitride Ceramics	175,000
In-Situ Toughened Silicon Nitride	150,000
Materials Properties, Behavior, Characterization or Testing	$ 1,762,000
Advanced Statistics Calculations	32,000
Component Verification	290,000
High Frequency Fatigue	220,000
Tensile Stress Rupture Testing	300,000
Ceramics Life Prediction	200,000
Life Prediction Methodology	0
Mechanical Behavior of Gas Turbine Ceramics	385,000
Ultrasonic NDE Development	335,000
Technology Transfer and Management Coordination	$ 300,000
Technical Project Management	300,000
Device or Component Fabrication, Behavior or Testing	$ 395,000
Corrosion-Resistant Coatings	175,000
Ceramic-Metal Joining	220,000
Lightweight Vehicle Materials	$11,400,000
Device or Component Fabrication, Behavior or Testing	$11,400,000
Low-Cost High Performance Aluminum Alloy Sheet for Automotive Applications	3,500,000
Low-Cost High Performance Cast Light Metals for Automotive Applications	1,700,000
Low-Cost High Performance Fiber Reinforced Polymer Composites	3,200,000
USAMP Cooperative Agreement	3,000,000
Advanced Battery Materials	$ 2,753,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 883,000
Advanced Electrode Research	300,000
Electrochemical Properties of Solid Electrolytes	200,000
Preparation and Characterization of New Polymer Electrolytes	210,000
New Cathode Materials	73,000
Structural Studies of Lithiated Transition-Metal Oxides	100,000

OFFICE OF TRANSPORTATION TECHNOLOGIES (continued)

	FY 1996
Automotive Materials Technology (continued)	
Advanced Battery Materials (continued)	
Materials Properties, Behavior, Characterization or Testing	$ 1,286,000
Carbon Electrochemistry	250,000
Fabrication and Testing of Carbon Electrodes as Lithium Intercalation Anodes	75,000
Battery Materials: Structure and Characterization	140,000
Polymer Electrolytes for Ambient Temperature Traction Batteries: Molecular Level Modeling for Conductivity Optimization	117,000
Analysis and Simulation of Electrochemical Systems	235,000
Corrosion of Current Collectors in Rechargeable Lithium Batteries	200,000
Electrode Surface Layers	200,000
Modeling of Highly Porous NiMH Battery Substrates	69,000
Device or Component Fabrication, Behavior or Testing	$ 584,000
Development of a Thin-Film Rechargeable Lithium Battery for Electric Vehicles	71,000
Applied Research on Novel Components for Advanced Capacitors	115,000
Sol-Gel Derived Metal Oxides for Electrochemical Capacitors	123,000
Optimization of Metal Hydride Properties in MH/NiOOH Cells for Electric Vehicle Applications	90,000
Preparation of Improved, Low Cost Metal Hydride Electrodes for Automotive Applications	185,000
Fuel Cell Materials	$ 1,400,000
Materials Properties, Behavior, Characterization or Testing	$ 1,400,000
Electrode Kinetics and Electrocatalysis	300,000
Poisoning of Fuel Cell Electrocatalyst Surfaces: NMR Spectroscopic Studies	100,000
Fuel Cells for Renewable Applications	1,000,000
Heavy Vehicle Materials Technology	$11,569,000
Propulsion Systems Materials	$ 9,080,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 6,271,000
Low Cost SRBSN	400,000
Cost Effective Silicon Nitride Powder	0
Continuous Sintering of Silicon Nitride Ceramics	135,000
Low Cost, High Toughness Ceramics	350,000
Characterization/Testing of Low CTE Materials	100,000
Low CTE Materials/Diesel Exhaust Insulation	328,000
Low Cost NZP Powder	433,000
Advanced Manufacturing of Diesel Engine Turborotors	0
Advanced Manufacturing of Ceramic Exhaust Valves for Diesel Engines	0
Insulating Structural Ceramics for High Efficiency, Low Emission Engines	535,000
Thick Thermal Barrier Coatings (TTBCS) for Low Emissions, High Efficiency Diesel Engine Components	723,000

OFFICE OF TRANSPORTATION TECHNOLOGIES (continued)

	FY 1996
Automotive Materials Technology (continued)	
Heavy Vehicle Materials Technology (continued)	
Propulsion Systems Materials (continued)	
Materials Preparation, Synthesis, Deposition, Growth or Forming (continued)	
Advanced Materials for Low Emissions, High Efficiency Diesel Engine Components	1,075,000
Advanced Materials for Low Emissions, High Efficiency Diesel Engine Components	1,075,000
High Strength Materials for Diesel Engine Fuel Injectors	1,117,000
Materials Properties, Behavior, Characterization or Testing	$ 1,130,000
Diesel Exhaust Catalyst Characterization	200,000
Computerized Mechanical Properties Database	240,000
Life Prediction of Ceramic Valves	200,000
High Temperature Tensile Testing	0
Computed Tomography	120,000
Nuclear Magnetic Resonance Imaging	80,000
On-Machine Inspection	200,000
Mechanical Properties of CMZP	90,000
Technology Transfer and Management Coordination	$ 800,000
Technical Project Management	300,000
International Exchange Agreement (IEA)	200,000
Standard Reference Materials	200,000
Mechanical Property Standardization	100,000
Device or Component Fabrication, Behavior or Testing	$ 879,000
Thick Thermal Barrier Seal Coatings	30,000
Characterization of Machined Ceramics	200,000
Next-Generation Grinding Wheel	0
Chemically Assisted Grinding of Ceramics	150,000
High Speed Grinding	0
Laser-Based NDE Methods	0
Grinding Machine Stiffness	0
Next Generation Grinding Spindle	0
Process Cost Model	0
Intelligent Grinding Wheel	499,000
High Strength Weight Reduction Materials	$ 2,489,000
Materials Properties, Behavior, Characterization or Testing	$ 695,000
Modeling of Transportation Materials Requirements and Physical Metallurgy of Magnesium	595,000
Study of Bonding Interfaces Between Reinforcing Materials and Cast Aluminum Alloy	100,000

OFFICE OF TRANSPORTATION TECHNOLOGIES (continued)

	FY 1996
Automotive Materials Technology (continued)	
Heavy Vehicle Materials Technology (continued)	
High Strength Weight Reduction Materials (continued)	
Device or Component Fabrication, Behavior or Testing	$ 1,794,000
Development of a Casting Process for Ultralarge Heavy Vehicle Components	1,444,000
Metal Compression Forming of Aluminum Alloys and Metal Matrix Composites	350,000

OFFICE OF TRANSPORTATION TECHNOLOGIES

The Office of Transportation Technologies seeks to develop, in cooperation with industry, advanced technologies that will enable the U.S. transportation sector to be energy efficient, shift to alternative fuels and electricity, and minimize the environmental impacts of transportation energy use. Timely availability of new materials and materials manufacturing technologies is critical for the development and engineering of these advanced transportation technologies. Materials research and development are conducted by the Office of Advanced Automotive Technologies (OAAT) and the Office of Heavy Vehicle Technologies to address critical needs of automobiles and heavy vehicles, respectively. Materials R&D activities are closely coordinated between the two offices to ensure non-duplication of efforts. Another important aspect of these activities is the partnership between the Federal government laboratories and U.S. industry, which ensures that the R&D is relevant and that federal research dollars are highly leveraged.

Within OAAT, materials R&D is carried out through the **Automotive Materials Technology** program, the **Advanced Battery Systems Program**, and the **Fuel Cell Systems Program**. The **Automotive Materials Technology** program develops: (a) ***Propulsion System Materials*** to enable advanced propulsion systems for hybrid vehicles, and (b) ***Lightweight Vehicle Materials*** to reduce vehicle weight and thereby decrease fuel consumption. The program seeks to develop advanced materials with the required properties and the processes needed to produce them at the costs and volumes needed by the automotive industries. Improved materials for body, chassis, and powertrain are critical to attaining the challenging performance standards for advanced automotive vehicles. The DOE contacts are Debbie Haught, (202) 586-2211, for automotive propulsion system materials and Toni Maréchaux, (202) 586-8501, for automotive lightweight vehicle materials. The **Advanced Battery Program** supports the development of rechargeable batteries and ultracapacitors for electric and hybrid vehicle applications. The DOE contact is Albert Landgrebe, (202) 586-1483. The OAAT **Fuel Cell Program** includes R&D of materials for proton-exchange membrane (PEM) fuel cells. The DOE contact is JoAnn Milliken, (202) 586-2480.

The **Heavy Vehicle Materials Technology** program focuses on two areas: (a) ***Heavy Vehicle Propulsion System Materials***, and (b) ***High Strength Weight Reduction Materials.*** In collaboration with U.S. industry and universities, efforts in propulsion system materials focus on the materials technology critical to the development of the low emissions, 55 percent efficient (LE-55) heavy-duty and multi-purpose Diesel engines, such as: manufacturing of ceramic and metal components for high-efficiency turbocharger and supercharger; thermal insulation, for reducing engine block cooling, lowering ring-liner friction and reducing wear; high-pressure fuel injection materials; and exhaust aftertreatment catalysts and particulate traps. In the area of high strength weight reduction materials, energy savings from commercial trucking is possible with high strength materials which can reduce the vehicle weight within the existing envelope so as to increase payload capacity, and thereby reducing the number of trucks needed on the highways. Increased safety can be obtained by new brake materials and by incorporating highly shock absorbent materials in truck structures for improved control and crashworthiness. The DOE contacts are Robert Schulz, (202) 586-8051, for heavy vehicle propulsion system materials and Sidney Diamond, (202) 586-8032, for high strength weight reduction materials.

The **High Temperature Materials Laboratory** (HTML) at the Oak Ridge National Laboratory is a modern research facility that houses in its six user centers a unique collection of instruments for characterizing materials. It supports a wide-variety of high-temperature ceramics and metals R & D. The HTML enables scientists and engineers to solve materials problems that limit the efficiency and reliability of advanced energy-conversion systems by providing access to sophisticated state-of-the-art equipment (which few individual companies and institutions can afford to purchase and maintain) and highly trained technical staff. The DOE contact is Robert Schulz, (202) 586-8051.

TRANSPORTATION MATERIALS TECHNOLOGY

AUTOMOTIVE MATERIALS TECHNOLOGY

PROPULSION SYSTEMS MATERIALS

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

38. **GELCASTING: SCALE-UP AND COMMERCIALIZATION**
$650,000
DOE Contact: D. A. Haught, (202) 586-2211
ORNL Contact: D. P. Stinton, (423) 574-4556
ORNL Contact: M. A. Janney, (423) 574-4281

The purpose of this work is to develop gelcasting as an advanced, near-net-shape ceramic forming process capable of manufacturing cost-effective, reliable silicon nitride components for vehicle propulsion systems. This program will address the technical aspects of the gelcasting process, evaluation of the applicability of gelcasting to a wide range of commercially available ceramic powders, and identification and assessment of manufacturing concerns and issues as they relate to commercialization of gelcasting. The emphasis of the program is on gelcasting of silicon nitride ceramics and developing industry acceptance of the process. Issues of practicality and ES&H will be addressed in the program. The technical feasibility of in-process and NDE testing methods for improving quality and reliability of gelcast ceramics will also be addressed.

Keywords: Silicon Nitride, Ceramics, Gelcasting, Forming

39. **OPTIMIZATION OF SILICON NITRIDE CERAMICS**
$175,000
DOE Contact: D. A. Haught, (202) 586-2211
ORNL Contact: D. P. Stinton, (423) 574-4556
University of Michigan Contact: T. Y. Tien, (313) 764-9449

The objective of this investigation is to synthesize silicon nitride ceramics with optimum flexural strength, fracture toughness, and creep resistance by using statistical experimental designs. The sintering conditions and the composition of the sintering additives can affect the microstructure of silicon nitride ceramics and the characteristics of the grain-boundary phase and, hence, the mechanical properties. It is believed that the mechanical properties of silicon nitride can be optimized by controlling the size and aspect ratio of β-Si_3N_4 and the nature of the grain- boundary phase. In a related study to optimize the surface finish of silicon nitride materials, the effect of annealing on bend strength of specimens is being investigated. It is believed that the strength of these materials can be further improved as well if surface grain growth could be prevented by using proper vapor environment during annealing.

Keywords: Physical/Mechanical Properties, Silicon Nitride, Toughened Ceramics

40. **IN-SITU TOUGHENED SILICON NITRIDE**
$150,000
DOE Contact: D. A. Haught, (202) 586-2211
ORNL Contact: T. N. Tiegs, (423) 574-5173
AlliedSignal Ceramic Components Contact: J. M. Wimmer, (310) 512-3183

The purpose of this effort is to develop an extensive property database for AS800 silicon nitride, to improve its high-temperature properties, and to develop advanced fabrication processes to allow this material to be commercialized in a timely manner. This work is being done to address cost and property requirements to accelerate the adoption of AS800 into engines, including hybrid electric vehicles.

Keywords: Physical/Mechanical Properties, Silicon Nitride, Toughened Ceramics

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

41. **ADVANCED STATISTICS CALCULATIONS**
$32,000
DOE Contact: D. A. Haught, (202) 586-2211
ORNL Contact: M. K. Ferber, (423) 576-0818
Contact: S. F. Duffy, (330) 678-7328

This effort has focused on issues relating to parameter estimation of the two- and three-parameter Weibull distribution. The scope includes updating and distributing existing macros, creating macros for Quattro-Pro, creating fractography graphics and updating existing graphics software, and investigating goodness-of-fit statistics to distinguish two-parameter failure populations from three-parameter failure populations.

Keywords: Design Codes, Life Prediction, Statistics, Weibull, Fracture, Structural Ceramics, Mechanical Properties

42. **COMPONENT VERIFICATION**
$290,000
DOE Contact: D. A. Haught, (202) 586-2211
ORNL Contact: D. P. Stinton, (423) 574-4556
ORNL Contact: P. F. Becher, (423) 574-5157

The objective of this effort is to develop test methodology to measure mechanical properties of ceramics from complex-shaped components (e.g., blades, nozzles) at elevated temperatures. This work will allow end-users to verify properties of actual components and allow database generated from simple-shaped specimen to be related to large components and advanced-design capabilities.

Keywords: Silicon Carbide, Silicon Nitride, Toughened Ceramics, Property Characterization

43. **HIGH FREQUENCY FATIGUE**
$220,000
DOE Contact: D. A. Haught, (202) 586-2211
ORNL Contact: D. P. Stinton, (423) 574-4556
ORNL Contact: K. C. Liu, (423) 574-5116

The objective of this task is to develop the baseline information on tensile and cyclic fatigue behavior of structural ceramics at room and elevated temperatures and at frequencies (>1000 Hz) of interest to automotive applications. Material behavior models for ceramic components design and life evaluation analysis are being developed. A benefit of this task will be a baseline database of candidate ceramic materials for use by ceramic materials manufacturers and ceramic components designers, fabricators, and users.

Keywords: Cyclic Fatigue, High Temperature Properties, Toughened Ceramics, Silicon Nitride, Time-Dependent

44. **TENSILE STRESS RUPTURE TESTING**
$300,000
DOE Contact: D. A. Haught, (202) 586-2211
ORNL Contact: D. P. Stinton, (423) 574-4556
ORNL Contact: K. C. Liu, (423) 574-5116

The objective of this task is to develop the baseline information of tensile stress rupture and time-dependent creep behavior of structural ceramics at elevated temperatures in the range of interest to automotive and advanced turbine engine applications. Another goal is to develop material behavior models to facilitate design analysis of high-temperature structural components and improve their reliability.

Keywords: High Temperature Properties, Silicon Nitride, Tensile Testing, Time-Dependent, Toughened Ceramics

45. **CERAMICS LIFE PREDICTION**
$200,000
DOE Contact: D. A. Haught, (202) 586-2211
ORNL Contact: D. P. Stinton, (423) 574-4556
NASA - Lewis Research Center Contact: J. A. Salem, (216) 433-3313

The objective of this research is to develop and verify models and test methods for life prediction of brittle materials such as *in situ* toughened ceramics, glasses, and intermetallics. The slow-crack-growth module of the CARES/LIFE code is being verified. Mixed-mode loading of precracked specimens are being performed in order to determine the significance of shear on two-dimensional machining cracks in lifetime prediction. On completion of the CARES/CREEP model, elevated temperature tensile, flexural, and biaxial testing of alumina will be performed in order to verify the code.

Keywords: Creep, Fracture Toughness, High Temperature Properties, Life Prediction, Silicon Nitride, Time-Dependent, Toughened Ceramics

46. **LIFE PREDICTION METHODOLOGY**
$0
DOE Contact: D. A. Haught, (202) 586-2211
ORNL Contact: C. R. Brinkman, (423) 574-5106
AlliedSignal Engines Contact: N. Menon, (602) 231-1230

The objective of this effort is to develop methodologies required to adequately predict the useful life of ceramic components in advanced heat engines. The Erica and Ceramic computer codes are being updated and verified via extensive mechanical property characterization, at ambient and high temperatures, of uni-and-multiaxial test specimens of AS800 silicon nitride.

Keywords: Creep, Failure Analysis, Failure Testing, Life Prediction, Nondestructive Evaluation, Silicon Nitride, Time-Dependent

47. **MECHANICAL BEHAVIOR OF GAS TURBINE CERAMICS**
$385,000
DOE Contact: D. A. Haught, (202) 586-2211
ORNL Contact: M. K. Ferber, (423) 576-0818
University of Dayton Contact: N. L. Hecht, (513) 229-4341

The objective of this task is to develop a database on mechanical behavior of existing and emerging ceramic materials for gas turbine applications. The fast fracture and time-dependent (dynamic fatigue and stress rupture) properties of AS800 and SN282 silicon nitride are being determined in tension and bending.

Keywords: Environmental Effects, Fatigue, Structural Ceramics, Tensile Testing, Time-Dependent

48. **UTRASONIC NDE DEVELOPMENT**
$335,000
DOE Contact: D. A. Haught, (202) 586-2211
ORNL Contact: D. P. Stinton, (423) 574-4556
ORNL Contact: W. A. Simpson, Jr., (423) 574-4421

The objective of this program is to develop nondestructive evaluation techniques capable of detecting critical flaws in structural ceramic components. Acoustic nonlinearity is being used to monitor the initial microstructural state of structural ceramics and to assess changes in that state as a function of in-service degradation. This approach appears sensitive to changes occurring at the lattice level (dislocations, vacancies, microcracking, etc.) and may provide a means of detecting early-stage (i.e., incipient) degradation. In addition, advanced techniques are being developed to detect and characterize critical flaws of particular interest to the ceramic community, i.e. surface and near-surface flaws.

Keywords: NDE, Structural Ceramics, Ultrasonics

TECHNOLOGY TRANSFER AND MANAGEMENT COORDINATION

49. **TECHNICAL PROJECT MANAGEMENT**
$300,000
DOE Contact: D. A. Haught, (202) 586-2211
ORNL Contact: D. P. Stinton, (423) 574-4556

The objective of this effort is to assess the ceramic technology needs for advanced automotive heat engines, formulate technical plans to meet these needs, and prioritize and implement a long-range research and development program.

Keywords: Advanced Heat Engines, Coordination, Management, Structural Ceramics

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

50. **CORROSION-RESISTANT COATINGS**
$175,000
DOE Contact: D. A. Haught, (202) 586-2211
ORNL Contact: D. P. Stinton, (423) 574-4556
ORNL Contact: W. Y. Lee, (423) 576-2894

The objective of this research program is to develop a coating system that will protect Si_3N_4 ceramics from hot corrosion. The corrosion behavior of candidate coating materials has been examined in both bulk and coating forms. Our study has indicated that mullite ($3Al_2O_3 \cdot 2SiO_2$) prepared by chemical vapor deposition (CVD) is an appropriate coating material. The materials and processing issues relating to the development of a thermochemically stable as well as thermomechanically durable mullite coating have been investigated by a team of researchers at Oak Ridge National Laboratory, AlliedSignal Engines, and Boston University.

Keywords: Coatings, Chemical Vapor Deposition, CVD, Engines, Silicon Carbide, Silicon Nitride, Structural Ceramics, Corrosion Resistance, Mullite

51. **CERAMIC-METAL JOINING**
$220,000
DOE Contact: D. A. Haught, (202) 586-2211
ORNL Contact: D.P. Stinton, (423) 574-4556
ORNL Contact: M. L. Santella, (423) 574-4805

The objective of this task is to develop joining technology for silicon nitride to metal alloys and silicon nitride to silicon nitride for gas turbine hot section applications. Experiments are being done to identify and understand the effects of chemical reactions that occur during active metal brazing on the mechanical properties of silicon nitride. A collaborative effort to study the technical issues relevant to attaching silicon nitride turbine rotors to metal shafts is being conducted with Teledyne Ryan.

Keywords: Brazing, Joining/Welding, Metals, Structural Ceramics, Silicon Carbide, Silicon Nitride

LIGHTWEIGHT VEHICLE MATERIALS

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

52. **LOW-COST HIGH PERFORMANCE ALUMINUM ALLOY SHEET FOR AUTOMOTIVE APPLICATIONS**
$3,500,000
DOE Contact: Toni Maréchaux, (202) 586-8501
ORNL Contact: Phil Sklad, (423) 574-5069
Laboratory Partners: ORNL, LANL, INEL, PNNL
Industry Partners: Alcoa, USAMP, Rockwell, University of Michigan, Michigan Technological University (MTI), University of Stuttgart (IFU), Erie Press Systems, Troy Design and Manufacturing, Imageware, AutoDie International, Advanced Technology Associates, Wyman Gordon, Uiversal Energy Systems, Reynolds Metals Company, American Society of Mechanical Engineers (ASME), Commonwealth Aluminum, ARCO Aluminum, Ravenswood Aluminum

The objectives of this project are: to evaluate and improve aluminum forming processes including conventional press forming, integral extruded forming, and warm forming for automotive applications; to develop and implement low-cost continuous casting technologies for production of high-quality aluminum sheet; and to develop a non-heat treatable aluminum alloy sheet product for automotive applications, such as exterior body panels or structural components, which combines resistance to stress corrosion cracking with strength, formability, joinability, and surface appearance similar to current compositions requiring heat treatment for full property development.

Keywords: Aluminum, Sheet Forming, Extrusion, Automotive

53. **LOW-COST HIGH PERFORMANCE CAST LIGHT METALS FOR AUTOMOTIVE APPLICATIONS**
$1,700,000
DOE Contact: Toni Maréchaux, (202) 586-8501
ORNL Contact: Phil Sklad, (423) 574-5069
Laboratory Partners: LLNL, ORNL, SNL, INEL
Industry Partners: USAMP (Ford, GM, Chrysler)

The objectives of this effort are: to optimize design knowledge and improve product capability for light-weight, high-strength, cast structural components; to develop a method for producing prototype tools for lightweight metals in metal mold processes such as die casting, injection molding, and stamping, which are cheaper and faster to produce than those currently used for production; and to develop a process to produce particulate reinforced aluminum via powder metallurgy techniques.

Keywords: Aluminum, Magnesium, Cast Metals, Powder Metallurgy, MMC, Rapid Prototyping, Automotive

54. **LOW-COST HIGH PERFORMANCE FIBER REINFORCED POLYMER COMPOSITES**
$3,200,000
DOE Contact: Toni Maréchaux, (202) 586-8501
ORNL Contact: Dave Warren, (423) 574-9693
Laboratory Partners: ORNL, INEL, LBNL
Industry Partners: USAMP/Automotive Composites Consortium, The University of Texas at Austin, The Budd Company

The objective of this effort is to develop Mode I, II, and Mixed Mode Fracture computer-based models for use by the domestic automotive industry. This work includes the characterization of bulk adhesives, sheet composite, and adhesive-adherend pairs using one composite adherend and two adhesives (epoxy and urethane). Models are to simulate the fracture behavior of bonded joints under a wide range of mode mixes. Develop experimentally-based, durability-driven design guidelines to assure the long-term (15 year) integrity of polymeric composite automotive structures. Develop and demonstrate reliable attachment technologies for use in lightweight composite structures for automotive applications. Develop industry standard adhesive joint test methods. Include bulk material characterization, fracture, fatigue, creep, and creep fracture. Develop NDE methods, advanced curing technologies and input for structural analysis models. Provide support for Focal Projects. Develop and model slurry preforming processes applicable to the automotive industry. After initial development, optimize the processes for repeatabilty of glass fiber positioning at increased production rates. Assisting implementation of the technology in ACC focal projects. Develop NDE technology to evaluate bonded joint integrity of automotive assemblies, such as a body-in-white.

Keywords: Polymer, Composites, Joining, Fracture, Durability, Preforming, Automotive

55. **USAMP COOPERATIVE AGREEMENT**
$3,000,000
DOE Contact: Toni Maréchaux, (202) 586-8501
ORO Contact: Harold Clark, (423) 576-0823
Industry Partner: US Automotive Materials Partnership (Chrysler, Ford, GM)

The objectives of this project are to define and conduct vehicle related R&D in materials and materials processing. Projects include Rapid Prototyping for Metal Mold Processes, Design and Product Optimization for Cast Light Metals, Powder Metallurgy of Particle Reinforced Aluminum, Non-Toxic Free Machining Steel, Slurry Process Scale-up, P4 Preforming, and Full Field NDT of Adhesive Bonding. Projects will be conducted by multi-organizational teams involving USAMP members, automotive suppliers, universities, and private research institutions.

Keywords: Polymer Composites, Aluminum, Magnesium, Free Machining Steel, Glass Fiber Preforming, Adhesive Bonding, Slurry Preforming, Powder Metallurgy, MMC, Rapid Prototyping, NDT, Automotive

ADVANCED BATTERY MATERIALS

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

56. **ADVANCED ELECTRODE RESEARCH**
$300,000
DOE Contact: Albert Landgrebe, (202) 586-1483
Lawrence Berkeley National Laboratory Contact: E. J. Cairns, (510) 486-5028

The objective of this project is to investigate the behavior of S electrodes in Li/polymer electrolyte/sulfur cells and improve their lifetime and performance. Interest in the Li/S couple stems from its high theoretical specific energy (~2600 Wh/kg) as well as its environmentally benign components. In principle, this system is well-suited to EV applications, however a practical Li/S battery showing promise for EVs has not beendeveloped. Modeling studies indicated that smaller

S particles are needed to improve the S utilization in the electrode.

Keywords: Batteries, Solid-State Cells, Electric Vehicles, Sulfur Electrode

57. **ELECTROCHEMICAL PROPERTIES OF SOLID ELECTROLYTES**
$200,000
DOE Contact: Albert Landgrebe, (202) 586-1483
Lawrence Berkeley National Laboratory Contact: L. C. De Jonghe, (510) 486-6138

The objective of this project is to fabricate and study novel composite electrolytes which combine the advantages of a protective thin-film single-ion conductor with a conventional elastomeric polymer electrolyte for EV applications. Synthesis of montmorillonite-PEO nanocomposites is also underway to form Li-ion conducting polymer electrolytes. X-ray diffraction was used to determine the inter-layer spacings; an increase in 00l d-spacings to about 0.74 nm indicates that poly(ethylene) oxide has been inserted between the alumino-silicate layers.

Keywords: Batteries, Solid-State Cells, Electric Vehicles, Polymeric Electrolytes

58. **PREPARATION AND CHARACTERIZATION OF NEW POLYMER ELECTROLYTES**
$210,000
DOE Contact: Albert Landgrebe, (202) 586-1483
Lawrence Berkeley National Laboratory Contact: J. Kerr, (510) 486-6279

The objectives of this project are to develop methods of preparation and purification of the comb-branch backbone structures to design new polymers for rapid ion transport in batteries and to measure lithium ion transference numbers as a function of polymer and Li salt structure. New initiative in FY 1997.

Keywords: Batteries, Solid-State Cells, Electric Vehicles, Polymeric Electrolytes

59. **NEW CATHODE MATERIALS**
$73,000
DOE Contact: Albert Landgrebe, (202) 586-1483
State University of New York Contact: M. S. Whittingham, (607) 777-4623

The objective of this project is to synthesize and evaluate oxides of tungsten, molybdenum, and first-row transition metals for alkali-metal intercalation electrodes which are useful as positive electrodes in advanced nonaqueous rechargeable batteries. Mild hydrothermal techniques are used for the synthesis of metal oxides. The mild hydrothermal aqueous decomposition reaction of potassium permanganate at 170C produce a layered structure. Electrochemical intercalation and deintercalation of lithium into the dehydrated potassium manganese oxide lattice shows a continuous curve indicative of single phase behavior.

Keywords: Intercalation Electrodes, Rechargeable Batteries

60. **STRUCTURAL STUDIES OF LITHIATED TRANSTION-METAL OXIDES**
$100,000
DOE Contact: Albert Landgrebe, (202) 586-1483
Deleware State University Contact: K. Wheeler, (302) 739-4934

The objective of this project is to investigate the mechanism of lithium intercalation of transition metal oxides for rechargeable lithium batteries by X-ray diffraction analysis. New initiative in FY 1997.

Keywords: Intercalation Electrodes, Rechargeable Batteries

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

61. **CARBON ELECTROCHEMISTRY**
$250,000
DOE Contact: Albert Landgrebe, (202) 586-1483
Lawrence Berkeley National Laboratory Contact: K. Kinoshita, (510) 486-7389

The objective of this project is to identify the critical parameters that control the reversible intercalation of Li in carbonaceous materials and to determine their maximum capacity for Li intercalation. This effort is coordinated with the research conducted at LLNL to evaluate the intercalation of Li in carbonaceous materials for rechargeable Li batteries. Samples obtained from commercial vendors, as well as several that were synthesized in-house, were systematically studied by utilizing electron microscopy (facilities at the National Center for Electron Microscopy) and X-Ray diffraction analysis. The results to date show that graphite powders, both natural and synthetic, which have d(002) spacing of 0.3354 nm, yield the theoretical capacity for Li intercalation, LiC_6.

Keywords: Carbon, Li Batteries, Li intercalation

62. **FABRICATION AND TESTING OF CARBON ELECTRODES AS LITHIUM INTERCALATION ANODES**
$75,000
DOE Contact: Albert Landgrebe, (202) 586-1483
Lawrence Livermore National Laboratory Contact: T. Tran, (510) 422-0915

The objectives of this work are to evaluate the performance of carbonaceous materials as hosts for lithium intercalation negative electrodes, and to develop reversible lithium intercalation negative electrodes for advanced rechargeable lithium batteries. The approach is to fabricate electrodes from various commercial carbons and graphites and evaluate them in small lithium-ion cells. Electrode performance will be correlated with carbon structure and properties in collaboration with LBNL. Electrodes fabricated from natural vein graphites (Superior Graphite Co.) yielded Li intercalation capacities that range from 320 to 360 mAh/g (equivalent to x in Li_xC_6 from 0.85 to 0.95), approaching the theoretical value of 372 mAh/g corresponding to LiC_6. Natural-flake and purified-flake graphites tend to have a lower capacity than the LiC_6 composition. Graphitized cokes from Superior Graphite exhibited reversible capacities of about 230 mAh/g (x near 0.62), comparable to that obtained with petroleum cokes from other sources.

Keywords: Carbon, Li Batteries, Intercalation

63. **BATTERY MATERIALS: STRUCTURE AND CHARACTERIZATION**
$140,000
DOE Contact: Albert Landgrebe, (202) 586-1483
Brookhaven National Laboratory Contact: J. McBreen, (516) 282-4071

The objective of this research is to elucidate the molecular aspects of materials and electrode processes in batteries and to use this information to develop electrode and electrolyte structures with good performance and long life. Current efforts have included *in situ* extended X-ray absorption fine structure (EXAFS) studies of Bi-doped manganese oxides and *ex situ* studies of lithium manganese oxides and nickel oxide electrodes that were cycled in Zn/NiOOH cells. An apparatus was set up for *in situ* high resolution XRD studies of battery electrodes. EXAFS shows that the structure of supersaturated zincate is identical to regular zincate solutions. XANES indicates ion pairing of zincate with the lighter alkali ions (Li^+ and Na^+). EXAFS shows that complete removal of Li from Li_xNiO_2 eliminates the long range order in the crystal.

Keywords: Electrodes, Batteries, EXAFS

64. **POLYMER ELECTROLYTES FOR AMBIENT TEMPERATURE TRACTION BATTERIES: MOLECULAR LEVEL MODELING FOR CONDUCTIVITY OPTIMIZATION**
$117,000
DOE Contact: Albert Landgrebe, (202) 586-1483
Northwestern University Contact: M. A. Ratner, (708) 491-5371

The goal of this research is to apply molecular dynamics (MD) and Monte Carlo simulations to understand the conduction process in polymer electrolytes, and its modification by such parameters as temperature, density, ion species, polymer chain basicity, and interionic correlations, The results of this study should be beneficial in the development of improved polymer electrolytes for rechargeable Li batteries for EV applications. It was demonstrated conclusively using hopping models within a relaxing environment that polymer electrolytes will generally exhibit higher mobilities than polyelectrolytes, although the transference properties are less attractive. A novel cluster analysis method showed that although few free ions exist in concentrated polymer electrolytes, modified single particle motions remain responsible for conduction.

Keywords: Batteries, Electric Vehicles, Polymeric Electrolytes

65. **ANALYSIS AND SIMULATION OF ELECTROCHEMICAL SYSTEMS**
$235,000
DOE Contact: Albert Landgrebe, (202) 586-1483
University of California, Berkeley Contact: J. Newman, (510) 642-4063

The objective of this program is to improve the performance of electrochemical cells used in the interconversion of electrical energy and chemical energy by identifying the phenomena which control the performance of a system. These phenomena are incorporated into a mathematical model which can predict system behavior. The models aid in the recognition of important parameters that are crucial to the optimization of a given electrochemical system. Mathematical models have been developed to explore the design and optimization of lithium and lithium-ion batteries, the discharge behavior of nickel oxide/KOH/ $LaNi_5$ battery systems and electrochemical capacitors, based on pseudohomogeneous porous-electrode theory.

Keywords: Electrochemical Phenomena, Galvanostatic Charge/Discharge

66. **CORROSION OF CURRENT COLLECTORS IN RECHARGEABLE LITHIUM BATTERIES**
$200,000
DOE Contact: Albert Landgrebe, (202) 586-1483
University of California, Berkeley Contact:
J. W. Evans, (510) 642-3807

The objective of this research is to investigate the corrosion behavior of current collectors for rechargeable Li batteries. Ion-implantation of tungsten was used to improve the corrosion resistance of Al current collectors. SEM studies of W-implanted Al after normal and overcharge operation in a Li/V oxide cell did not show evidence of pitting. This finding suggests that W-implanted Al alloys have higher corrosion resistance than Al in current collectors.

Keywords: Current Collectors, Advanced Batteries

67. **ELECTRODE SURFACE LAYERS**
$200,000
DOE Contact: Albert Landgrebe, (202) 586-1483
Lawrence Berkeley National Laboratory Contact:
F. R. McLarnon, (510) 486-4636

Advanced *in situ* and *ex situ* characterization techniques are being used to study the structure, composition, and mode of formation of surface layers on electrodes used in rechargeable batteries. The objective of this research is to identify film properties that improve the rechargeability, cycle-life performance, specific power, specific energy, stability, and energy efficiency of electrochemical cells. Sensitive techniques such as ellipsometry, light scattering, Raman spectroscopy and scanning electron microscopy are utilized to monitor the formation of surface layers on secondary battery electrodes. In addition, foreign ions are incorporated in porous nickel electrodes to improve the cycle performance in an alkaline electrolyte. The co-precipitation of Co^{2+} ions into the $Ni/Ni(OH)_2$ electrode reduced the drop in charge efficiency to ~25% after long-term cycling, compared to ~50% drop in electrodes without Co. Low-energy ion implantation and plasma-assisted deposition was used to form compact and homogeneous nitrided lithium surface layers on a Li electrode surface. SEM images of as-grown nitrided Li surfaces showed island structures with characteristic sizes of ~20 µm, and no macroscopic cracks or other inhomogeneities were detected. Preliminary tests with unoptimized electrodes clearly demonstrate the beneficial effects of using protective Li_3N layers in rechargeable cells with liquid organic electrolytes.

Keywords: Ion Implantation, Electrodes, Rechargeable Batteries

68. **MODELING OF HIGHLY POROUS NiMH BATTERY SUBSTRATES**
$69,000
DOE Contact: Albert Landgrebe, (202) 586-1483
University of Michigan Contact: Ann Marie Sastry,
(313) 764-3061

The objective of this research is to develop predictive capability for determining performance of MH/NiOOH secondary cells through microstructural modeling of the NiOOH electrode. These studies should lead to improved energy densities in MH/NiOOH batteries by determining optimal microstructures for NiOOH substrates. The study is focused on the effects of the microstructure of fibrous composite electrodes on thermal and electrical conductivity, strength, and lifetime. Materials under study are comprised of a variety of fibers, including carbon (7-12 mm diameter) and polypropylene (~10 mm diameter) fibers, both coated with nickel and sinter-bonded, and pure sinter-bonded nickel fibers. A technique for calculating both local and continuum elastic properties has been established, and significant differences between the local properties and those predicted by classic approaches have been identified.

Keywords: MH/NIOOH Batteries, Modeling, Microstructural Characterization

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

69. **DEVELOPMENT OF A THIN-FILM RECHARGEABLE LITHIUM BATTERY FOR ELECTRIC VEHICLES**
$71,000
DOE Contact: Albert Landgrebe, (202) 586-1483
Oak Ridge National Laboratory Contact:
J. B. Bates, (615) 574-4143

The objective of this research is to identify methods for depositing acceptable thin-film electrodes for rechargeable Li batteries. These methods are being applied to develop solid-state $Li/Li_xMn_2O_4$ rechargeable thin-film Li batteries for EV applications. The batteries are expected to have several important advantages as power sources: high specific energy and energy density, long cycle lifetimes, and a wide temperature range of operation. $Li/Li_xMn_2O_4$ cathodes were fabricated at temperatures below 180°C by rf magnetron and assembled in 4 V thin-film solid-state Li cells. The shape of the constant-current discharge curves indicate that the cathode films deposited on substrates at 100°C were not fully stable. Cycling results have also shown evidence of a true hysteresis in the lithium insertion reaction.

Keywords: Electric Vehicles, Thin-Film Batteries, Solid-State Electrodes

70. **APPLIED RESEARCH ON NOVEL CELL COMPONENTS FOR ADVANCED CAPACITORS**
$115,000
DOE Contact: Albert Landgrebe, (202) 586-1483
SAFT Research & Development Center Contact: Guy Chagnon, (410) 771-3200

The objective of this research is to evaluate the double-layer capacitance of high-surface-area carbons, and to develop low-cost carbon electrodes for electrochemical double-layer capacitors that meet the DOE goal of 1600 W/kg, 10 Wh/kg and $1/kW. Coin-size capacitors fabricated with active carbons achieved 4.8 Wh/kg, 4.1 kW/kg. These cells were submitted to INEL for evaluation.

Keywords: Electrochemical Capacitors, Carbon Electrodes

71. **SOL-GEL DERIVED METAL OXIDES FOR ELECTROCHEMICAL CAPACITORS**
$123,000
DOE Contact: Albert Landgrebe, (202) 586-1483
University of Wisconsin - Madison Contact: Marc A. Anderson, (608) 262-2470

The objective of this research is to improve the chemical and materials properties of the NiO/Ni system for electrochemical capacitors (ultracapacitors). The specific capacitance of NiO/Ni electrodes in 1 M LiOH was as high as 120 F/g of active material per cell, double the value obtrained in 1 M KOH. These cells were submitted to INEL for evaluation.

Keywords: Electrochemical Capacitors, NiO Electrodes

72. **OPTIMIZATION OF METAL HYDRIDE PROPERTIES IN MH/NiOOH CELLS FOR ELECTRIC VEHICLE APPLICATIONS**
$90,000
DOE Contact: Albert Landgrebe, (202) 586-1483
University of South Carolina Contact: R. E. White, (803) 777-7314

The objective of this research is to optimize the alloy composition of metal hydride electrodes by microencapsulation of hydrogen storage alloys for MH/NiOOH batteries. The polarization resistance of a copper-coated $LaNi_{4.27}Sn_{0.24}$ alloy was found to be lower when compared with the corresponding resistance estimated for the bare alloy for the same state of charge. Galvanostatic discharge curves were used to estimate the hydrogen diffusion coefficient. For an average particle radius a =15 mm, the effective diffusion coefficient through $LaNi_{4.27}Sn_{0.24}$ was calculated to be 6.75x10 cm^2/s.

Keywords: MH/NiOOH Batteries, Hydrogen Storage, $LaNi_{4.27}Sn_{0.24}$ Alloy, Microencapsulation

73. **PREPARATION OF IMPROVED, LOW COST METAL HYDRIDE ELECTRODES FOR AUTOMOTIVE APPLICATIONS**
$185,000
DOE Contact: Albert Landgrebe, (202) 586-1483
Brookhaven National Laboratory Contact: J. Reilly, (516) 344-4502

The objective of this research is to increase the energy density of metal hydride electrodes for MH/NiOOH batteries by preparing improved AB_5 and AB_2 electrodes. A second objective is to develop improved mathematical model for the electrochemical behavior of the MH_x electrode.The thermodynamic properties of two hydride alloys were determined and related to their performance as electrodes. X-ray absorption spectroscopy (XAS) studies of AB_2 alloy hydrides indicated the presence of strong interactions between the interstitial H atom and Ti, V and Zr. Very little interaction between H and Ni was observed, suggesting that the role of Ni in the AB_2 alloys is primarily catalytic in nature.

Keywords: MH/NiOOH Batteries, AB_5 and AB_2 Electrodes, Hydrogen Storage, X-Ray Absorption Spectroscopy

FUEL CELL MATERIALS

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

74. **ELECTRODE KINETICS AND ELECTROCATALYSIS**
$300,000
DOE Contact: JoAnn Milliken, (202) 586-2480
Lawrence Berkeley National Laboratory Contact: P. N. Ross, (510) 486-6226

Physically meaningful mechanistic models are essential for the interpretation of electrode behavior and are useful in directing the research on new classes of materials for electrochemical energy conversion and storage devices. The objective of this project is to develop an atomic-level understanding of the processes taking place in complex electrochemical reactions at electrode surfaces. Researchers are employing low energy electron diffraction (LEED) to study single crystals; high resolution electron microscopy (HREM) for carbon electrode materials; and X-ray absoption fine structure (EXAFS) for organometallic catalysts. Low Energy Ion Scattering (LEIS) and Auger Electron Spectroscopy (AES) are being utilized to study the composition of sputtered and UHV-annealed polycrystalline Pt-Ru bulk alloys for methanol electrocatalysis. It was found that both the structure sensitivity and the high catalytic activity of the Pt_3Sn surface to CO oxidation is attributed to an adsorbed state of CO unique to this alloy and occurs at relatively high coverage on the (111) surface.

Keywords: Spectrographic Analysis, Electrocatalysts, Electrooxidation

75. **POISONING OF FUEL CELL ELECTROCATALYST SURFACES: NMR SPECTROSCOPIC STUDIES**
$100,000
DOE Contact: JoAnn Milliken, (202) 586-2480
Lawrence Berkeley National Laboratory Contact: E. J. Cairns, (510) 486-5028

Platinum is the most active single-component catalyst for CH_3OH electrooxidation in DMFCs; however, poisoning reactions at the surface render the anode ineffective under target operation conditions. The objective of this research is to obtain information on the nature of the poisoning intermediate(s) in CH_3OH electrooxidation on Pt-based electrocatalysts by NMR. A glass 3-electrode electrochemical cell for use in a narrow-bore (5 cm) spectrometer operating at a proton frequency of 270 MHz was fabricated. The ^{13}C NMR signal arising from ^{13}CO adsorbed on the electrodes under open-circuit conditions was detected.

Keywords: NMR, Electrooxidation, Fuel Cells

76. **FUEL CELLS FOR RENEWABLE APPLICATIONS**
$1,000,000
DOE Contact: Robert B. Schulz, (202) 586-8051

Project description currently unavailable.

HEAVY VEHICLE MATERIALS TECHNOLOGY

PROPULSION SYSTEMS MATERIALS

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

77. **LOW COST SRBSN**
$400,000
ORNL Contact: D. R. Johnson, (423) 576-6832
ORNL Contact: T. N. Tiegs, (423) 574-5173

There are two major objectives of this research element: the first objective is the development of new sintered reaction-bonded silicon nitride materials that will serve as cost-effective materials for use in suitable applications; the second is the investigation of properties of dense silicon nitride materials annealed in the microwave furnace. Primary investigations have shown that microwave annealing of dense silicon nitride materials results in improved high-temperature creep properties in these materials. This study seeks to find the reasons for these improved properties.

Keywords: Annealing, Cost Effective Ceramics, Microwave Processing, Microwave Sintering, Silicon Nitride, SRBSN

78. **COST EFFECTIVE SILICON NITRIDE POWDER**
$0
DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: S. G. Winslow, (423) 574-0965
Dow Contact: G. A. Eisman, (517) 638-7864

The objective of this program was to further advance the carbothermal nitridation process for producing silicon nitride powder developed under Phase I by focusing on issues relating to the overall cost of manufacturing the powder. Phase II tasks were designed to: (1) determine feasibility of using low-cost raw materials and their impact on the final product quality; (2) reduce processing costs; and (3) characterize, process, fabricate MOR test specimens, and evaluate the mechanical properties of the lower cost powder. A powder which met project goals was developed.

Keywords: Cost Effective Ceramics, Silicon Nitride, Powder Synthesis, Powder Characterization

79. **CONTINUOUS SINTERING OF SILICON NITRIDE CERAMICS**
$135,000
DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: T. N. Tiegs, (423) 574-5173
Southern Illinois University Contact: D. E. Wittmer, (618) 453-7006/7924

The objective of this effort is to investigate the potential of cost-effective sintering of Si_3N_4 through the development of continuous sintering techniques and the use of lower cost Si_3N_4 powders and sintering aids.

Keywords: Cost Effective Ceramics, Silicon Nitride, Sintering

80. **LOW COST, HIGH TOUGHNESS CERAMICS**
$350,000
DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. R. Johnson, (423) 576-6832
ORNL Contact: T. N. Tiegs, (423) 574-5173

In silicon nitride, acicular or elongated grains can be generated by in situ growth and these can provide significant toughening on the same order as the whisker-toughened materials.

Microstructural development to promote growth of in situ toughened microstructures in silicon nitride is the current emphasis of this project.

Keywords: Alumina, Composites, Silicon Carbide, SiAlON, Toughened Ceramics

81. **CHARACTERIZATION/TESTING OF LOW CTE MATERIALS**
$100,000
DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. R. Johnson, (423) 576-6832
ORNL Contact: D. P. Stinton, (423) 574-4556

Insulated exhaust portliners are needed in advanced diesel engines to increase engine fuel efficiency by increasing the combustion temperatures and reducing the combustion heat that is lost through the head and into the water cooling system. Low-expansion materials have potential for this application due to their very low thermal conductivity, extraordinary thermal-shock resistance, and reduction of attachment stresses. Thermal-shock resistance is critical because the shape of the portliners requires that they be cast into the metallic cylinder head. Functioning exhaust portliners are inaccessible after they are cast into cylinder heads and, hence, must not require maintenance for the life of the head (~1 million miles). A contract has been placed with LoTEC to develop cost-effective processes for the fabrication of the portliners. LoTEC is investigating $Ba_{1+x}Zr_4P_{6-2x}Si_{2x}O_{24}$ (BaZPS) and $Ca_{1-x}Sr_xZr_4P_6O_{24}$. ORNL is assisting with the characterization and evaluation of the LoTEC compositions.

Keywords: Physical/Mechanical Properties, Structural Ceramics, Ultra-low Expansion, Zirconia

82. **LOW CTE MATERIALS/DIESEL EXHAUST INSULATION**
$328,000
DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D.R. Johnson, (423) 576-6832
LoTEC, Inc. Contact: Santosh Limaye, (801) 277-6940

The overall objective of this effort is to develop sodium-zirconium-phosphate (NZP) ceramic-based, "cast-in-place," diesel-engine portliners. Specific objectives are: (1) development and optimization of the overall insulation system, (2) refinement of the compliant layer formation process around the ceramic insulation system, (3) development and adaptation of cost-effective powder and material fabrication processes, and (4) creation of a database of high-temperature properties (stability in diesel exhaust environment, thermal cycling, thermal shock, etc.). LoTEC will continue to develop and scale up production of sodium-zirconium-phosphate (NZP) materials developed at Penn State University.

Keywords: Structural Ceramics, Ultra-low Expansion, Zirconia

83. **LOW COST NZP POWDER**
$433,000
DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D.R. Johnson, (423) 576-6832
LoTEC, Inc. Contact: Santosh Limaye, (801) 277-6940

The overall objective of this work is to develop a suitable technology for low-cost synthesis and processing of NZP materials. The two NZP materials of primary interest are BS-25 ($Ba_{1.25}Zr_4Si_{0.5}P_{5.5}O_{24}$) and CS-50 ($Ca_{0.5}Sr_{0.5}Zr_4P_6O_{24}$). Specific objectives to be accomplished are: (1) preliminary assessment of powder techniques of specialist vendors for cost-effective NZP powder synthesis; (2) evaluation of NZP powder samples for phase and impurity content, particle size and distribution, surface area, thermal stability, dispersability, flowability, sinterability after green forming, and synthesis costs; (3) selection of up to two finalist powder suppliers based on results of initial evaluation, commercial viability of the process, and scale-up costs; (4) advanced evaluation of powders supplied by two companies based on results of material properties testing such as thermal expansion, strength, elastic modulus, etc.; and (5) metal-casting trials involving NZP prototype parts and testing of the prototypes for diesel-engine worthiness. A secondary objective will be to set up a hydrothermal (or other) low-cost powder synthesis facility at LoTEC as a parallel effort.

Keywords: Powder Characterization, Powders, Structural Ceramics, Ultra-low Expansion, Zirconia

84. **ADVANCED MANUFACTURING OF DIESEL ENGINE TURBOROTORS**
$0
DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. R. Johnson, (423) 576-6832
Kyocera Contact: E. Kraft, (206) 750-6147

The objective of this program is to develop the cost-effective manufacturing technology required for ceramic turbine rotors for use in turbochargers for heavy duty diesel truck and bus applications. A team, led by Kyocera and including Schwitzer U.S., Inc. and Caterpillar Inc., will develop and demonstrate production readiness for reliable, cost affordable, turbochargers with ceramic turborotors. Program goals include a nominal order of magnitude reduction in cost over the present cost for small quantities, and process capability for critical component attributes which is adequate for the performance and reliability specifications of the application.

Keywords: Components, Cost Effective Ceramics, Process Control, Silicon Nitride

85. **ADVANCED MANUFACTURING OF CERAMIC EXHAUST VALVES FOR DIESEL ENGINES**
$0
DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: A. E. Pasto, (423) 574-4956
Norton Contact: Vimal Pujari, (508) 351-7929

The objectives of this program are to design, develop, and demonstrate advanced manufacturing technology for the production of ceramic valves. A production manufacturing process for a ceramic exhaust valve for DDC's Series 149 diesel engine is being developed under this program. Specific objectives are to: (1) reduce manufacturing costs by at least an order of magnitude over current levels; (2) develop and demonstrate performance ratio values of 0.7 or less for all critical component attributes; and (3) to validate ceramic valve performance, durability, and reliability in rig and engine testing.

Keywords: Components, Cost Effective Ceramics, Process Control, SiAlON

86. **INSULATING STRUCTURAL CERAMICS FOR HIGH EFFICIENCY, LOW EMISSION ENGINES**
$535,000
DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. R. Johnson, (423) 576-6832
Caterpillar Contact: Michael Haselkorn, (309) 578-2953

The overall objective of this new program is to develop a commercially viable, zirconia-toughened mullite cylinder-head insert for advanced diesel engines using an innovative tape cast and pressureless sintering process.

Keywords: Ceramics, Components, Diesel, Engines, Mullite, Zirconia

87. **THICK THERMAL BARRIER COATINGS (TTBCS) FOR LOW EMISSIONS, HIGH EFFICIENCY DIESEL ENGINE COMPONENTS**
$723,000
DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. R. Johnson, (423) 576-6832
Caterpillar Contact: M. Brad Beardsley, (309) 578-8514

The objective of this new program is to develop durable, thick thermal barrier coating (TTBC) technologies for higher efficiency and lower-emission heavy duty diesel engines.

Keywords: Ceramics, Coatings and Films, Components, Diesel, Engines

88. **ADVANCED MATERIALS FOR LOW EMISSIONS, HIGH EFFICIENCY DIESEL ENGINE COMPONENTS**
$1,075,000
DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. R. Johnson, (423) 576-6832
Cummins Contact: Paul Becker, (812) 377-4701

The goal of this new program is to develop advanced material applications in diesel engine components to enable the design of cleaner, more efficient engines. Advanced materials may include ceramics, intermetallic alloys, advanced metal alloys, or ceramic or metal coatings. Components may include in-cylinder components, valve-train components, fuel-system components, exhaust system components, and air handling systems.

Keywords: Alloys, Ceramics, Coatings and Films, Components, Diesel, Engines, Intermetallics

89. **ADVANCED MATERIALS FOR LOW EMISSIONS, HIGH EFFICIENCY DIESEL ENGINE COMPONENTS**
$1,075,000
DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. R. Johnson, (423) 576-6832
Detroit Diesel Contact: Yuri Kalish, (313) 592-7825

The goal of this new program is to develop advanced material applications in diesel engine components to enable the design of cleaner, more efficient engines. Advanced materials may include ceramics, intermetallic alloys, advanced metal alloys, or ceramic or metal coatings. Components may include in-cylinder components, valve-train components, fuel-system components, exhaust system components, and air handling systems.

Keywords: Alloys, Ceramics, Coatings and Films, Components, Diesel, Engines, Intermetallics

90. **HIGH STRENGTH MATERIALS FOR DIESEL ENGINE FUEL INJECTORS**
$1,117,000
DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: R. L. Beatty, (423) 574-4536
Cummins Contact: Thomas Yonushonis, (812) 377-7078

The objective of this new program is to develop materials for next-generation diesel fuel injectors.

Keywords: Ceramics, Cermets, Components, Diesel

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

91. **DIESEL EXHAUST CATALYST CHARACTERIZATION**
$200,000
DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. R. Johnson, (423) 576-6832
ORNL Contact: T. A. Nolan, (423) 574-0811

The purpose of this work is to use analytical and high-resolution electron microscopy to characterize the microstructures of emission control catalysts. Emphasis is placed on relating microstructural changes to performance.

Keywords: Catalyst Performance, Catalysts, Diesel, Microstructure, Chemical Analysis, Mechanical Properties, Scanning Electron Microscopy

92. **COMPUTERIZED MECHANICAL PROPERTIES DATABASE**
$240,000
DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. R. Johnson, (423) 576-6832

The objective of this effort was to develop a comprehensive computer database containing experimental data on the properties of ceramic materials generated for the Ceramic Technology Project to provide a convenient and efficient mechanism for the compilation and distribution of the large amounts of data involved. The database was available in electronic form to project participants. In addition, periodic hard copy summaries of the data, including graphical representation and tabulation of raw data, were issued to provide convenient information sources for project participants.

Keywords: Database, Mechanical Properties, Structural Ceramics

93. **LIFE PREDICTION OF CERAMIC VALVES**
$200,000
DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. R. Johnson, (423) 576-6832
ORNL Contact: A. A. Wereszczak, (423) 574-7601

There are three central goals of the proposed research program: generation of engineering data from high-temperature mechanical testing, microstructural characterization of failure phenomena, and the implementation and verification of life-prediction methods involving structural ceramics.

Keywords: Components, Engines, Failure Analysis, Failure Testing, High Temperature Service, Life Prediction, Mechanical Properties, Structural Ceramics, Tensile Testing, SiAlON, Silicon Nitride

94. **HIGH TEMPERATURE TENSILE TESTING**
$0
DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. R. Johnson, (423) 576-6832
North Carolina A&T State University Contact: J. Sankar, (919) 334-7620

The objective of this research is to test and evaluate the long-term mechanical reliability of Si_3N_4 at high temperatures. Microstructural/microchemical analysis of the fracture surfaces using scanning electron microscopy (SEM), transmission electron microscopy (TEM), and energy-dispersive spectral analysis (EDS) is an integral part of this effort.

Keywords: Creep, Fracture, Microscopy, Silicon Nitride, Tensile Testing

95. **COMPUTED TOMOGRAPHY**
$120,000
DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. R. Johnson, (423) 576-6832
Argonne National Lab Contact: W. A. Ellingson, (312) 972-5068

The objective of this project is to apply X-ray CT techniques for cost-effective NDE inspection of diesel engine components.

Keywords: Components, Computed Tomography, Diesel, Engine, Nondestructive Evaluation

96. **NUCLEAR MAGNETIC RESONANCE IMAGING**
$80,000
DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. R. Johnson, (423) 576-6832
Argonne National Lab Contact: W. A. Ellingson, (312) 972-5068

The purpose of this work is to evaluate the potential of NMR imaging to impact the development and process control of near-net-shape gelcast ceramic components. The specific objectives of this work are to determine the utility of NMR imaging for: (1) 3D mapping of polymerization homogeneity; (2) real-time imaging of the polymerization process; (3) nondestructive evaluation of voids and flaws in the resultant components; and (4) measurement of physical properties such as degree of polymerization, viscosity, and specimen strength via correlation of these properties with measurable NMR parameters. This work is being performed in conjunction with Metals and Ceramics Division staff at Oak Ridge National Laboratory.

Keywords: Defect Structure, Gelcasting, Nondestructive Evaluation, Nuclear Magnetic Resonance, Silicon Nitride

97. **ON-MACHINE INSPECTION**
$200,000
DOE Contact: Robert B. Schulz,
(202) 586-8051
ORNL Contact: D. R. Johnson,
(423) 576-6832
Caterpillar Contact: M. K. Haselkorn,
(309) 578-6624

The primary objective of this new program is to establish a correlation between nondestructive evaluation techniques and the properties and performance of machined ceramic surfaces.

Keywords: Machining, Nondestructive Evaluation, Structural Ceramics

98. **MECHANICAL PROPERTIES OF CMZP**
$90,000
DOE Contact: Robert B. Schulz,
(202) 586-8051
ORNL Contact: D. R. Johnson,
(423) 576-6832
Caterpillar Contact: M. K. Haselkorn,
(309) 578-6624

The primary objective of this new program is to determine the effect of long-term exposure to a diesel-engine-exhaust environment of a particular low-expansion ceramic known as calcium magnesium zirconium phosphate (CMZP).

Keywords: CMZP, Diesel, Physical/Mechanical Properties, Stability

TECHNOLOGY TRANSFER AND MANAGEMENT COORDINATION

99. **TECHNICAL PROJECT MANAGEMENT**
$300,000
DOE Contact: Robert B. Schulz,
(202) 586-8051
ORNL Contact: D. R. Johnson,
(423) 576-6832

The objective of this effort is to assess the ceramic technology needs for advanced automotive heat engines, formulate technical plans to meet these needs, and prioritize and implement a long-range research and development program.

Keywords: AGT, Advanced Heat Engines, Coordination, Diesel, Management, Structural Ceramics

100. **INTERNATIONAL EXCHANGE AGREEMENT (IEA)**
$200,000
DOE Contact: Robert B. Schulz,
(202) 586-8051
ORNL Contact: D. R. Johnson,
(423) 576-6832
ORNL Contact: M. K. Ferber,
(423) 576-0818

The purpose of this effort is to organize, assist, and facilitate international research cooperation on the characterization of advanced structural ceramic materials. A major objective of this research is the evolution of measurement standards. Participants in Annex II are the United States, Germany, Sweden, Japan, and Belgium. Current research is focused on Subtask 7, Ceramic Machining, and Subtask 8, Ceramic Powder Characterization.

Keywords: IEA, Mechanical Properties, Powder Characterization

101. **STANDARD REFERENCE MATERIALS**
$200,000
DOE Contact: Robert B. Schulz,
(202) 586-8051
ORNL Contact: D. R. Johnson,
(423) 576-6832
NIST Contact: G. Onoda, (301) 975-4489

This project is directed toward a critical assessment and modeling of ceramic powder characterization methodology and toward the establishment of an international basis for standard materials and methods for the evaluation of powders prior to processing. The objectives of this program are: (1) to assist with the division and distribution of ceramic starting powders for an international round robin on powder characterization; (2) to provide reliable data on physical (dimensional), chemical, and phase characteristics of powders; and (3) to conduct statistical assessment, analysis, and modeling of round-robin data. The round-robin is to be conducted through the auspices of the International Energy Agency.

Keywords: IEA, Reference Material, Powder Characterization

102. **MECHANICAL PROPERTY STANDARDIZATION**
$100,000
DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. R. Johnson, (423) 576-6832
NIST Contact: G. Quinn, (301) 975-5765

The purpose of this effort is to develop mechanical test standards in support of the Heavy Vehicle Propulsion System Materials Program and the Advanced Turbine Technology Applications Program.

Keywords: Mechanical Properties, Test Procedures

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

103. **THICK THERMAL BARRIER SEAL COATINGS**
$30,000
DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. R. Johnson, (423) 576-6832
ORNL Contact: W. Y. Lee, (423) 576-2894

The purpose of this exploratory research program is to assess the possibility for sealing the surface of porous thermal barrier coatings (TBCs) with a thin oxide coating prepared by chemical vapor deposition. Al_2O_3, SiO_2, mullite, and ZrO_2 will be evaluated as candidate seal coating materials. The high-temperature stability of the sealed TBC structures will be studied by performing cyclic oxidation experiments at ORNL and gas permeability measurements at Caterpillar.

Keywords: Coatings, Chemical Vapor Deposition, CVD, Diesel, Engines, Thermal Barrier Coatings

104. **CHARACTERIZATION OF MACHINED CERAMICS**
$200,000
DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. R. Johnson, (423) 576-6832
ORNL Contact: P. J. Blau, (423) 574-5377

The purpose of this task is to develop, in conjunction with U.S. industry, advanced technologies and the associated scientific and economic concepts necessary to reduce costs associated with the machining of structural ceramics, especially as related to component parts for energy-efficient, low-emissions transportation systems. This effort is conducted by industry, other national laboratories, and in-house at ORNL. The ORNL research concerns two technical areas: (1) investigating the effects of machining practices on the durability of ceramics for valve and valve-seat applications, (2) understanding and characterizing the detailed nature of machining-induced surface and subsurface damage and their evolution in advanced ceramic materials using a range of analytical tools.

Keywords: Cost Effective Ceramics, Machining, Silicon Nitride, Structural Ceramics

105. **NEXT-GENERATION GRINDING WHEEL**
$0
DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: P. J. Blau, (423) 574-5377
Norton Contact: Robert H. Licht, (508) 351-7815

This effort is aimed at the engineering design and development of a next-generation, superabrasive grinding wheel specifically tailored for the cylindrical grinding of silicon nitride and other advanced structural ceramic parts for automotive and truck engine applications. The intent of this effort is to significantly reduce manufacturing cost of ceramic parts and to enhance the competitiveness of U.S. industry by providing an optimized grinding wheel for ceramics. The Phase I objectives to define requirements, and design, develop, and evaluate a next-generation grinding wheel for cost-effective cylindrical grinding of advanced ceramics have been met. The overall objectives of the Phase II effort are: (1) to scale up the manufacturing process for the Phase I experimental wheel composition in order to manufacture 356mm (14-in.) diameter grinding wheels, and to validate the performance of the new wheels in cylindrical grinding of advanced ceramics at independent test sites.

Keywords: Cost Effective Ceramics, Machining, Silicon Nitride, Structural Ceramics, Surface Characterization and Treatment

106. CHEMICALLY ASSISTED GRINDING OF CERAMICS
$150,000
DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: P. J. Blau, (423) 574-5377
NIST Contact: Steven M. Hsu, (301) 975-6119

The objective of this effort was to reduce ceramic machining costs by increasing the machining rate of ceramics using chemical reactions at the interface. The approach was to use chemistry to control the machining process. The ceramic surface can be chemically modified to form a soft reaction layer which can be removed rapidly with minimum substrate penetration, thus reducing stresses and minimizing residual cracks. Si_3N_4 is the material of focus. Efforts focused on the role of coolants in the machining of ceramics including testing coolants under actual production conditions.

Keywords: Chemical Reaction, Cost Effective Ceramics, Machining, Silicon Nitride, Structural Ceramics, Surface Characterization and Treatment

107. HIGH SPEED GRINDING
$0
DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: P. J. Blau, (423) 574-5377
Eaton Contact: Joseph A. Kovach, (216) 523-6766

The purpose of this effort is to develop a single step, rough finishing process suitable for producing high-quality silicon nitride ceramic parts at high material removal rates and at substantially lower cost than traditional, multi-stage grinding processes. Initial implications from Phase I have suggested that HSLD grinding of Si_3N_4 is technically feasible. Accordingly, the Phase II effort is focused on: (1) continued expansion of the HSLD science base, (2) further development of the enabling HSLD technologies required for successful implementation, and (3) economic analysis of the HSLD production cost drivers.

Keywords: Cost Effective Ceramics, Machining, Silicon Nitride, Structural Ceramics, Surface Characterization and Treatment

108. LASER-BASED NDE METHODS
$0
DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. R. Johnson, (423) 576-6832
Argonne National Lab Contact: J. G. Sun, (708) 252-5169

The primary objective of this program is to develop a laser-based, elastic optical scattering procedure which would provide a direct (near-real-time) method to detect machining-induced damage in monolithic ceramics. Median and lateral crack detection are of primary importance. The laser-based elastic optical scattering program is being executed in three steps. The first is to optimize the elastic scattering procedure by examining specimens machined using innovative machining techniques. The second step involves correlation of the elastic scattering results with mechanical properties in "real" machined ceramic specimens. The final step involves the development of a prototype instrument to be evaluated for on-line implementation in a production environment.

Keywords: Machining, Nondestructive Evaluation, Structural Ceramics

109. GRINDING MACHINE STIFFNESS
$0
DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: P. J. Blau, (423) 574-5377
University of Connecticut Contact: Bi Zhang, (203) 486-3576

The objective of this effort is to determine the minimum required grinding machine stiffness to meet acceptable quality requirements for ground silicon nitride ceramic parts.

Keywords: Machining, Silicon Nitride

110. NEXT GENERATION GRINDING SPINDLE
$0
DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: P. J. Blau, (423) 574-5377
Eaton Contact: J. A. Kovach, (216) 523-6766

The objective of this effort is to design, develop, test, and demonstrate the operation of a next generation, high-stiffness, high-speed spindle to be used for centerless grinding of ceramic parts.

Keywords: Machining, Structural Ceramics

111. **PROCESS COST MODEL**
$0
DOE Contact: Robert B. Schulz,
(202) 586-8051
ORNL Contact: S. G. Winslow,
(423) 574-0965
AlliedSignal Ceramic Components Contact:
B. S. Draskovich, (312) 512-5654

The objective of this effort was to refine and utilize a process cost model for the evaluation of various fabrication methods used to manufacture diesel engine and aerospace/industrial turbomachinery structural ceramic components and provide a report containing an analysis of the process cost modeling effort.

Keywords: Cost-Effective Ceramics, Cost Reduction, Modeling, Processing, Structural Ceramics

112. **INTELLIGENT GRINDING WHEEL**
$499,000
DOE Contact: Robert B. Schulz,
(202) 586-8051
ORNL Contact: P. J. Blau, (423) 574-5377
University of Massachusetts Contact:
Stephen Malkin, (413) 545-3687

The objective of this effort is to develop an "intelligent grinding wheel" for in-process monitoring of ceramic grinding processes. Such a wheel will be smart enough to monitor its "state" or "condition" during truing, dressing, and grinding; to identify the prevailing grinding mechanisms (ductile versus brittle); and to use this real-time information as a feedback signal for process control and optimization. In order to monitor the wheel working condition and the grinding processes in a real-time and on-line fashion, without additional instrumentation, both acoustic emission sensors and dynamic force sensors, together with the primary signal-processing electronics, will be embedded in the core of the grinding wheel.

Keywords: Cost Effective Ceramics, Machining, Structural Ceramics

HIGH STRENGTH WEIGHT REDUCTION MATERIALS

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

113. **MODELING OF TRANSPORTATION MATERIALS REQUIREMENTS AND PHYSICAL METALLURGY OF MAGNESIUM**
$595,000
DOE Contact: Sidney Diamond,
(202) 586-8032
ORNL Contact: P. Sklad, (423) 574-5069
ANL Contact: Frank Stodolsky,
(202) 288-2431

The objective of this effort is to perform an assessment of aluminum forming costs and assess feasibility of alternative engine materials and to evaluate novel magnesium forming processes.

Keywords: Aluminum Forming, Magnesium Forming

114. **STUDY OF BONDING INTERFACES BETWEEN REINFORCING MATERIALS AND CAST ALUMINUM ALLOY**
$100,000
DOE Contact: Sidney Diamond,
(202) 586-8032
ORNL Contact: P. Sklad, (423) 574-5069
ORNL Contact: K. Moore, (423) 574-7788
Cummins Engine Co. Contact: P. Becker,
(812) 377-4701

The objective of this effort is to develop and evaluate interfaces between various reinforcing materials and cast aluminum alloys.

Keywords: Bonding Interfaces, Cast Aluminum Alloys

DEVICE OF COMPONENT FABRICATION, BEHAVIOR OR TESTING

115. **DEVELOPMENT OF A CASTING PROCESS FOR ULTRALARGE HEAVY VEHICLE COMPONENTS**
$1,444,000
DOE Contact: Sidney Diamond, (202) 586-8032
ORNL Contact: P. Sklad, (423) 574-5069
ORNL Contact: S. Viswanathan, (423) 576-9917
Alcoa/CMI Contact: T. Meyer, (412) 337-2580

The objective of this effort is to develop cost effective high volume production process of ultra large castings for frame and other structural components in vehicular applications.

Keywords: Cost Effective Casting, Ultralarge Components

116. **METAL COMPRESSION FORMING OF ALUMINUM ALLOYS AND METAL MATRIX COMPOSITES**
$350,000
DOE Contact: Sidney Diamond, (202) 586-8032
ORNL Contact: P. Sklad, (423) 574-5069
ORNL Contact: S. Viswanathan, (423) 576-9917
Thompson Aluminum Castings Contact: R. M. Purgert, (216) 581-9200

The objective of this effort is to validate metal compression forming as a cost-effective, high volume, net shape processing technology for aluminum alloys and metal matrix composites.

Keywords: Metal Compression Forming, Aluminum Alloys, Metal Matrix Composites

OFFICE OF UTILITY TECHNOLOGIES

	FY 1996
Office of Utility Technologies - Grand Total	$34,790,000
Office of Solar Energy Conversion	$16,200,000
Photovoltaic Energy Technology Division	$16,200,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$10,700,000
Amorphous Silicon for Solar Cells	5,300,000
Polycrystalline Thin Film Materials for Solar Cells	4,900,000
Deposition of III-V Semiconductors for High-Efficiency Solar Cells	500,000
Materials Properties, Behavior, Characterization or Testing	$ 4,000,000
Materials and Device Characterization	4,000,000
Device or Component Fabrication, Behavior or Testing	$ 1,500,000
High-Efficiency Crystal Silicon Solar Cells	1,500,000
Office of Geothermal Technologies	$ 590,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 100,000
Thermally Conductive Composites for Heat Exchangers	100,000
Materials Properties, Behavior, Characterization or Testing	$ 490,000
Advanced High Temperature Geothermal Well Cements	250,000
Corrosion Mitigation in Highly Acidic Steam Condensates	100,000
Advanced Coating Materials	140,000
Office of Energy Management	$18,000,000
Advanced Utility Concepts Division	$18,000,000
High Temperature Superconductivity for Electric Systems	$18,000,000
Device or Component Fabrication, Behavior or Testing	$18,000,000
Wire Technology	4,000,000
Systems Technology	6,000,000
Superconductivity Partnership Initiative	8,000,000

OFFICE OF UTILITY TECHNOLOGIES

OFFICE OF SOLAR ENERGY CONVERSION

PHOTOVOLTAIC ENERGY TECHNOLOGY DIVISION

The National Photovoltaics program sponsors high-risk, potentially high-payoff research and development in photovoltaic energy technology that will result in a technology base from which private enterprise can choose options for further development and competitive application in U.S. electrical markets. The objective of materials research is to overcome the technical barriers currently limiting the efficiency and cost of photovoltaic cells. Theoretical conversion efficiency of photovoltaic cells is limited by the portion of the solar spectrum to which the cell's semiconductor material can respond, and by the extent to which these materials can convert each photon to electricity. The practical efficiency is constrained by the amount of light captured by the cell, the cell's uniformity, and a variety of loss mechanisms for the photo-generated carriers. Cost is affected by the expense and amount of materials required, the complexity of processes for fabricating the appropriate materials, and the complexity and efficiency of converting these materials into cells and modules.

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

117. **AMORPHOUS SILICON FOR SOLAR CELLS**
$5,300,000
DOE Contact Jeffrey Mazer: (202) 586-2455
NREL Contact: Bolko von Roedern, (303) 384-6480

This project performs applied research upon the deposition of amorphous silicon alloys to improve solar cell properties. Efficient solar energy conversion is hindered by improper impurities or undesired structure in the deposited films and the level of uniformity of the films over large (1000 cm^2) areas. The films are deposited by plasma enhanced chemical vapor deposition (glow discharge), thermal chemical vapor deposition and sputtering. The long term goal of this effort is to develop the technology for 15 percent efficient solar cells with an area of about 1000 cm^2. Achieving that goal will enable amorphous silicon to be a cost-effective electrical generator.

Keywords: Amorphous Materials, Coatings and Films, Semiconductors, Chemical Vapor Deposition, Sputtering and Solar Cells

118. **POLYCRYSTALLINE THIN FILM MATERIALS FOR SOLAR CELLS**
$4,900,000
DOE Contact: Jeffrey Mazer, (202) 586-2455
NREL Contact: Kenneth Zweibel, (303) 384-6441

This project performs applied research upon the deposition of $CuInSe_2$ and CdTe thin films for solar cells. Research centers upon improving solar cell conversion efficiency by depositing more nearly stoichiometric films, by controlling interlayer diffusion and lattice matching in heterojunction structures and by controlling the uniformity of deposition over large (1000 cm^2) areas. The films are deposited by chemical and physical vapor deposition, electrodeposition and sputtering. The long term goal for this effort is to develop the technology for 15 percent efficient solar cells with areas of about 1000 cm^2. Achieving this goal would enable polycrystalline thin film material to be a cost-effective electrical generator.

Keywords: Coatings and Films, Semiconductors, Chemical Vapor Deposition, Physical Vapor Deposition, Electrodeposition, Sputtering and Solar Cells

119. **DEPOSITION OF III-V SEMICONDUCTORS FOR HIGH-EFFICIENCY SOLAR CELLS**
$500,000
DOE Contact: Jeffrey Mazer, (202) 586-2455
NREL Contact: John Benner, (303) 384-6496

This project performs applied research upon deposition of III-V semiconductors for high efficiency solar cells, both thin film for flat plate applications and multilayer cells for concentrator applications. Research centers upon depositing layers precisely controlled in terms of composition, thickness and uniformity and studying the interfaces between the layers. The materials are deposited by chemical vapor deposition, liquid phase epitaxial growth and molecular beam epitaxial growth. The long term goal of this area is to develop 35 percent efficient concentrator cells and 24 percent 100 cm^2 one-sun cells for flat plate applications. Achieving these goals would enable systems using these technologies to be cost-effective electrical generators.

Keywords: Semiconductors, Chemical Vapor Deposition, Solar Cells

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

120. MATERIALS AND DEVICE CHARACTERIZATION
$4,000,000
DOE Contact: Jeffrey Mazer, (202) 586-2455
NREL Contact: Larry Kazmerski, (303) 384-6600

This project measures and characterizes materials and device properties. The project performs surface and interface analysis, electro-optical characterization and cell performance and material evaluation to study critical material/cell parameters such as impurities, layer mismatch and other defects that limit performance and lifetime. Techniques that are used include deep level transient spectroscopy, electron beam induced current, secondary ion mass spectroscopy, scanning electron microscopy and scanning transmission electron microscopy.

Keywords: Semiconductors, Nondestructive Evaluation, Surface Characterization, Microstructure and Solar Cells

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

121. HIGH-EFFICIENCY CRYSTAL SILICON SOLAR CELLS
$1,500,000
DOE Contact: Jeffrey Mazer, (202) 586-2455
NREL Contact: John Benner, (303) 384-649
SNLA Contact: Margie Tatro, (505) 844-3154

This project performs applied research upon crystal silicon devices to improve solar-to-electric conversion efficiency. The project employs new coatings and/or dopants and other treatments to reduce electron-hole recombination at cell surfaces or in the bulk material. Control of point defects in crystalline silicon is being studied by a variety of techniques.

Keywords: Semiconductors, Solar Cells, Crystal Silicon

OFFICE OF GEOTHERMAL TECHNOLOGIES

The primary goal of the geothermal materials program is to ensure that the private sector development of geothermal energy resources is not constrained by the availability of technologically and economically viable materials of construction. This requires the performance of intermediate and long-term high risk materials research and development, which is sponsored by the Office of Geothermal Technologies.

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

122. THERMALLY CONDUCTIVE COMPOSITES FOR HEAT EXCHANGERS
$100,000
DOE Contact: R. LaSala, (202) 586-4198
BNL Contact: L. E. Kukacka, (516) 282-3065

This project is investigating thin thermally conductive polymer-based composites for use as corrosion and scale-resistant liner materials on carbon steel tubing used in shell and tube heat exchangers in binary geothermal processes or for bottoming cycles in multi-stage flash plants. Corrosion and scaling on the brine side of carbon steel tubing in shell and tube heat exchangers have been major problems in the operation of geothermal processes. Compared to the cost of high alloy steels, a considerable economic benefit could result from the utilization of a proven corrosion resistant polymer concrete material if sufficient heat transfer and anti-fouling properties can be derived. The work consists of determinations of the effects of compositional and processing variables on the thermal and fouling properties of the composite, and measurements of the physical and mechanical properties after exposure to hot brine in the laboratory and in plant operations. The effects of anti-oxidant additives on the fouling coefficient and scale adherence are also being evaluated. Results to date from field tests with flowing hypersaline brine under heat exchange conditions indicate heat transfer coefficients similar to those for high alloy stainless steels. The liner provided excellent corrosion protection to the carbon steel substrate, and no deterioration or debonding of it were apparent. Further improvements in the fouling coefficients by the inclusion of anti-oxidants are anticipated. Additional field tests are scheduled for FY1997. The results from preliminary design, manufacturing and cost studies indicate that contingent upon the development of a method for joining the composite lined tubes to the tube sheets, reductions in the cost of heat exchangers up to 65 percent could be realized.

Keywords: Composites, Polymers, Corrosion, Heat Transfer, Scale-Resistant, Fabrication Technology, Fouling Coefficient

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

123. **ADVANCED HIGH TEMPERATURE GEOTHERMAL WELL CEMENTS**
$250,000
DOE Contact: R. LaSala, (202) 586-4198
BNL Contact: L. E. Kukacka, (516) 282-3065

Lightweight (<1.2 g/cc), environmentally benign, chemically and thermally resistant well cements are needed to reduce the potential for lost circulation problems during well completion operations and to insure long-term well integrity. Materials designed for temperatures >400°C will be needed as higher temperature resources are developed. Cements resistant to brines containing high concentrations of CO_2 at temperatures >150°C are also needed. Emphasis is being placed on high temperature rheology, phase chemistry, and the mechanical, physical, and chemical resistance properties of the cured materials. Retarding admixtures required to maintain pumpability during placement operations are also being identified. The most promising cement formulation identified to date consists of 23.7 wt% Class F flyash; 15.8 wt% calcium aluminate cement, 31.4 wt% of a 40 wt% sodium metaphosphate solution, and 29.1 wt% Al_2O_3. The latter is in the form of lightweight, hollow ceramic micropheres. This formulation, which has a slurry density of approximately 1.2g/cc, and after hydrothermal curing forms a strong, CO_2-resistant cement, will be used in a well completion in FY1997.

Keywords: Cements, Material Degradation, Strength, Phase Transformation, Bulk Characterization, Drilling, Carbonation, Retarders, Rheology, Well Completions

124. **CORROSION MITIGATION IN HIGHLY ACIDIC STEAM CONDENSATES**
$100,000
DOE Contact: R. LaSala, (202) 586-4198
BNL Contact: L. E. Kukacka, (526) 282-3065

Increased HCl gas concentrations in the steam produced from geothermal wells at The Geysers in Northern California have resulted in severe corrosion problems in casings in the upper regions of wells where condensation may occur, in the well-head, transmission piping, turbines, and cooling towers. The objective of the program is to optimize and field test polymers, polymer matrix composites, and ceramic matrix composites for utilization as corrosion resistive liners on components exposed to low pH steam condensates at temperatures up to~200°C. Emphasis is being placed on polymer and composite composition, metal surface modification and installation procedures.

Keywords: Corrosion Protection, Polymers, Composites, Ceramics, Well Casing, Turbine Components, Piping, Acid Condensate

125. **ADVANCED COATING MATERIALS**
$140,000
DOE Contact: R. LaSala, (202) 586-4198
BNL Contact: L. E. Kukacka, (516) 282-3065

Corrosion of plant components is a problem that is encountered in most geothermal processes, and low cost solutions are needed in order to maintain the economic competitiveness of this large and environmentally benign energy source. The objective of this task is to optimize and field test polymers and polymer, ceramic, and metallic-matrix composites, developed in other parts of the Geothermal Materials Development Program, as corrosion protective systems for use in brine dominated geothermal electric generation processes and for the biochemical treatment of plant wastes. Successful evaluations and subsequent technology transfer will result in reduced plant construction and operation costs, increased generation efficiencies and utilization factors, and enhanced environmental acceptance.

Keywords: Corrosion Protection, Polymers, Composites, Placement Techniques, Field Tests, Biochemical Processes

OFFICE OF ENERGY MANAGEMENT

ADVANCED UTILITY CONCEPTS DIVISION

The Advanced Utility Concepts Division supports research and development of advanced energy storage and electrochemical conversion systems that will facilitate the substitution of renewable energy sources for fossil fuels-measures that will increase the reliability and efficiency of the energy economy. The goal is to provide reliable, inexpensive devices to mitigate the temporal and spatial mismatches between energy supply and energy demand. The research is divided into four subprograms: Superconductivity Systems, Utility Battery Storage, Thermal Storage, and Hydrogen Energy.

HIGH TEMPERATURE SUPERCONDUCTIVITY FOR ELECTRIC SYSTEMS

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

126. **WIRE TECHNOLOGY**
$4,000,000
DOE Contact: Jim Daley, (202) 586-1165
Argonne National Laboratory Contact:
U. Balachandran, (708) 252-4250
Brookhaven National Laboratory Contact:
David Welch, (516) 282-3517
LANL Contact: Dean Peterson,
(505) 665-3030
National Renewable Energy Laboratory
Contact: Richard Blaugher, (303) 384-6518
ORNL Contact: Robert Hawsey,
(423) 574-8057
SNL Contact: Peter Roth, (505) 845-9301
American Superconductor Contact:
G. N. Riley, (508) 836-4200
Intermagnetics General Corp. Contact:
Paradeep Haldar, (518) 782-1122

The wire technology goal is improvement in short wire samples (1 cm to 10 cm) through: improved powder synthesis, improved fundamental understanding of critical currents in high temperature superconductors, and investigation of new wire processing methods. Improvement in long wire length uniformity is included in the Systems Technology project below.

The wire development project is the key to eventual commercialization of superconductivity system. Subtasks in the project are as follows:

(1) Ink development and spray deposition - To develop high quality, low cost methods for the delivery of superconductor precursor materials in a commercially scalable thick-film process using ink-spray techniques.

(2) Thallination and advanced substrate development - Continue to optimize the thallination parameters leading to high Jc superconducting films and develop and evaluate a textured substrate to permit the synthesis of a bi-axially textured oxide film. To scale up the thallination apparatus to allow longer length development of superconducting samples leading eventually to a continuous thallination process.

(3) Development of Thallium based conductors - The purpose of the Tl-based conductor development project is to develop materials and processes which will lead to the practical production of wires and tapes capable of carrying high currents in the presence of typical operating magnetic fields a liquid nitrogen temperatures.

(4) Practical conductor development for electrical power systems utilizing high Tc oxides; characterization of aligned Bi(2223) in AG PIT tapes - The purposes of this project is to make detailed characterization of electrical magnetic properties, such as ac losses and critical currents, of cuprate conductors in order to make critical assessments of the conductors, as well as to provide pertinent data for the design of various electrical devices.

(5) Development of high Ic and Jc BSCCO conductors - The main part of the project is aimed at understanding the effects of optimal defect geometry and density on the high temperature, high field performance of Bi-2223 tapes. The defects are produced by the recoil of proton induced fission fragments in the Bi-2223 cores of the tapes, which result in splayed columnar defects.

(6) High rate deposition technology for long-length conductors - The purpose of this project is to develop metal-organic chemical vapor deposition processes to fabricate high-quality superconductor coatings on long-length substrates. Film composition, crystalinity, morphology, and superconducting properties as a function of chemical precursor, gas pressure, flow rate, substrate materials, and deposition

temperatures will be systematically investigated.

(7) High current YBCO coated-conductor development - The objectives of this project included: Development of continuous processing of both the IBAD buffer layer and the laser-deposited YBCO layers at lengths of one meter. Investigation of means to accelerate and economize the deposition of IBAD layer. Investigation of accelerated deposition of the YBCO layer.

(8) Deposited conductors on textured metal substrates - The purpose of the project is to develop scalable processes for fabrication of conductors for high temperature, high field applications. The objectives for FY1996 are: to obtain proof-of-principle for the RABITS (rolling-assisted biaxially textured substrate) approach to conductor fabrication by demonstrating high critical current densities in a reproducible manner. For this purpose, primarily pulsed laser deposition has been used for oxide buffer layers and $YBa_2Cu_3O_7$.

Keywords: Superconductor, Thallium Conductor, Bismuth Conductor, Coated Conductor

127. **SYSTEMS TECHNOLOGY**
$6,000,000
DOE Contact: Jim Daley, (202) 586-1165
Argonne National Laboratory Contact:
U. Balachandran, (708) 252-4250
Brookhaven National Laboratory Contact:
David Welch, (516) 282-3517
LANL Contact: Dean Peterson,
(505) 665-3030
National Renewable Energy Laboratory
Contact: Richard Blaugher,
(303) 384-6518
ORNL Contact: Robert Hawsey,
(423) 574-8057
SNL Contact: Thomas Bickel,
(505) 845-9301
American Superconductor Contact:
G. N. Riley, (508) 836-4200
Intermagnetics General Corp. Contact:
Paradeep Haldar, (518) 782-1122
General Electric Research & Development
Contact: J. E. Tkaczyk, (518) 387-5004
Oxford Instruments, Inc. Contact:
K. R. Marken, (908) 541-1300

Systems technology goals include: improved uniformity in long (10 meter to 1000 meter) HTS wires, development of high field (2-5 telsa) coils, and design of high efficiency electric power devices.

The electric power application project includes development of long length wire manufacture and coil manufacture. Some preliminary systems development is also done. Project subtasks are as follows:

(1) AC-loss calorimeter system for HTS power transmission cables - The objective of this project is to develop an ac-loss calorimetric measurement system capable of determining the total ac-losses (hysteretic eddy current and coupling) of an HTS cable conductor operating in a 3-phase environment.

(2) Practical conductor development for electrical power systems utilizing high Tc oxides: characterization of electrical and magnetic properties - The purposes of this project are two fold: to make detailed characterization of electrical and magnetic properties, such as ac losses and critical currents, of cuprate conductors in order to make critical assessments of the conductors, as well as to provide pertinent data for the design of various electrical devices.

(3) Power applications of high temperature superconductors - To develop HTS components relating to electric power applications. Evaluate techniques and approaches to manufacture HTS coils and magnets for use in power related applications such as transformers, motors, generators, fault current limiters, SMES and transmission cable. Manufacture long lengths of Bi-2223 multi filament conductor and Bi-2212 surface coated conductor for use in the demonstration of prototype systems.

(4) Long-length HTS conductors - The purpose of this project is to develop technology to fabricate long-length conductors with superconducting and mechanical properties suitable for commercial operation at temperature approaching 77K.

(5) Resistive Fault current limiter - The purpose of the project is to develop a resistive 100A fault current limiter from sinter YBCO. The device would be an intermediate step in the development of a commercial FCL(600 A/12 kV) for distribution lines of an electric utility.

(6) HTS transmission cable - The purpose of this project is to develop the technology necessary to proceed to commercialization of high temperature superconducting transmission cable. The objectives are to design and construct a low-cost, 2000 A ac,

bare 1m HTS cable prototype, and test its performance.

(7) Conductor, coil, and apparatus development for utility an commercial applications - The purpose of this project is to establish the technical and economic feasibility and benefits to society of HTS transformers of medium(30 MVA) to large rating. The objective is to design and begin the construction of a nominal 1 MVA HTS demonstration transformer incorporating the concepts developed in FY95.

(8) AC wires and AC coils for power applications - The objective of this AC loss effort is to support the development of a high temperature superconductor developed for AC applications. FY95 data indicated filament decoupling in twisted conductor. The low level of loss observed in FY95 indicated that improvements in the AC apparatus would be required to characterize long continuous lengths of conductor. The main concern was the variation in the field homogeneity for long sample lengths when the sample was exposed to AC fields perpendicular to the wide face of the conductor.

(9) High gradient magnetic separation - The objective is to design and build a prototype industrial HTS high gradient magnetic separation system. The copper coils used in conventional industrial magnetic separation systems consume large amounts of electrical power. Significant energy savings are possible if superconducting magnet systems are used.

Keywords: Long Length Conductor, Bearing, Flywheels, Superconducting Tape, Power Transmission Cable, Resistive Fault Current Limiter, Magnetic Separation, Transformer

128. **SUPERCONDUCTIVITY PARTNERSHIP INITIATIVE**
$8,000,000

The Superconductivity Partnership Initiative (SPI) is an industry-led venture between the Department of Energy and four industrial consortia intended to accelerate the use of high temperature superconductivity in energy applications. Each SPI team includes a vertical integration of non-competing companies that represent the entire spectrum of the R&D cycle. That is, the teams include the ultimate user of the technology-the electric utilities—as well as a major manufacturing company and a small company supplier of superconducting components. Each team also includes one or more national laboratories who perform specific tasks defined by the team. The SPI goal is to design cost-effective HTS systems for electricity generation, delivery and use. The funding below amount below includes the Department's share of the SPI design activities as well as parallel HTS technology development that directly supports the SPI teams. In FY95, projects are underway for a superconducting 100 MVA generator (General Electric), fault-current limiter (General Dynamics), and 100 HP motor (Reliance, Electric Company). In addition, a transmission cable project, led by the Electric Power Research Institute and Pirelli Cable was funded. All of these projects will incorporate high-temperature superconducting wire. Four Department of Energy National Laboratories are currently directly supporting the Superconductivity Partnership Projects: Argonne, Los Alamos, Oak Ridge, and Sandia.

Project subtasks are as follows:

(1) Generator - Results of the generator project, included generator assessment activities including defining the applications, establishing a conceptual generator design, developing a preliminary generator design and initiating the performance analysis of the generator in the utility system. In addition, wire and coil development activities will be started and include wire development, fabrication, and coil design and development. Generators represent a large established worldwide market with growth projections forecasting that over 1000GW of new generation capacity will be needed in the next 10 years, with 173 GW needed in the U.S.

General Electric Co. Contact: Kenneth Lay, (518) 387-6147

(2) Fault Current Limiter - The fault-current limiter project undertook conceptual studies of various device designs, provide a market survey for current limiter applications, complete an energy benefit assessment, conduct a network interface assessment, determine conductor requirements, and analyze the economic potential of fault current limiters. Fault current limiters can be used on transmission and distribution systems to improve system flexibility, reliability and performance.

Lockheed Martin Contact: Eddie Leung, (619) 974-1166

(3) Motor - Electrical and mechanical design and thermal analysis completed. In addition, the construction of the components for a motor prototype will be nearly completed, with assembly and testing. Superconducting motors can have a large impact on electrical energy utilization through reduced losses and size compared to conventional iron core motors. This reduced losses and smaller size will be the driving force for the commercial introduction of superconducting motors in industrial applications.

Reliance Electric Company Contact:
Rich Schiferl, (216) 266-6253

(4) High Temperature Superconducting Power Cable - The first phase of the contract calls for the development and fabrication of a 30-meter prototype 115KV HTS underground power transmission cable which will be tested at a utility test site. Additionally, the project will conclude with design of a 3-phase, 100 meter cable system.

Electric Power Research Institute Contact:
Don Von Dollen, (415) 855-2679

Keywords: Generator, Motor, Fault Current Limiter, Transmission Cable

OFFICE OF ENERGY RESEARCH

	FY 1996
Office of Energy Research - Grand Total	$417,462,697
Office of Basic Energy Sciences	$393,943,766
Division of Materials Sciences	$332,060,000
Division of Chemical Sciences	$ 5,300,000
Division of Engineering and Geosciences	$ 6,583,766
Engineering Sciences Research	$ 3,946,973
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 1,009,868
Fundamentals of Thermal Plasma Processing	478,000
Multivariable Control of the Gas-Metal Arc Welding Process	153,000
Metal Transfer in Gas-Metal Arc Welding	124,000
Thermal Plasma Chemical Vapor Deposition of Advanced Materials	157,975
Research on Combustion-Driven HVOF Thermal Sprays	96,893
Effect of Forced and Natural Convection on Solidification of Binary Mixtures	0
Materials Properties, Behavior, Characterization or Testing	$ 2,579,682
Continuum Damage Mechanics - Critical States	0
An Investigation of History-Dependent Damage in Time-Dependent Fracture Mechanics	99,729
Intelligent Control of Thermal Processes	517,000
Elastic-Plastic Fracture Analysis Emphasis on Surface Flaws	132,000
Nondestructive Evaluation of Superconductors	205,000
Origins of Asymmetric Stress-Strain Response in Phase Transformations	80,535
Modeling and Analysis of Surface Cracks	192,000
Development of Measurement Capabilities for the Thermophysical Properties of Energy-Related Fluids	425,000
High-T_c Superconductor-Semiconductor Integration and Contact Technology	116,800
Thin Film Characterization and Flaw Detection	0
Transport Properties of Disordered Porous Media From the Microstructure	116,959
Inelastic Constitutive Equation: Deformation Induced Anistropy and the Behavior at High Homologous Temperature	149,828
Stress and Stability Analysis of Surface Morphology of Elastic and Piezoelectric Materials	137,700
Optical Techniques for Characterization of High Temperature Superconductors	231,000
3-D Experimental Fracture Analysis at High Temperatures	76,721
Simulation and Analysis of Dynamic Failure in Ductile Materials	99,410

OFFICE OF ENERGY RESEARCH (continued)

	FY 1996
Office of Basic Energy Sciences (continued)	
Division of Materials Sciences (continued)	
Division of Chemical Sciences (continued)	
Division of Engineering and Geosciences (continued)	
Engineering Sciences Research (continued)	
Device or Component Fabrication, Behavior or Testing	$ 357,423
An Analytical-Numerical Alternating Method for 3-D Inelastic Fracture and Integrity Analysis of Pressure-Vessels and Piping at Elevated Temperatures	85,000
Pulse Propagation in Inhomogeneous Optical Waveguides	200,493
Flux Flow, Pinning and Resistive Behavior in Superconducting Networks	71,930
Geosciences Research	$ 2,636,793
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 435,170
An Investigation of Organic Anion-Mineral Surface Interactions During Diagenesis	200,000
Transition Metal Catalysis in the Generation of Petroleum and Natural Gas	104,538
Mineral Dissolution and Precipitation Kinetics: A Combined Atomic-Scale and Macro-Scale Investigation	130,632
Materials Structure and Composition	$ 572,212
Reaction Mechanisms of Clay Minerals and Organic Diagenesis: An HRTEM/AEM Study	132,386
Infrared Spectroscopy and Hydrogen Isotope Geochemistry of Hydrous Silicate Glasses	139,826
Biomineralization: Systematics of Organic-Directed Controls on Carbonate Growth Morphologies and Kinetics Determined by *In Situ* Atomic Force Microscopy	0
Reactions and Transport of Toxic Metals in Rock-Forming Silicates at 25°C	200,000
The Crystal Chemistry and Structural Analysis of Uranium Oxide Hydrates	100,000
Materials Properties, Behavior, Characterization or Testing	$ 1,629,411
Oxygen and Cation Diffusion in Oxide Materials	224,179
Structure and Reactivity of Ferric Oxide and Oxyhydroxide Surfaces: Quantum Chemistry and Molecular Dynamics	200,000
Cation Diffusion Rates in Selected Silicate Minerals	130,000
Grain Boundary Transport and Related Processes in Natural Fine-Grained Aggregates	152,460
New Method for Determining Thermodynamic Properties of Carbonate Solid-Solution Minerals	150,552
Micromechanics of Failure in Brittle Geomaterials	181,098
Three-Dimensional Imaging of Drill Core Samples Using Synchrotron-Computed Microtomography	150,000

OFFICE OF ENERGY RESEARCH (continued)

	FY 1996
Office of Basic Energy Sciences (continued)	
Division of Materials Sciences (continued)	
Division of Chemical Sciences (continued)	
Division of Engineering and Geosciences (continued)	
Geosciences Research (continued)	
Materials Properties, Behavior, Characterization or Testing (continued)	
Thermodynamics of Minerals Stable Near the Earth's Surface	150,000
Theoretical Studies of the Adsorption of Gold Complexes and Flotation Collectors onto Sulfide Mineral Surfaces	27,547
Shear Strain Localization and Fracture Evolution in Rocks	0
Transport Phenomena in Fluid-bearing Rocks	146,273
Cation Chemisorption at Oxide Surfaces and Oxide-Water Interfaces: X-ray Spectroscopic Studies and Modeling	0
Dissolution Rates and Surface Chemistry of Feldspar Glass and Crystal	117,302
Office of Computational and Technology Research	$56,309,931
Division of Advanced Energy Projects and Technology Research	$56,309,931
Laboratory Technology Research (LTR) Program	$ 4,897,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 1,837,000
Lumeloid, A New Solar Energy Conversion Material (ANL94-42)	100,000
Cold Cathode Electron Emission From Diamond and Diamond-Like Carbon Thin Films for Flat Panel Computer Displays (ANL95-02)	140,000
Giant Magnetoresistance Wire Sensor (ANL95-07)	150,000
Composite Metal-Hydrogen Electrodes for Metal-Hydrogen Batteries (BNL94-06)	115,000
Development of CdTe/CdZnTe Materials for Radiation Detectors (BNL94-09)	115,000
Corrosion Resistance of New Alloys for Biomedical Applications (BNL94-20)	25,000
Novel Biocompatible "Smart" Contact Lens Material (LBNL94-28)	75,000
Alloy Design of Neodymium ($Nd_2Fe_{14}B$) Permanent Magnets (ORL94-15)	282,000
Development of Aluminum Bridge Deck System (ORL94-56)	100,000
New Thermoelectric Materials for Solid State Refrigeration (ORN95-10)	180,000
Manufacturing of Ni-Base Superalloys with Improved High-Temperature Performance (ORL95-05)	150,000
Polymer Multilayer (PML) Film Applications in Optics, Electrolytes, and Glazings (PNNL94-06)	65,000
Development of Mixed Metal Oxides (PNNL94-28)	25,000
Development of Tape Calendaring Technology for Separation Membranes (PNNL95-04)	40,000
Innovative Multilayer Thermal Barrier Coatings for Gas Turbine Engines (PNNL95-07)	275,000

OFFICE OF ENERGY RESEARCH (continued)

	FY 1996
Office of Computational and Technology Research (continued)	
Division of Advanced Energy Projects and Technology Research (continued)	
Laboratory Technology Research (LTR) Program (continued)	
Device or Component Fabrication, Behavior or Testing	$ 1,450,000
Application of High Performance Computing to Automotive Design and Manufacturing (ANL94-54)	250,000
Microfabrication of a Multi-Axis Microaccelerometer Using High Aspect Ratio Microfabrication (HARM) and Silicon Micromachining (BNL94-02)	250,000
Nondestructive X-ray Scattering Characterization of High Temperature Superconducting Wires (BNL95-10)	140,000
Thin Film Lithium Batteries (BNL95-11)	90,000
New Catalysts for Direct Methanol Oxidation Fuel Cells (BNL95-14)	15,000
Rechargeable Zinc/Air Batteries for Consumer Applications (LBNL94-43)	15,000
Micromagnetic Structures (LBNL95-12)	71,000
Development of Zinc/Nickel Oxide Batteries for Electric Vehicle Applications (LBNL95-27)	90,000
Catalytic Conversion of Chlorofluorocarbons Over Palladium-Carbon Catalysts (LBNL95-45)	104,000
Development of a Thin-Film Battery Powered Hazard Card and Other Microelectronic Devices (ORL94-39)	70,000
Ion Implantation Processing Technologies (ORL94-72)	100,000
Rapid Prototyping of Ceramics (ORL94-95)	150,000
Rapid Prototyping of Bioceramics for Implants (ORL95-12)	105,000
Instrumentation and Facilities	$ 1,240,000
Micro-Spectroscopy Facility for New Infrared Imaging Materials (BNL94-60)	25,000
Development of Environmentally Conscious Machining Fluids (ORL94-91)	445,000
Novel Methods for Fabrication Cost Reduction of Pressure Infiltration Cast Metal Matrix Composite Components (ORL95-01)	200,000
Ultra-Precision Automated Measurement for Manufacturing (ORL95-08)	80,000
Neural Network Model (ORL95-90)	150,000
Modeling and Simulation of Advanced Sheet Metal Forming (PNNL94-38)	340,000
Materials Properties, Behavior, Characterization or Testing	$ 370,000
In-Line Aluminum Sensors (ORL95-04)	90,000
The Role of Yttrium in Improving the Oxidation Resistance in Advanced Single Crystal Nickel-Based Superalloys for Turbine Applications (ORL95-07)	45,000
Processing/Property Relationships in Centrifugally Cast Al-Metal Matrix Composites (MMC) (PNNL94-02)	80,000
Bioactive and Porous Metal Coatings for Improved Tissue Regeneration (PNNL95-23)	155,000

OFFICE OF ENERGY RESEARCH (continued)

	FY 1996
Office of Computational and Technology Research (continued)	
Division of Advanced Energy Projects and Technology Research (continued)	
Advanced Energy Projects Program	$ 8,034,851
Device or Component Fabrication, Behavior or Testing	$ 3,991,851
Magnetic Refrigeration for Sub-Room Temperature Cooling	310,000
Composite Magnetostrictive Materials for Advanced Automotive Magnetomechanical Sensors	101,000
Energy Related Applications of Selective Line Emitters	254,000
A Novel Tandem Homojunction Solar Cell: An Advanced Technology for High Efficiency Photovoltaics	268,000
Two-Dimensional Synthesis: Ultrathin Porous Membranes	300,000
Blue-Emitting Devices Based on Galllium Nitride	332,000
Magnetically Enhanced Thermoelectric Cooling	250,000
PV-Powered, Electrochromic Windows	330,000
Hot Carrier Solar Cells	330,000
Atomic and Nanoscale Engineering of Thermophotovoltaic Semiconductors Using Scanning Probe Microscopy Techniques	315,000
Photochemical Solar Cells	150,000
Biomolecular Optoelectronic Devices	370,000
Semiconductor Broadband Light Emitters	382,000
A Thermo-Photovoltaic Generator for Use in a Lightweight Electric Car	299,851
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 3,333,000
Photorefractive Liquid Crystals: New Materials for Energy-Efficient Imaging Technology	300,000
Evaporation Through Tungsten to Achieve High-Rate Vapor Phase Processing of Intermetallics	318,000
Supported Molten Metal Catalysts: Development of a New Class of Catalysts	316,000
Ultrasonic and Dielectric Noninvasive Diagnostics for Sintering of Ceramic Composites	290,000
Compact MEV Ion Implanter	298,000
Combinatorial Synthesis of High T_c Superconductors	144,000
Thermoelectric Quantum Wells	350,000
Porous Carbons: Controlling Structure, Composition and Performance	374,000
Fabrication and Characterization of Micron Scale Ferromagnetic Features	101,000
Micro-Hollow Cathode Discharge Arrays: High Pressure, Nonthermal Plasma Sources	229,000
Rapid Melt and Resolidification of Surface Layers Using Intense, Pulsed Ion Beams	300,000
Experimental and Theoretical Investigation of Duel-Laser Ablation for Stoichiometric Large-Area Multicomponent Film Growth	147,000
"Off-Diagonal" Thermoelectricity for Cooling and Power Generation	166,000
Materials Properties, Behavior, Characterization or Testing	$ 710,000
Exploitation of Room Temperature Molecule/Polymer Magnets for Magnetic and Electromagnetic Interference Shielding and Electromagnetic Induction Applications	322,000
Molecular Surface Modification as a Means of Corrosion Control	388,000

OFFICE OF ENERGY RESEARCH (continued)

	FY 1996
Small Business Innovation Research Program	$40,399,742
Materials, Preparation, Synthesis, Deposition, Growth or Forming	$13,909,822
Phase I Projects	$1,796,412
Control of Glycol Dehydrator Benzene, Toluene, Ethylbenzene, and Xylene Emissions	75,000
Composite Ceria Electrolytes for Solid Oxide Fuel Cells	75,000
Nitrogen Selective Adsorption for Natural Gas Upgrading	75,000
Gas-Solid Reaction and Separation Process for Simultaneous Removal of Toxic Metals and Particulates in Coal-Based Power Systems	75,000
An Attrition-Resistant Zinc Titanate Sorbent for a Transport Reactor	75,000
Noncontact Viscosity Measurement of Molten Glass Using Laser-Generated Ultrasound for Process Control During Melting and Forming Operations	75,000
A Light Scattering Based Sensor for On-Line Monitoring of Fiber Diameter Distribution During Fiberglass Manufacturing	74,999
Advanced Materials for Higher Temperature Glass Forming	75,000
Novel Use of Gas Jet Plasma to Prepare Amorphous Silicon Alloy	75,000
High Rate Deposition of Transparent Conducting Zinc Oxide Using Activated Oxygen for Photovoltaic Manufacturing Cost Reduction	75,000
Innovative Bonding and Spray-Forming Techniques for Cost-Effectively Producing High Performance Induction Motors	74,607
Tungsten Trioxide Films for Detection of Nitrogen Oxide in Automotive Exhaust Streams	72,420
Development and Testing of Environmentally-Safe Extractive Scintillator Solutions for Alpha Spectrometry	75,000
Binary-Chalcogenides as Evaporation Source Material For Cu(In, Ga) $(Se,S)_2$ Thin-Film Deposition	74,847
Development of Optimal SnO_2 Contacts for CdTe Photovoltaic Applications	75,000
Large Area, Low Cost Processing for CIS Photovoltaics	74,658
Improved Processes for Forming CIS Films	75,000
Ultrafast Polysilylene Scintillators	74,975
Highly Branched, Lightly Crosslinked, Solid Polymer Electrolytes	74,992
An Innovative Approach to Synthesis of Porous Intermetallic Matrix Composites for Regenerative Cooling Below 20K	75,000
Development of Artificial Pinning Center NbTiTa Conductor for High Field Applications	74,984
NbTi Ternary and Quarternary Alloys for High Field (>8T) Applications	74,937
Development of a New High-Field NbTi Superconductor with Mechanically Introduced Ta Inclusions	74,996
Improved Ultrafast Scintillators for Nuclear Physics	74,997
Phase II Projects (First Year)	$8,074,120
Low Cost, Contamination-Tolerant Electrocatalysts for Low-Temperature Fuel Cells	750,000
A Low Cost, High Temperature Superconductor Wire Manufacturing Technology	750,000
A Low Cost Receiver Plate Manufacturing Process for High Concentration Photovoltaic Systems	680,000
An Intumescent Mat Material for Joining of Ceramics to Metals at High Temperatures	750,000
Development of Modulator Quality Rubidium Titanyl Arsenate Crystals for Remote Sensing Laser Systems	750,000

OFFICE OF ENERGY RESEARCH (continued)

	FY 1996
Small Business Innovation Research Program (continued)	
Materials, Preparation, Synthesis, Deposition, Growth or Forming (continued)	
A Novel Method to Recycle Thin Film Semiconductor Materials	600,000
An Improved Material and Low-Cost Fabrication Options for Candle Filters	750,000
An Integrated Catalyst/Collector Structure for Regenerative Proton-Exchange Membrane Fuel Cells	719,147
Nanostructured Interstitial Alloys as Catalysts for Direct Energy Applications	750,000
Environmentally Responsible Recycling of Thin-Film Cadmium Telluride Modules	75,000
Low-Cost, Large-Area, High-Resistivity Substrates for Gas Microstrip Detectors	749,973
An Economic Sorbent for the Removal of Mercury, Chlorine, and Hydrogen Chloride from Coal Combustion Flue Gases	750,000
Phase II Projects (Second Year)	$4,039,290
A Ceramic Material and Process for Use in Monolithic Ceramic Cross-Flow Filters	617,274
Jet Vapor Deposition of Multilayer and Nanocluster Thick Film Targets for Radioactive Nuclear Beams and Medical Applications	750,000
Design and Application of Close-Spaced Thermionic Converters with Novel Isothermal Electrodes	750,000
A Multilayer Silicon Carbide Fiber Coating for Toughened, Neutron Radiation-Resistant Silicon Carbide/Silicon Carbide Composites	422,016
Economical and Reliable Niobium-Tin Conductors via Innovations in Stabilizers	750,000
Carbon-Carbon to Copper Joining for Fusion Reactor Applications	750,000
Materials, Properties, Behavior, Characterization or Testing	$ 8,962,093
Phase I Projects	$1,797,948
Thermally Stable Nitrogen-Absorbents	75,000
Improved Sealing Molten Carbonate Fuel Cell Electrolyte Matrix	74,946
Intermediate Temperature (~650 Degrees Celsius), High Power Density Solid Oxide	74,977
Carbon Monoxide Tolerant Anodes for Proton Exchange Membrane (PEM) Fuel Cells	75,000
Novel Proton Exchange Membrane (PEM) for Fuel Cell Application	75,000
Low Cost Advanced Bipolar Plates for Proton Exchange Membrane Fuel Cells	75,000
Natural Gas Reformer Cleanup System for Proton Exchange Membrane Fuel Cells	75,000
Improved Bi-2223 Flux Pinning Through Chemical Doping	75,000
Low Cost Multifilament Composite Process	75,000
High Temperature Superconducting Composites With Low Alternating Current Loss	75,000
Template-Mediated Synthesis of Periodic Membranes for Improved Liquid-Phase Separations	75,000
Novel Fiber-Based Adsorbent Technology	75,000

OFFICE OF ENERGY RESEARCH (continued)

	FY 1996
Small Business Innovation Research Program (continued)	
Materials, Properties, Behavior, Characterization or Testing (continued)	
Phase I Projects (continued)	
Recyclable Bio-Reagent for Rapid and Selective Extraction of Contaminants from Soil	74,937
Innovative Method to Stabilize Liquid Membranes for Removal of Radionuclides from Groundwater	75,000
Metal-Binding Silica Materials for Wastewater Cleanup	74,999
A Low Cost Process for the Concentration and Stabilization of Mixed Low Level Waste	75,000
A Reusable, Non-Toxic, Non-Lethal Activated Barrier to Delay Unauthorized Intruders by Vision Obscuration	75,000
Coating Capillary Optics to Improve X-ray and Neutron Transmission	75,000
Monolithic Polycapillary Optic for Bending and Microfocusing Neutron Beams	73,429
Superhard Nanophase Cutter Materials for Rock Drilling Applications	75,000
Evaluation and Constitutive Modeling of Unidirectional SiC/SiC Composites with Engineered SiC Fiber Coatings Subjected to Neutron Irradiation	75,000
Innovative Fabrication of SiC/SiC Composites with High Through-the-Thickness Thermal Conductivity	75,000
High Numerical Aperture Scintillating Fibers	74,660
Low Loss Silicon Nitride Technology for High Power Rf Transmission Windows	75,000
Phase II Projects (First Year)	$2,989,171
Rotating, In-Plane Magnetization and Magneto-Optic Imaging of Cracks Under Coatings on Ferromagnetic Metals	750,000
Development of Laser Materials and Rugged Coatings as Components for Tunable Ultraviolet Laser Systems	739,171
Application of Raman Spectroscopy to Identification and Sorting of Post-Consumer Plastics for Recycling	750,000
A Sensor for Automated Plastics Sorting	750,000
Phase II Projects (Second Year)	$4,174,974
An Apparatus for Structural Analysis of High Temperature Materials Using Synchrotron Radiation	750,000
A Novel High Strength Ceria-Zirconia Toughened Alumina Ceramic with Superior High Temperature Corrosion and Erosion Resistance	425,165
Improvements in the Characteristics of Ternary Niobium Titanium Tantalum Alloys	750,000
X-Ray Absorption Spectroscopy for Trace Analysis of Chemical Phase and Composition	749,809
High Temperature Thermally Stable Multi-Layer Quantum Well Films	750,000
A Long Life Zinc-Oxide Titanium-Oxide Sorbent	750,000

OFFICE OF ENERGY RESEARCH (continued)

	FY 1996
Small Business Innovation Research Program (continued)	
Device or Component Fabrication, Behavior or Testing	$17,527,827
Phase I Projects	$ 5,016,195
Catalytic Membrane for High Temperature Hydrogen Separations	75,000
Low Cost, Environmental Friendly Carbonate Fuel Cell Matrix Fabrication	75,000
High Speed Manufacturing for Molten Carbonate Fuel Cell Components	74,593
High Performance Membranes for Removal of Carbon Dioxide from Natural Gas	75,000
Advanced Coal Based Power System Components Using Reaction Bonded Silicon Carbide	74,819
A Real Time Hydrocarbon Emissions Sensor for Hybrid Electric Vehicles	75,000
A Sensor for In-Situ Detection, Identification, and Quantification of TCE for Cone Penetrometers	74,796
Cone Penetrometer Deployable Solid Phase Optical Chemical Sensor for Subsurface Detection of Halohydrocarbons	74,999
Real Time Monitor for the Laser-Based Coatings Removal System	74,999
A New Separation and Treatment Method for Soil and Groundwater Restoration	75,000
Continuous Analyzer for Monitoring Hydrogen Chloride and Chlorine During Site Cleanup Activity	74,703
A Practical Laser Induced Breakdown Spectrometer for Real Time On-Line Monitoring of Aqueous Process Streams	74,392
A Low Level Tritium Monitor Based on a Multi-Phase Scintillator Material	75,000
A Miniaturized Flow-Injection System for Unattended Monitoring of Uranium by Electrochemical Detection	74,998
Long-Life Electrical Neutron Generator	75,000
Tracktag-A GPS/RFID Tag for Location and Status Monitoring	75,000
Development of an RF Tagging Method for Use in Monitoring International Nonproliferation Treaty Compliance	74,834
A Compact Neutron Generator	74,971
Intelligent Sensing and Control System for Ethylene Production Using Laser Ultrasonic Coke Detention	74,941
Thin-Film, Micron-Scale Transformers	74,742
Passive Electronic Components from Nanostructured Materials	75,000
A Novel On-Line Ammonia Sensor for Energy Conversion Applications	74,995
A Multicore Optical Fiber Sensor for Mass Transport and Particulates	75,000
Infrared Hollow Waveguide Organic Solvent Analyzer	74,583
Stratospheric Water Vapor Microsensor	75,000
A Simple, Inexpensive Approach to Real-Time Calibration of Radiometric Instrumentation	74,977
High Altitude Water Vapor Concentration Measurement Using Diode Laser Interferometry	74,407
Miniature Spectrometer Based on a Novel Optical Filter with Spectral Selectivity Distributed Along the Aperture	74,970
A High Resolution Bug Eye Orientation Sensor Based on Fuzzy Optical Metrology	74,995
Compact, Airborne Laser Multigas Sensor	74,970
Microwave Radiometer for Passively and Remotely Measuring Atmospheric Water Vapor	74,843
Advanced Water Sensor for Unmanned Aerial Vehicles	75,000
High-Gain Monocapillary Optics	75,000
High Performance X-Ray and Neutron Microfocusing Optics	74,850

OFFICE OF ENERGY RESEARCH (continued)

Small Business Innovation Research Program (continued)

Device or Component Fabrication, Behavior or Testing (continued)

Phase I Projects (continued)

	FY 1996
Thermally Stable Polycrystalline Diamond Cutters for Hard Rock Drilling	75,000
Very Low Friction Small Radius Domed Cutters for Percussion Drill Bits	75,000
Development and Testing of a Jet Assisted Polycrystalline Diamond Drilling Bit	75,000
Advanced Low-Stress Bonding of Thermally Stable Polycrystalline Diamond Cutters to Tungsten Carbide Substrates	74,929
Nanocrystalline Superhard, Ductile Ceramic Coatings for Roller Cone Bit Bearings	74,962
Solid-State Ultracapacitors for Electric Vehicles and Consumer Electronics	75,000
A Four Volt per Cell Ultracapacitor with High Energy Density	75,000
A High Power Battery Based on Insertion Electrodes	75,000
A High Power Bipolar Ni-MH Battery for a Hybrid Vehicle	75,000
Synergetic Ultracapacitor	75,000
High Surface Area Non-Oxide Ceramic Electrodes for Ultracapacitors	75,000
Novel Ultracapacitor Electrodes for High Power Applications	75,000
Wrappable Inorganic Electrical Insulators for Superconducting Magnets	75,000
Novel Composite Insulators for Radio-Frequency Antenna Limiters	75,000
Pulsed Induction Joining of Sapphire to Metal for Gyrotron Windows	74,900
Joining of Tungsten Armor Using Functional Gradients	75,000
A Cost-Effective Technical Approach to Fabricating High Jc Bronze-Route $(Nb,Ti)_3Sn$ Superconducting Wire for Fusion Applications	74,996
Fabrication of a Copper-Backed Beryllium PFC Armor with a Built-In Diffusion Barrier Structure	75,000
Development and Evaluation of Mineral Insulated Diagnostic Probes Subjected to High Dose Neutron Irradiation	75,000
Silicon Detectors with 40Å Entrance Window for Low Energy Ions and Neutral Particles	71,080
Carbon Thermostructure for Silicon-Based Particle Detectors	75,000
Light Amplifier	74,186
High Performance Optical Detectors for Calorimetry	75,000
Design, Development, and Fabrication of Hybrid High Temperature Superconducting Current Leads	75,000
Design of Novel Induction Accelerator Gaps	75,000
A LaF_3:Nd + Photosensitive Wire Chamber for Gamma-Ray Imaging	74,971
Large Area Pixelated and Tiled X-Ray and Gamma-Ray Detector	75,000
Improved Cost and Radiation Hardness for Silicon Detectors	75,000
Coplanar CdZnTe p-i-n, Gamma-Ray Detectors for Nuclear Spectroscopy	74,982
Large Room Temperature $Cd_{1-x}Zn_xTe$ Detectors	75,000
High Power Target Design for a Next Generation Radioactive Beam ISOL-Type Facility	74,873
In-Situ Nondestructive Measurements of Key Mechanical Properties of Reactor Pressure Vessels Using Innovative SSM Technology	75,000
Oxidation Induction Time Technology for Electric Cable Condition Monitoring and Life-Assessment	74,939

OFFICE OF ENERGY RESEARCH (continued)

	FY 1996
Small Business Innovation Research Program (continued)	
Device or Component Fabrication, Behavior or Testing (continued)	
Phase II Projects (First Year)	$6,540,879
Advanced High Power Silicon Carbide Internally Cooled X-ray	749,291
Chemical Microsensor Array as Integrated Chip Compatible Devices for Chemical Weapons Nonproliferation Inspection	600,787
A High Resolution Multi-hit Time to Digital Converter Integrated Circuit	749,890
A Helium-Cooled Faraday Shield Using Porous Metal Cooling	695,343
Low Cost Fabrication of Large Silicon Carbide/Silicon Carbide Composite Structures	750,000
Bandgap-Engineered Thermophotovoltaic Devices for High Efficiency Radioisotope Power	747,791
Rugged, Tunable Infrared Laser Sources	750,000
An Innovative Membrane and Process for Removal and Recovery of Natural Gas Liquids	750,000
A Lower Cost Molten Carbonate Matrix	747,777
Phase II Projects (Second Year)	
Economical Photo Films Based on Metal Oxides	736,720
A Continuous Cryopump/Pellet-Fabrication Apparatus for Fusion	748,826
Development of Expansive Cements Using Dry Flue Gas Desulfurization Solid Wastes	748,476
Highly Selective Membranes for the Separation of Organic Vapors Using Super-glassy Polymers	750,000
A Long Life Perovskite Oxygen Electrode for Calcium and Lithium Oxide Processing in Nuclear Fuel Cycles	749,994
Fullerene Based Catalysts for Heavy Oil Upgrading	750,000
A Low Emission Alkali Metal Thermal to Electric Converter Automotive Power System	749,857
An Acoustic Plate Mode Sensor for Aqueous Mercury	736,880
Small Business Technology Transfer Program	$2,978,338
Materials Preparation, Synthesis, Deposition, Growth or Forming	$1,699,000
Phase I Projects	$ 199,000
Cabled Monofilament Subelements for Improved Multifilament Niobium Tin Performance and Reduced Cost	99,000
Two-Phase Homogeneous Catalysis in Ionic Liquid and Liquid Cathrate Solvents	100,000
Phase II (First Year)	$1,500,000
Laser Processing of Thermal Sprayed Beryllium Plasma Facing Components	500,000
Amorphous Silicon/Crystalline Silicon Heterojunctions for Nuclear Radiation Detector Applications	500,000
Low Loss Sapphire Windows for High Power Microwave Transmission	500,000

OFFICE OF ENERGY RESEARCH (continued)

	FY 1996
Small Business Technology Transfer Program (continued)	
Device or Component Fabrication, Behavior or Testing	$1,279,338
Phase I Projects	$ 779,338
Fuzzy Carbon Electrode Structures for Electrochemical Double Layer Capacitors	99,545
High Speed Motor Alternators for Hybrid Electric Vehicle Energy Storage	99,830
A Flywheel Motor Alternator for Hybrid Electric Vehicles	100,000
Feasibility of Correlating Vanadium-Chromium-Titanium Alloy Weld Strength with Weld Chemistry	99,968
Development of Focusing Crystal Spectrometers for Extended X-ray Sources	100,000
Ultra-High Vacuum Radio Frequency Load	99,995
Advanced Electron Cyclotron Resonance Ion Source with Large Resonant Plasma Volume	100,000
Two-Phase Homogeneous Catalysis in Ionic Liquid and Liquid Cathrate Solvents	100,000
Phase II (First Year)	$ 500,000
Environmentally Benign Manufacturing of Compact Disk Stampers	500,000
Office of Fusion Energy Sciences	$17,209,000
Materials Properties, Behavior, Characterization or Testing	$17,209,000
Structural Materials Development	1,250,000
Insulating Ceramics for Fusion	30,000
Modeling Irradiation Effects in Solids	80,000
Fusion Systems Materials	3,493,000
Structural Materials for Fusion Systems	1,100,000
Development of Radiation-Hardened Ceramic Composites for Fusion Applications	36,000
Radiation Effects and Micromechanics of SiC/SiC Composites	40,000
Damage Analysis and Fundamental Studies for Fusion Reactor Materials Development	200,000
Development of Lithium-Bearing Ceramic Materials for Tritium Breeding in Fusion Reactors	40,000
Post-Irradiation Examination of Lithium-Bearing Ceramic Materials for Tritium Breeding in Fusion Reactors	70,000
International Thermonuclear Experimental Reactor (ITER) Materials Development for Plasma Facing Components	5,500,000
ITER Ceramic Materials	190,000
ITER Materials Evaluation	380,000
ITER Structural Materials Evaluation	200,000
Development of Nb_3Sn Superconducting Wire for the ITER Magnet Program	4,000,000
Structural Materials Development for the Conduit of ITER Cable-in-Conduit-Conductors	600,000

OFFICE OF ENERGY RESEARCH

The Office of Energy Research (ER) advances the science and technology foundation for the Department and the Nation to achieve efficiency in energy use, diverse and reliable energy sources, a productive and competitive economy, improved health and environmental quality, and a fundamental understanding of matter and energy. The Director of Energy Research is responsible for six major outlay programs: Basic Energy Sciences, Fusion Energy, Health and Environmental Research, High Energy and Nuclear Physics and Computational and Technology Research. The Director also advises the Secretary on DOE physical research programs, university-based education and training activities, grants, and other forms of financial assistance.

The Office of Energy Research conducts materials research in the following offices and divisions:

- Office of Basic Energy Sciences - Division of Engineering and Geosciences; Division of Materials Sciences; and Division of Chemical Sciences
- Office of Computational and Technology Research - Division of Advanced Energy Projects and Technology Research
- Office of Health and Environmental Research - Division of Physical and Technology Research
- Office of Fusion Energy - Division of Advanced Physics and Technology

Materials research is carried out through the DOE national laboratories, other federal laboratories, and grants to universities and industry.

OFFICE OF BASIC ENERGY SCIENCES

The Office of Basic Energy Sciences (BES) supports basic research in the natural sciences leading to new and improved energy technologies and to understanding and mitigating the environmental impacts of energy technologies. The BES program is one of the Nation's foremost sponsors of fundamental research in broad areas of materials sciences, chemical sciences, geosciences, biosciences, and engineering sciences. The BES program underpins the DOE missions in energy and the environment, advances energy-related basic science on a broad front, and provides unique national user facilities for the scientific community.

The program supports two distinct but interrelated activities: (1) research operations, primarily at U.S. universities and 11 DOE national laboratories and (2) user-facility operations, design, and construction. Encompassing more than 2,400 researchers in 200 institutions and 17 of the Nation's premier user facilities, the program involves extensive interactions at the interagency, national, and international levels. All research activities supported by BES undergo rigorous peer evaluation through competitive grant proposals, program reviews, and advisory panels. The challenge of the BES program is to simultaneously achieve excellence in basic research with high relevance to the Nation's energy future, while providing strong stewardship of the Nation's research performers and the institutions that house them to ensure stable, essential research communities and premier national user facilities.

DIVISION OF MATERIALS SCIENCES

The Division of Materials Sciences conducts a broad program of materials research to increase the understanding of phenomena and properties important to materials behavior that will contribute to meeting the needs of present and future energy technologies. The Division supports fundamental research in materials at DOE national laboratories and plans, constructs, and operates national scientific user facilities needed for materials research. In addition, the Division funds over 200 grants, mostly with universities, on a wide range of topics in materials research.

Fundamental materials research is carried out at twelve DOE laboratories: Ames Laboratory at Iowa State University, Argonne National Laboratory, Brookhaven National Laboratory, Idaho National Engineering Laboratory, Lawrence Berkeley National Laboratory, Los Alamos National Laboratory, National Renewable Energy Laboratory, Oak Ridge National Laboratory, Pacific Northwest National Laboratory, and Sandia National Laboratories in New Mexico and California, and the Stanford Synchrotron Radiation Laboratory. The laboratories also conduct significant research activities for other DOE programs such as Energy Efficiency, Fossil Energy, Nuclear Energy, Environmental Management and Defense Programs. The Division of Materials Sciences also funds a program consisting of 50 research projects at the University of Illinois Frederick Seitz Materials Research Laboratory.

The performance parameters, economics, environmental acceptability and safety of all energy generation, conversion, transmission, and conservation technologies are limited by the discovery and optimization of the behavior and performance of materials in these energy technologies. Fundamental materials research seeks to understand the synergistic relationship between the synthesis, processing, structure, properties, behavior, performance of materials of importance to energy technology applications and recycling of materials. Such understanding is necessary in order to develop the cost-effective capability to discover technological and economically desirable new materials and cost-competitive and environmentally acceptable methods for their synthesis, processing, fabrication, quality manufacture and recycling. The materials program supports strategically relevant basic scientific research that is necessary to discover new materials and processes and to eventually find optimal synthesis, processing, fabricating, and manufacturing parameters for materials. Materials Science research enables sustainable development so that economic growth can be achieved while improving environmental quality.

Specific information on the Materials Sciences sub-program is contained in the DOE publication DOE/ER-0703 Materials Sciences Programs FY 1996 (published June 1997). This 168-page publication contains program descriptions for 478 research programs that were funded in Fiscal Year 1996 by the Division of Materials Sciences. Five cross-cutting indices identify all 478 programs according to Principal Investigator(s), Materials, Techniques, Phenomena and Environment. Other contents include identification of the Division of Materials Sciences Staff structure and expertise; a bibliographical listing of 48 scientific workshop, topical, descriptive, Research Assistance Task Force and research facilities reports on select topics that identify materials sciences research needs and opportunities; a descriptive summary of the DOE Center of Excellence for the Synthesis and Processing of Advanced Materials; a descriptive summary and access information on 15 National Research User Facilities including synchrotron light sources, neutron beam sources, electron beam microcharacterization instruments, materials preparation and combustion research; and an analytical summary of research funding levels. Limited copies may be obtained by calling (301) 903-3427 and requesting DOE publication DOE/ER-0703. Project summaries are also available under the Division's home page on the Worldwide Web (www.er.doe.gov/production/bes/dms/portfolio.html).

NATIONAL USER FACILITIES UNDER THE OFFICE OF BASIC ENERGY SCIENCES

Basic Energy Sciences (BES) is responsible for the planning, construction, and operation of many of the Nation's most sophisticated research facilities, including third-generation synchrotron light sources and high-flux neutron sources as well as specialized facilities for microcharacterization, materials synthesis and processing, combustion research, and ion beam studies. These facilities are unmatched in the world in their breadth of capabilities and number of scientific users. BES facilities have enormous impact of science and technology, ranging from the structure of superconductors and biological molecules to the development of wear-resistant prostheses, from atomic-scale characterization of environmental samples to elucidation of geological processes, and from the production of unique isotopes for defense applications and cancer therapy to the development of new medical imaging technologies.

BES research facilities serve over 4,500 researchers from universities, industry, and government laboratories each year. These users conducted forefront research in physics, materials sciences, chemical sciences, earth sciences, structural biology, engineering, medical and other sciences. The costs for the construction and the safe, user-friendly operation of these world class facilities are substantially beyond the capability of individual academic and private industrial research laboratories. They are made available to all qualified users from academia, industry, and both DOE and non-DOE government laboratories, most generally without charge for non-proprietary research that will be published in the open literature.

The research facilities permit the Nation's science and technology enterprise to have access to research instruments that are required for world-competitive forefront research that would not otherwise be possible. Included amongst the numerous honors and distinctions to the research that has been carried out at the BES national user facilities was the 1994 Nobel Prize in Physics, shared by Dr. Clifford G. Shull, who carried out pioneering investigations in neutron scattering at Oak Ridge National Laboratory. All of the BES national user facilities have been constructed within cost, on schedule, and with rigorous compliance to all environmental, safety and health regulations. Further information about the National User Facilities can be found in "Scientific Research Facilities," published by the U.S. Department of Energy; available from the Office of Basic Energy Sciences, (301) 903-3081.

DIVISION OF CHEMICAL SCIENCES

The Division of Chemical Sciences supports research important to fossil chemistry, combustion, advanced fusion concepts, photoconversion, catalysis, separations chemistry, actinide and lanthanide chemistry, thermophysical properties of complex fluids, nuclear waste processing, and environmental remediation. Research related to materials is carried out in the areas of heterogeneous catalysis, advanced battery technology, and materials precursor chemistry. The operating budget for FY 1996 for materials-related programs was $5,300,000 and was allocated to 42 projects in heterogeneous catalysis, advanced batteries and materials precursor chemistry.

The program in catalysis emphasizes fundamental chemical, physical, materials and engineering aspects related to catalytic chemistry. Research into fundamental aspects of heterogeneous catalysis overlaps in several areas with complementary efforts in the Division of Materials Sciences. Among these areas are the synthesis of oxides having large surface areas and large pore volumes, but fairly small pores. This includes single and mixed oxides which are either crystalline or amorphous. Another area of overlap is the characterization of thin oxide films on metals. These materials not only have important relationships to industrial catalysts but also are intrinsically interesting and allow the types of detailed studies of ceramic type properties normally associated with single crystals. Structural studies on bimetallic crystals as model catalysts constitutes a second area of overlap. This area is closely tied to alloy physics. Finally, the reactive decomposition chemistry of chlorocarbons on single crystals has a strong relationship to corrosion and lubrication.

The Advanced Battery Research program supports fundamental research to help develop new generic battery technology focused on the non-automotive consumer market with emphasis on improvements in battery size, weight, life, and recharge cycles. Areas of research include materials development and characterization, battery component development and interactions, characterization methodologies, and systems development and modeling. Although both primary and secondary battery systems are considered, the greatest emphasis is placed on rechargeable (i.e., secondary) battery systems. The program covers a broad spectrum of research including investigations of lithium cells, metal hydrides, fundamental studies of composite electrode structures, failure and degradation of active electrode materials, thin-film electrodes, electrolytes, and interfaces. Characterization and methodologies include problems of electrode morphology, corrosion, separator/electrolyte stability, stable microelectrodes, and the transport properties of electrode and electrolyte materials and surface films. Investigations in computational chemistry, modeling, and simulations, including property predictions, phenomenological studies of reactions and interactions at critical interfaces, film formation, phase change effects on electrodes and characterization of crystalline and amorphous materials are also of interest.

Chemical Sciences-supported materials precursor chemistry centers on the chemistry of advanced materials precursors, including the synthesis of novel inorganic and organometallic and polymeric structures which could serve as precursors to ceramics and other advanced materials. The research is represented by the following areas: catalysis to link monomeric/ polymer building blocks; the mechanisms of oligomerization steps; electronic theories to predict precursors for new ceramics; emerging advanced materials based on complex oxides; single source precursors to multicomponent oxides; the design of materials with tailored properties; and the synthesis and characterization of complex 3-dimensional structures.

The Division of Chemical Sciences manages several large scientific facilities. Four of these are user-oriented: the Combustion Research Facility at Sandia/California, the High Flux Isotope Reactor at Oak Ridge National Laboratory, the Stanford Synchrotron Radiation Laboratory at Stanford University and the National Synchrotron Light Source at Brookhaven National Laboratory. The National Synchrotron Light Source is operated in conjunction with the Division of Materials Sciences.

For information about specific programs the DOE contact is William S. Millman, (301) 903-3285. The reader also is referred to the Worldwide Web for the publication <u>Summaries of FY 1996 Research in the Chemical Sciences</u> (www.er.doe.gov/ production/bes/chmhome.html) for summaries of all funded programs, summaries of Small Business Innovation Research programs; and descriptions of major user and other special facilities.

DIVISION OF ENGINEERING AND GEOSCIENCES

Materials research in the Division of Engineering and Geosciences is sponsored by two different programs as described below.

The BES Engineering Research Program was started in 1979 to help resolve the numerous serious engineering issues impeding efforts to meet U.S. long-term energy needs. The program supports fundamental research on broad, generic topics in energy related engineering-topics not as narrowly scoped as those addressed by the shorter term engineering research projects sponsored by the various DOE technology programs. Special emphasis is placed on projects which, if successfully concluded, will benefit more than one energy technology.

The broad goals of the BES Engineering Research Program are: (1) to extend the body of knowledge underlying the current engineering practice so as to create new options for enhancing energy savings and production, for prolonging useful equipment life, and for reducing costs without degradation of industrial production and performance quality; and (2) to broaden the technical and conceptual base for solving future engineering problems in the energy technologies. The DOE contact for this program is Robert E. Price, (301) 903-5822.

ENGINEERING SCIENCES RESEARCH

A brief description of Engineering Sciences supported programs is found in DOE/ER-0704, "Summaries of FY 1996 Engineering Research," which was published in June 1997. Limited copies may be obtained by calling (301) 903-5822.

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

129. **FUNDAMENTALS OF THERMAL PLASMA PROCESSING**
$478,000
DOE Contact: Robert E. Price, (301) 903-5822
Idaho National Engineering Laboratory Contact: J. R. Fincke, (208) 526-2031

This project is the experimental portion of a coordinated experimental-theoretical research project on thermal plasma processing of materials. This work is primarily focused on the development of advanced diagnostic and computational techniques and their application to obtain a better and more detailed understanding of the fundamental physical and chemical processes occurring in nonequilibrium thermal plasmas with entrained particles. The techniques thus developed and the information and insights they provide, can then be directly applied to process design, optimization, and scale-up. The diagnostic and computational techniques already developed under this project now represent the state of the art in this area.

During the next five years of this project, we propose to further extend and generalize these techniques to permit their application to several additional topics of timely importance in the thermal plasma processing of materials, namely (1) functionally gradient materials (FGMs), (2) reactive plasma spraying, and (3) plasma chemical synthesis of nanophase materials. These topics share some common features and physics which make it efficient and cost-effective to consider them together. They forma a natural progression and will be pursued sequentially in the above order, but with significant overlap.

Keywords: Plasma Processing, Functionally Gradient Materials

130. **MULTIVARIABLE CONTROL OF THE GAS-METAL ARC WELDING PROCESS**
$153,000
DOE Contact: Robert E. Price, (301) 903-5822
MIT Contact: David E. Hardt, (617) 253-2429

Continuing from last year we have been pursuing three related topics: development of a unique high bandwidth are—furnace, development of a "variable footprint" welding torch, and exploration of distributed parameter models, sensors and controllers. These topics are all motivated by the need to have greater control over the spatial distributions, owing to the limitations imposed by a lumped parameter modeling approach. The arc furnace work was completed this year, with demonstration of de-coupled temperature and flowrate control. A U.S. patent has been issued for this furnace concept and the attendant control system.

The work on the variable footprint torch is pursuing a Gas-Modulated Plasma Arc approach. Characteristics of the new hardware include decoupled heat and filler metal delivery, variable heat output distribution and modular construction for multi-functionality. A physically-based model is currently under development as an aid in designing an appropriate controller for the said torch. The model will be tested and verified upon completion of the torch, currently under in-house fabrication.

In the area of distributed parameter control, we are considering both the basic modeling form along with a multivariable optimal control philosophy. Techniques are being developed for optimally locating and shaping (in space and time) heating/cooling sources (e.g., cooling passages in a mold). The theory for optimal location of measurements has been studied, and simulations and experiments were conducted to study the findings. As an example application, transient temperature control was implemented on a model used by Bethlehem Steel Corporation for a hot slab mill. The techniques being developed are being used as guidelines for developing new actuators (heaters, torches etc.) and sensors for a variety of industrial processes.

Keywords: Gas-Metal Arc, Welding

131. **METAL TRANSFER IN GAS-METAL ARC WELDING**
$124,000
DOE Contact: Robert E. Price, (301) 903-5822
MIT Contacts: T. W. Eagar and J. Lang, (617) 253-3229

Three projects have been undertaken, all aimed at improved control of the final properties of a weld.

The first project, now completed, was a study to model droplet detachment dynamics. Experimental data was generated using a specially developed GMAW system with laser imaging, high speed video, and electrode vibration mechanics. Simulations based on a lumped parameter model were also conducted and good results with the experiments attained.

The second project is to develop a semi-transferred plasma welding system. This system is presently under construction. It will consist of two independent plasmas. A transferred plasma is used for substrate heating, while a second non-transferred plasma is used to provide a spray coating stream. Each will be independently controlled with a separate power supply.

The third project is to model and predict the physics of the weld pool during GMAW. The first phase of the experimental component of this project has been completed. The theoretical part is currently under way. Present efforts are focused on determining the shape of the free surface of the molten metal and its influence in the fluid flow, and the influence of Marangoni flows due to compositional differences between the impinging droplet and the substrate.

Keywords: Gas-Metal Arc, Welding

132. **THERMAL PLASMA CHEMICAL VAPOR DEPOSITION OF ADVANCED MATERIALS**
$157,975
DOE Contact: Robert E. Price, (301) 903-5822
University of Minnesota Contact: J. Heberlein

The objectives of this program include the characterization of plasma reactors used for materials processing in particular for the deposition of diamond films and the generation of ultrafine particles.

For characterizing a particular diamond deposition reactor, a realistic model has been developed for liquid precursor injection into the plasma in front of the substrate. This three-dimensional model is based on a fluid dynamic description of the plasma jet and the injection gas streams, an energy transfer model including evaporation of the droplets, dissociation of the vapors, and recombination reactions according to chemical kinetics. A surface kinetics model describes the diamond film growth. Initial results show reasonable agreement with experiments.

The theoretical description of rf reactors for ultrafine powder production has been completed, and temperature and velocity profiles for different reactor configurations and operating conditions provide a basis for future optimal reactor design.

In order to meet needs for spatially and temporally resolved measurements of the characteristics of turbulent plasma jets, a diagnostic capability has been established based on laser scattering techniques. Results of these measurements will be compared with findings obtained at INEL.

For determining transport coefficients of gas mixtures at plasma temperatures, the influence of different interaction potentials during binary collisions has been established and recommendations have been made for potentials providing the most reliable data.

Keywords: Plasma, CVD, Diamond

133. **RESEARCH ON COMBUSTION-DRIVEN HVOF THERMAL SPRAYS**
$96,893
DOE Contact: Robert E. Price, (301) 903-5822
Pennsylvania State University Contact: G. Settles, (814) 863-1504

The High-Velocity Oxy-Fuel (HVOF) thermal spray process combines the fields of materials, combustion, and gas dynamics. It relies on combustion to melt and propel solid particles at high speeds onto a surface to be coated. The goal of this research is to understand and improve the HVOF deposition of corrosion-resistant coatings, which are important in many energy-related industries. This involves both experimentation and modeling.

HVOF spraygun nozzle design and operating parameters have been found with which to vary the kinetic and thermal energies of the spray particles independently. Through metallographic analysis, the resulting coating properties are now being studied. The ability to do this is apparently unique, with results which are expected to be of direct use to HVOF users. For example, it should be possible to tailor coatings to produce desirable properties such as low porosity, high density, and high corrosion resistance. An early result is that stainless steel particles already molten before impact tend to produce less desirable coatings than solid particles which fuse upon impact due to their kinetic energy.

Results of the research are presented annually at the National Thermal Spray Conference. One Ph.D. has been educated and a second graduate student is currently working on this project.

Keywords: Combustion, Oxy-Fuel

134. **EFFECT OF FORCED AND NATURAL CONVECTION ON SOLIDIFICATION OF BINARY MIXTURES**
$0
DOE Contact: Robert E. Price, (301) 903-5822
Purdue University Contact: F. Incropera, (317) 494-5688

This study deals with the influence of combined convection mechanisms on the solidification of binary systems. A major accomplishment of research performed to date has been the development and numerical solution of a continuum model, which uses a single set of equations to predict transport phenomena in the liquid, "mushy" (two-phase), and solid regions of the mixture. Calculations have been performed for aqueous salt solutions and/or lead/tin alloys involving forced convection, thermo/solutal natural convection, and/or thermo/diffusocapillary convection. The calculations have revealed a wide variety of rich and robust flow conditions, including important physical features of the solidification process which have been observed experimentally but have heretofore eluded prediction. These features include double-diffusive layering in the melt, development of an irregular liquidus front, remelting of solid, development of flow channels in the mushy region, and the establishment of characteristic macrosegregation patterns (regions of significantly different composition) in the final solid. Theoretical and experimental studies have also revealed means by which macrosegregation may be actively suppressed, as, for example, through the application of a magnetic field or intermittent rotation of the mold.

Keywords: Mixture, Convection

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

135. **CONTINUUM DAMAGE MECHANICS - CRITICAL STATES**
$ 0
DOE Contact: Robert E. Price, (301) 903-5822
Arizona State Contact: D. Krajcinovic, (602) 965-8656

Objective: Primary objective of the current research program is to examine a variety of critical states in mechanical response of brittle and quasi-brittle solids containing a large number of crack-like micro-defects. More specifically, the focus of the ongoing research is placed on the determination of circumstances (type of loading, confinement level, shape and size of the specimen, thermal and environmental conditions, etc.) leading to the onset of critical states defined as a threshold connectivity at which a solid ceases to support external loads.

Technical Approach: Current applied mechanics / engineering practice in evaluating the mechanical failures of brittle and quasi-brittle solids emphasizes use of effective continuum theories coupled with the deterministic and highly idealized description of the defect geometry (such as doubly periodic arrays of penny-shaped cracks). In contrast, the approach selected in this research program accentuates the stochastic geometry of the microstructural disorder and its effect on the onset of macro-fracture and the type of the failure mode.

One of the important aspects of this research is to explore applicability of the novel methods of statistical physics (percolation theory, models of self-organized criticality, etc.) to micromechanical models. Some of the already obtained results provide connection between the mechanical parameters such as stiffness and damage variable and the percolation theory concepts such as the order parameter, excluded volume, etc. This provides a set of rational criteria for the selection of the universal dimensional invariants needed to describe the onset of a certain class of failures. Secondly, use of the statistical methods (such as fractal and multifractal formalism) provide a superior and size-independent (intrinsic) description of the fluctuations in the stress field (stress concentrations) in the vicinity of the critical states. This aspect alone should provide a definitive answer related to the dependence of the order-disorder transition on the microstructuraltexture and/or boundary conditions. In summary, the selected approach provides the best hope of description of the universal aspects of the stochastic nature of the damage and its evolution in the vicinity of the critical state.

Keywords: Continuum Mechanics, Fractals, Brittle Materials

136. **AN INVESTIGATION OF HISTORY-DEPENDENT DAMAGE IN TIME-DEPENDENT FRACTURE MECHANICS**
$99,729
DOE Contact: Robert E. Price, (301) 903-5822
Battelle Memorial Institute Contact: F. Brust, (614) 424-5034

In order to meet the demand imposed by future technology, new plants with increased energy efficiency must operate at relatively high temperatures. Additionally, the existing power generation equipment in the United States continues to age and is being used far beyond its intended life. Some recent failures have clearly demonstrated that the current methods for insuring safety and reliability of high temperature equipment is inadequate. Owing to these concerns, a thorough understanding of high temperature failure initiation and propagation in materials exposed to variable mechanical and thermal loading is very important.

In the past, the evolution of damage has been addressed through a macroscopic theoretical model (developed as part of this effort) which attempt to predict the crack growth and failure response of material components exposed to high temperature conditions. However, micromechanical processes such as diffusion of atomic flux into grain boundaries, elastic accommodation and creep deformation of the material and grain boundary sliding do contribute significantly to the nucleation and growth of voids leading to failure. Understanding gained by consideration of micromechanics of cavity growth is crucial for developing damage-based constitutive models as well as methodologies for life prediction of structural components. While the application of this understanding in estimating life of structural materials experiencing high temperature creep has met with some success, it is of limited use for structural components experiencing complex load histories under high temperature conditions.

A micro-mechanical model accounting for rate-controlling microscopic processes has been developed as part of this effort. To date, both sustained and variable load histories have been investigated in two-dimensional geometries. The results illustrate the importance of accounting for nonlinear changes in geometry, grain-boundary diffusion processes, elastic accommodation of the surrounding material as well as more realistic constitutive laws for creep deformation. Current efforts involve investigating different load histories and three-dimensional effects. In addition, the ultimate goal of this effort is to establish a firm connection between the micro- and macro-mechanical models thereby leading to the development of appropriate methodology for life prediction of structural components exposed to high temperature conditions involving complex load histories.

Keywords: Damage, Fracture Mechanics

137. **INTELLIGENT CONTROL OF THERMAL PROCESSES**
$517,000
DOE Contact: Robert E. Price, (301) 903-5822
Idaho National Engineering Laboratory Contact: J. R. Fincke, (208) 526-2031

This project addresses intelligent control of thermal processes as applied to gas metal arc welding. Intelligent control is defined as the combined application of process modeling, sensing, artificial intelligence, and control theory to process control. The intent of intelligent control is to produce a good product without relying on post-process inspection and statistical quality control procedures, by integrating knowledge of process engineering practice and process physics into sensing and control algorithms. The gas metal arc welding process is used as a model system; considerable fundamental information on the process has been developed at INEL and MIT during the past ten years. Research is being conducted on analytical modeling of nonlinear aspects of molten metal droplet formation and transfer, and integration of knowledge-based control methods (including artificial neural networks and fuzzy logic based connectionist systems) with iterative learning control methods. Results are being transferred to industrial partners through a related EE-OTT CRADA on Intelligent Diagnostics, Sensing, and Control of Thin Section Welding.

New work has been started on control methods for distributed thermal processes. The focus of this work is specifically on processes employing one or more point sources of heat and or mass with spatial rastering and temporal modulation of the source(s) to produce a distributed temperature field in a distributed mass. The prototypical process is plasma hearth melting of metals. The initial work is investigating iterative learning control to control the trajectory of a heat source through state space (including both the spatial terajectory of the heat source and the thermal parameter trajectory).

This project is part of a collaborative research program with the Massachusetts Institute of Technology.

Keywords: Fuzzy Logic, Neural Networks

138. **ELASTIC-PLASTIC FRACTURE ANALYSIS EMPHASIS ON SURFACE FLAWS**
$132,000
DOE Contact: Robert E. Price,
(301) 903-5822
Idaho National Engineering Laboratory
Contacts: W. G. Reuter, J. Epstein,
W. Lloyd, (205) 526-0111

The objective is to improve design and analytical techniques for predicting the integrity of flawed structural components. The research is primarily experimental, with analytical evaluations guiding the direction of experimental testing. Tests are being conducted on materials ranging from linear elastic to fully plastic. The latter extends beyond the range of a J-controlled field. Specimens containing surface cracks are used to simulate the fracture process (crack growth initiation, subcritical growth, and catastrophic failure) that may occur in structural components.

Metallography and microtopography techniques have been developed to measure crack tip opening displacement and crack tip opening angle for comparison with analytical models. Moiré interferometry techniques are used to evaluate and quantify the deformation in the crack region. These studies have resulted in the ability to predict crack growth initiation of specimens containing surface cracks using constraint and fracture toughness data obtained from standard fracture toughness specimens. Results are being transferred to industry in the form of an ASTM Test Standard on Surface Cracked Specimens (Structures) that is presently being developed. Future research will focus on predicting the stable crack growth process in base metal and in weldments.

Due to the complexity of studying the fracture process in weldments, diffusion bonded specimens were used initially to simulate a weldment. This provided an opportunity to study the fracture process in a model weldment (two dissimilar materials, e.g., base metal and weld metal) of either a butt weld or a single "V" groove geometry that contained neither a heat affected zone nor residual stresses. This work has been completed and now the focus is on actual weldments of A710 steel. Two weldments have been fabricated with one having matched weld metal and the second an overmatched weld metal. Characterization of the microstructure and of local tensile properties is presently in progress. Testing of fracture toughness specimens, specimens containing surface cracks, and modified specimen geometries is planned for the future.

Keywords: Fracture Mechanics, Welding

139. **NONDESTRUCTIVE EVALUATION OF SUPERCONDUCTORS**
$205,000
DOE Contact: Robert E. Price,
(301) 903-5822
Idaho National Engineering Laboratory
Contact: K. L. Telschow,
(208) 526-1254

This project is concerned with the development and application of new nondestructive evaluation (NDE) techniques and devices for the characterization of materials, particularly high-temperature superconducting materials in tape form. Microstructural and, particularly, superconducting properties, need to be measured noninvasively and spatially in order to aid the fabrication process.

Two approaches that are both noncontacting and potentially applicable to the industrial environment are being investigated separately and together. One approach uses noncontacting induced current for determination of critical currents on a local scale. This technique can be used alone or in conjunction with external applied fields and DC transport currents to determine spatial variations in critical current density. Its operation is based on inducing the critical state and determining full penetration through the tape with a small probe coil. A new integral equation approach has been found and solved iteratively that determines the flux front profile in geometries with azimuthal symmetry accounting for demagnetization effects. The capability of high temperature SQUID sensors for measurements in long length tapes is being investigated for increased sensitivity and full hysteresis behavior determination. The second approach uses lasers to generate and detect ultrasonic wave modes in tape geometries. Specific elastic wave modes are employed both analytically and experimentally to determine layer thickness, elastic constants and grain orientation. The stability of the critical state to elastic strain is being investigated using both approaches simultaneously in a coupled mode.

Keywords: Nondestructive Evaluation, Superconductors

140. **ORIGINS OF ASYMMETRIC STRESS-STRAIN RESPONSE IN PHASE TRANSFORMATIONS**
$80,535
DOE Contact: Robert E. Price, (301) 903-5822
University of Illinois Contact: H. Sehitoglu, (217) 333-4112

A number of uniaxial and stress state experiments on the NiTi alloys that are known to undergo thermo-elastic phase transformations were conducted. Unlike steels which exhibit virtually no recoverable transformation strains, the transformation strains in this class of materials are partially recovered upon unloading, depending on the applied strain levels. Using a servohydraulic intensifier, a servohydraulic test machine, and a novel pressurized test chamber; pressures of 750MPa and axial stresses of almost any magnitude are simultaneously generated and applied to the gage section of a solid, cylindrical NiTi specimens. The work utilizes a robust internal load cell that can measure axial forces without the effect of seal friction and demonstrate innovative ways of calibrating this load cell, and methods of axial and circumferential strain measurement in a pressure environment and verify accuracy of these results. Constitutive models proposed in the literature for thermo-elastic transformation were evaluated in light of these results. The current models predict that the volume fraction of martensite is solely dependent on the effective stress. Our experimental results indicate that there is a dependence of the transformations strain on the hydrostatic stress component with strong asymmetry in tension versus compression. In view of these experimental findings, new transformation models are being developed incorporating the low symmetry of the twinning planes. The stress-induced phase transformation of CuZnAl was also found to be stress state dependent but less so than NiTi.

Keywords: Alloys, Phase Transformations

141. **MODELING AND ANALYSIS OF SURFACE CRACKS**
$192,000
DOE Contact: Robert E. Price, (301) 903-5822
MIT Contacts: David M. Parks, (617) 253-0033 and F. A. McClintock, (617) 253-2219

We are developing a mechanics basis for analyzing the fracture behavior of cracks located on or near the fusion zones of structural weldments. Such welds are often characterized by significant strength mismatch between base plate and weld metal, as well as by local strength gradients associated with metallurgical details of the heat-affected zones. Moreover, the local gradients in microstructure, and the accompanying gradients in material resistance to both ductile hole growth and cleavage fracture mechanisms provide additional complexity, compared to the corresponding fracture mechanics models of macroscopically homogeneous crack-tip microstructures and properties.

Under macroscopic mode I loading, strength-mismatched interface crack-tip stress and deformation fields show considerable differences from the corresponding fields in mechanically homogeneous media. In particular, both triaxial stress and plastic strain levels in the softer domain (e.g., an undermatched baseplate) are elevated. Families of mismatched fields have been characterized by finite element and slip-line solutions, and have been shown to apply from small-scale yielding through fully-plastic conditions.

The mismatched fields are being coupled with local models of cleavage and ductile fracture in the inhomogeneous crack-tip region, and the results compared with experiments on both model weldments created by diffusion-bonding and with actual welds in A710 steel.

Keywords: Fracture Mechanics, Welding

142. **DEVELOPMENT OF MEASUREMENT CAPABILITIES FOR THE THERMO-PHYSICAL PROPERTIES OF ENERGY-RELATED FLUIDS**
$425,000
DOE Contact: Robert E. Price, (301) 903-5822
National Institute of Standard and Technology Contacts: R. Kayser and W. Haynes , (301) 975-2583

The major objectives of this new three-year project are to develop state-of-the-art experimental apparatus for measuring the thermophysical properties of a wide range of fluids and fluid mixtures important to the energy, chemical, and energy-related industries. The specific measurement capabilities to be developed are the following: Small-Volume, Dual-Cell Dew-Bubble Point Apparatus; Heat-of-Vaporization Calorimeter and Effusion Cell for Vapor-Pressure Determinations; Solubility Measurements Using Magnetic Levitation; Thermal Diffusivity from Light Scattering; and Phase-Equilibria Apparatus for Azeotropic Aqueous-Organic-Salt Mixtures. These new apparatus will extend significantly the state of the art for properties measurements and make it possible to study a wide range of complex fluid systems (e.g., highly involatile, very insoluble, highly polar, electrically conducting, reacting) under conditions which have been previously inaccessible.

Keywords: Thermophysical Properties, Fluids

143. **HIGH-T_c SUPERCONDUCTOR-SEMICONDUCTOR INTEGRATION AND CONTACT TECHNOLOGY**
$116,800
DOE Contact: Robert E. Price, (301) 903-5822
National Institute of Standard and Technology Contacts: J. Moreland, (303) 497-3641 and J. W. Elkin, (303) 497-5448

The purpose of this project is to study materials problems faced in integrating high-T_c superconductor (HTS) thin-film technology with conventional semiconducting technologies. The emphasis of the research is to investigate HTS-semiconductor contact systems and novel HTS-semiconductor devices. The ultimate goal is to develop HTS thin-film technology to its fullest potential for multi chip module interconnections, future ULSI source and drain connections, and microelectronic microwave filters. These potential applications provide the motivation for a thorough investigation of HTS thin-film materials development of these hybrid systems. Determining the compatibility of HTS thin-film deposition and patterning processing with that of standard Si processing is crucial for expanding the applications of these hybrid technologies.

The nanostuctural properties of HTS materials have proven to have a principal influence on the electrical properties of HTS materials and devices. For this reason the use of scanned probe microscopies are being emphasized for evaluating HTS-semiconductor epitaxy as well as electrical conduction in interconnects and contacts to hybrid device structures. The further development of scanned probe microscopies, specifically for electronic device imaging will be invaluable not only for the HTS-semiconductor integration studies but for all developments in microelectronics in the foreseeable future. The current emphasis is on developing scanning potentiometry based on atomic force microscopy with resolution and sensitivity levels better than 50 nm and 1 mV, respectively. Also, investigations regarding adapting scanning potentiometry for high frequency applications up to 100 GHz are under way.

Keywords: High T_c Superconductors, Contacts

144. **THIN FILM CHARACTERIZATION AND FLAW DETECTION**
$0
DOE Contact: Robert E. Price, (301) 903-5822
Northwestern University Contact: J. D. Achenbach, (312) 491-5527

This work is concerned with the determination of the elastic constants of thin films deposited on substrates, with the measurement of residual stresses in such films and with the detection and characterization of defects in thin film substrate configurations.

There are many present and potential applications of configurations consisting of a thin film deposited on a substrate. Thin films that are deposited to improve the hardness and/or the thermal properties of surfaces are of principal interest in this work. Thin film technology does, however, also include high Tc superconductor films, films for magnetic recording, superlattices and films for band-gap engineering and quantum devices. The studies carried out on this project also have relevance to those applications.

Both the film and the substrate are generally anisotropic. A line-focus acoustic microscope, is being used to measure the speed of wave modes in the thin film/substrate system. This microscope has unique advantages for measurements in anisotropic media. Analytical and numerical techniques are employed to extract the desired information on the thin film from the measured data. Recent results include: (1) use of multiple wave modes to determine thin film constants, (2) measurements of superlattice film constants, and (3) investigation of the effect of surface roughness.

Keywords: Thin Films, Superlattices, Surface Roughness

145. **TRANSPORT PROPERTIES OF DISORDERED POROUS MEDIA FROM THE MICROSTRUCTURE**
$116,959
DOE Contact: Robert E. Price, (301) 903-5822
Princeton University Contact: S. Torquato, (609) 258-4600

This research program is concerned with the quantitative relationship between transport properties of a disordered heterogeneous medium that arise in various energy-related problems (e.g., thermal or electrical conductivity, trapping rate, and the fluid permeability) and its microstructure. In particular, we shall focus our attention on studying the effect of: porosity, spatial distribution of the phase elements, interfacial surface statistics, anisotropy, and size distribution of the phase elements, on the effective properties of models of both unconsolidated media (e.g., soils and packed beds of discrete particles) and consolidated media (e.g., sandstones and sintered materials).

Both theoretical, computer-simulation, and experimental techniques have been employed to quantitatively characterize the microstructure and compute the transport properties of disordered media. Statistical-mechanical theory has been used to obtain n-point distribution functions and to study percolation phenomena in continuum random-media models. For example, the pore-size distribution, lineal path function, and the chord-length distribution function have been investigated and computed. This has led to accurate predictions of transport properties of realistic models of isotropic as well as anisotropic heterogeneous media. Cross property relations have been derived. Rigorous relations which link the fluid permeability to length scales obtainable from Nuclear Magnetic Resonance experiments and the effective electrical conductivity have been derived. Moreover, the effective conductivity has been related to the effective elastic moduli. Recently, 3-D images of a sandstone have been obtained using X-ray tomographic techniques and statistical corrleation funcations have been extracted from them.

Keywords: Porous Media, Transport Properties

146. **INELASTIC CONSTITUTIVE EQUATION: DEFORMATION INDUCED ANISTROPY AND THE BEHAVIOR AT HIGH HOMOLOGOUS TEMPERATURE**
$149,828
DOE Contact: Robert E. Price, (301) 903-5822
Rensselaer Polytechnic Institute Contact: Erhard Krempl, (518) 266-6432

Using experimental results obtained with computer-controlled, servohydraulic testing machines, continuum mechanics and materials science as backgrounds, constitutive equations (mathematical models of material deformation behavior that are used in stress and life-time analyses) are being developed with emphasis on two aspects: Deformation induced anisotropy for large deformation on the one hand and high homologous temperature on the other. Both areas extend the modeling capability of the previously developed "unified," state variable viscoplasticity theory based on overstress (VBO).

A mathematical framework and a formulation for the representation of deformation induced anisotropy has been developed and this theory is now being applied to rolling of metals. In this case an isotropic metal can be deformed into metal with elastic and inelastic orthotropy. Simulation of this process is underway.

The small strain version of VBO has been extended to high homologous temperature and applied to Alloy 600 H at temperatures above 0.7. The model can simulate the experimentally observed creep and tensile behavior. It is also shown that the transition from the solid to the fluid state can be accomplished easily with VBO. Applications to solder materials for which ambient temperature is a high homologous temperature and an effort to reduce the number of needed constants in the model are underway.

Keywords: Deformation, Viscoplasticity

147. **STRESS AND STABILITY ANALYSIS OF SURFACE MORPHOLOGY OF ELASTIC AND PIEZOELECTRIC MATERIALS**
$137,000
DOE Contact: Robert E. Price, (301) 903-5822
Stanford University Contacts: H. Gao and D. Barnett, (415) 725-2560

The objective of this research has been to study morphological stabilities and instabilities in elastic and piezoelectric solid. In morphologies are included surface shapes, cracks, and defect patterns. In this past year the conditions for stability or instability of surfaces and interfaces in piezoelectric materials (including arbitrary elastic and piezoelectric anisotropy) have been developed.[1] This work has shown that piezoelectric coupling may tend to either stabilize or destabilize an initial flat boundary or interface. A destabilized surface evolves toward the formation of crack-like flaw. This study suggests that piezoelectric coupling could be utilized to control diffusive initiation of surface defects. A portion of future work will be directed toward corroborating theory with experiments and identifying whether more sophisticated theoretical models for defect generation need to be explored. Another direction which this research has taken is the study of fracture in piezoelectric solids. A strip saturation model and the concept of multiscale energy release rates have been introduced[2,3] to explain some existing experimental observations of the behavior of cracks in piezoelectric ceramics. Extensions of this work are underway.

Patterns of equilibrium 2-dimensional arrangements of large numbers of dislocations have been computed by using numerical methods to minimize the potential energy of the dislocation distributions. Efficiency of computation has been greatly enhanced by studying doubly periodic arrangements of dislocation cells for which some analytic reduction is possible. It has been found that many possible equilibrium patterns exist under zero applied stress, i.e., nearby equilibrium arrangements are always available. A study of the stabilty of these arrays under application of applied stresses is now underway.

Keywords: Surfaces, Interfaces, Stress Analysis, Piezoelectrics

[1]N. Y. Chien, H. Gao, G. Herrmann, and D. M. Barnett, "Diffusive Surface Instabilities Induced by Electromechanical Loading," Proceedings of the Royal Society, London, A452, pp. 527-541 (1995).

[2]H. Gao, T.-Y. Zhang, and P. Tong, "Local and Global Energy Release Rates for an Electrically Yielded Crack in Piezoelectric Ceramics," Journal of the Mechanics and Physics of Solids (in review).

[3]H. Gao and D. M. Barnett, "An Invariance Property of Local Energy Release Rates in a Strip Saturation Model of Piezoelectric Fracture," International Journal of Fracture (in review).

148. **OPTICAL TECHNIQUES FOR CHARACTERIZATION OF HIGH TEMPERATURE SUPERCONDUCTORS**
$231,000
DOE Contact: Robert E. Price, (301) 903-5822
Stanford University: G. S. Kino, (415) 497-0205

Photothermal techniques are used to measure the normal carrier density below the transition temperature T_c in high-temperature superconductors, to study the nature of the phase transition, and to measure the homogeneity and quality of these materials. A modulated focused laser beam incident on the sample varies its temperature periodically, and a second probe beam a few microns away measures the differential reflectivity associated with the thermal wave propagating along the sample. Changes in critical temperature in regions less than 100 μm apart have been measured, and the difference in quality of different samples can clearly be seen. Measurement of thermal diffusivity in single-YBCO crystals yields good estimates of the variation of normal electron density with temperature. Observations of small changes in the phase variation yield the transition temperature of the material. Polarized light observations of single-crystal YBCO near the transition point yield curves as a function of temperature with shapes that are very different, depending on the polarization of the probe beam relative to the A and B directions. Twinned samples do not show this anisotropy. The shape and sign of these curves also appears to provide a very sensitive measurement of the state of doping of the material. By measuring the modulated signals at the second harmonic of the input signal, the temperature modulation of the sample by the laser beam can be determined. During the last year the system has been rebuilt to give more accurate results, to work at lower temperatures so that we can make measurements of normal superconductors and compare with theory, and to make more rapid measurements of the quality of thin film superconductors.

Keywords: High T_c Superconductors, Thin Films

149. **3-D EXPERIMENTAL FRACTURE ANALYSIS AT HIGH TEMPERATURES**
$76,721
DOE Contact: Robert E. Price, (301) 903-5822
University of Washington Contact: Albert Kobayashi, (206) 543-5488

The objective of this three year project is to assess experimentally, the validity of T* integral and its applicability to quasi-static and dynamic ductile fracture. Early in the second year, a protocol for extracting the T* integral values from the surface displacement fields obtained by moiré interferometry was established. The procedure consists of numerically evaluating the integral along a partial contour, a small distance, ϵ, in front of the crack tip, In order to assure a state of plane stress, ϵ is equated to one plate thickness and the resultant T* is designated T^*_ϵ. The procedure was verified through numerical experiments conducted at the Georgia Institute of Technology (GIT) under a parallel DOE grant.

The established procedure was used to determine T^*_ϵ's of A606 HSLA steel, single-edge notched (SEN) specimens with small stable crack growth, $\approx$ 2 mm, and 2024-T3 aluminum, compact (CT) of large crack growth, $\approx$ 8 mm. Parallel numerical analysis of these two sets of experiments were conducted at GIT where the experimentally and numerically determined T^*_ϵ were found to be in excellent agreement. T^*_ϵ of the A606 HSLA SEN specimen continued to increase with stable crack growth, possibly due to the lack of constraint in the SEN specimen. T^*_ϵ of the 2024-T3 CT specimen reached a steady state value of $\approx$ 140 MPa-mm. The CT specimen results suggest that T^*_ϵ could be a viable fracture parameter which controls stable crack growth. The crack tip opening angles (CTOA) for the two materials immediately reached steady state values with crack growth. However, results from a FAA funded study showed that CTOA is insensitive to the inherent decrease in ductility due to increased thickness and therefore may not be a proper fracture parameter.

Keywords: Fracture Mechanics, Crack Growth

150. **SIMULATION AND ANALYSIS OF DYNAMIC FAILURE OF DUCTILE MATERIALS**
$99,410
DOE Contact: Robert E. Price, (301) 903-5822
Brown University Contact: B. Freund, (401) 863-1157

A central goal in the mechanics of materials is the determination of parameters which characterize macroscopic failure of materials in terms quantifiable characteristics of their microstructure. The motivation is to establish which characteristics account for macroscopic failure, with a view toward improvement of failure resistance through material selection or microstructural design. In the present project, emphasis is on the behavior of ductile structural alloys under high rate loading conditions. Thus, the dominant mechanism of plastic deformation is crystallographic slip and material strength degrades through nucleation, growth and coalescence of micro-voids. Plastic strains in such processes can be large and strain localization is common. The approach is to adapt methodologies for analysis of elastic-viscoplastic systems to problems selected on the basis of their relevance to safety of pressure vessel and piping systems, to materials processing and metal forming technologies, and to structural reliability under dynamic loading. Initial emphasis has been on failure of an explosively loaded ring expanding under plane strain conditions, a configuration which has been studied experimentally. Calculations reveal that strain localization sites, or necks, are more pervasive under rapid loading, and the spacing of necks decreases with increase in loading rate. The influence of inertia on bifurcation of deformation states is also being investigated theoretically. The project is being carried out in collaboration with colleagues involved in experimental research on dynamic ductile failure at the California Institute of Technology.

Keywords: Dynamic Failure, Ductile Materials

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

151. **AN ANALYTICAL-NUMERICAL ALTERNATING METHOD FOR 3-D INELASTIC FRACTURE AND INTEGRITY ANALYSIS OF PRESSURE-VESSELS AND PIPING AT ELEVATED TEMPERATURES**
$85,000
DOE Contact: Robert E. Price, (301) 903-5822
Georgia Institute of Technology Contact: S. Atluri, (404) 894-2758

Current and future power generation plants require efficient operation so that energy savings may be realized. In addition, power generation equipment in the US continues to age, creating operational dangers for the working staff as well as greater potential for power outages. Current methods to ensure safe operation of these plant components which operate in the nonlinear material regime are simplistic, and hence, not very reliable. This program is developing advanced analytical tools which can be used to reliably assure safety of future plants as well as aging plants. The finite element alternating method is the state-of-the-art methodology for determining stress intensity factors for two and three dimensional crack growth problems. This method has permitted accurate and simple analyses of linear fracture problems to be made so that sophisticated reliability assessments of operating equipment may be made. This program has extended the finite element alternating method so that it may now be used in the non-linear regime, i.e., the non-linear finite element alternating method. With this new methodology, sophisticated damage and fracture assessments can be made for components which experience failures in the elastic-plastic and high temperature creep regime. This is truly a revolutionary advance to the fracture assessment field.

Currently, sophisticated fracture assessments are being made using advanced fracture theories such as the T*-integral which were previously unattainable. The methods are being verified by comparison of predictions to experimental results. It is anticipated that these advances will permit the designer to make sophisticated fracture assessments in the future with a minimum of effort.

Keywords: Fracture, Pressure Vessels, Piping

152. **PULSE PROPAGATION IN INHOMOGENEOUS OPTICAL WAVEGUIDES**
$200,493
DOE Contact: Robert E. Price, (301) 903-5822
University of Maryland Contact: C. Menyuk, (301) 455-3501

We are presently working on two principal projects. First, we are studying randomly varying birefringence in optical fibers and its impact on both soliton and NRZ communications. We have derived a set of equations (modified Manakov equations) that allow us to simulate the propagation through a fiber with rapidly and randomly varying birefringence on the much longer length scale on which the signals varying due to chromatic dispersion, polarization mode dispersion, and nonlinearity. These equations also yield considerable physical insight into the behavior of these systems. We have benchmarked these codes carefully, and we have demonstrated that they yield the same results as computer codes that use far shorter step sizes and are far less efficient. In addition to Monte Carlo methods, we are now using analytical methods based on the theory of stochastic differential equations to completely characterize the probability distribution functions for the evolution of the signal's state of polarization and the corresponding terms in the modified Manakov equation that describes the complete evolution.

The second project is quasi-phase-matched waveguides. We are using a Green's function approach to determine the rate at which radiation leaks from the quasi-phase-matched guides. In the future we will look at oblique guides and guides with other unusual cross-sections that appear in the experiments to reduce unwanted Bragg reflections.

Keywords: Optical Waveguides, Monte Carlo

153. **FLUX FLOW, PINNING AND RESISTIVE BEHAVIOR IN SUPERCONDUCTING NETWORKS**
$71,930
DOE Contact: Robert E. Price, (301) 903-5822
University of Rochester Contact: S. Teitel, (716) 275-4039

The fluctuation of vortices and vortex lines has been shown to be a major source of electrical resistance for superconducting networks when placed in magnetic fields. Systems of particular interest include the new high temperature type II superconductors, and periodic arrays of Josephson junctions. Numerical simulations are being carried out to identify and characterize the nature of the various vortex structures present in such systems, as a function of temperature and applied magnetic field, and to understand the nature of the phase transitions between them.

Particular attention has recently been given to studying the equilibrium fluctuation of vortex lines in models of bulk high temperature superconductors.

Simulations have shown that there can be two distinct phase transitions describing the superconducting ordering parallel versus perpendicular to the applied magnetic field. The loss of order in the perpendicular direction has been associated with a melting of the ground state vortex line lattice. The loss of order in the parallel direction has been associated with the onset of a vortex line tangle percolating throughout the entire system. New simulations, relaxing earlier approximations, are being carried out to clarify this issue. The effect of applied currents and random vortex pinning sites will be added in future work. The dynamic behavior of vortices in two dimensional Josephson arrays has also recently been investigated using a detailed finite size analysis to verify proposed scaling equations.

This research will greatly enhance the fundamental understanding of behavior in strongly fluctuating superconducting materials. The results will have impact in understanding the magnetic properties of the new high temperature superconductors, and in the design of Josephson junction arrays for use as microwave detectors and generators.

Keywords: Superconductors, Flux Flow, Josephson Junctions

GEOSCIENCES RESEARCH

The BES Geosciences Research Program supports research that is fundamental in nature and of long-term relevance to one or more energy technologies, national security, energy conservation, or the safety objectives of the Department of Energy. It is also concerned with the extraction and utilization of such resources in an environmentally acceptable way. The purpose of this program is to develop geoscience or geosciences-related information in support of one or more of these Department of Energy objectives or to develop the broad, basic understanding of geologic materials and processes necessary for the attainment of long-term Department of Energy goals. In general individual research efforts supported by this program may involve elements of several different energy objectives. The DOE contact for this program is Paula M. Davidson, (301) 903-5822.

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

154. **AN INVESTIGATION OF ORGANIC ANION-MINERAL SURFACE INTERACTIONS DURING DIAGENESIS**
$200,000
DOE Contact: P. M. Davidson, (301) 903-5822
SNL Contacts: Patrick Brady, (505) 844-7216 and Randall Cygan, (505) 844-7216

The research is to investigate adsorption of anionic carboxylate and phenolate groups onto aluminosilicate surfaces in order to evaluate the role of organic acids as: (1) catalysts for mineral dissolution and porosity evolution in deep basins, and (2) controlling agents of coupled dissolution and growth of during diagenesis. Combined experimental and theoretical approaches are used to investigate the mechanisms and reaction rates of organic anion adsorption. T-dependent adsorption of oxalate, acetate, salicylate and benzoate anions onto selected aluminosilicate surfaces are being measured, as are dissolution rates of alumina (as corundum), tremolite, albite, kaolinite and precipitation rates of kaolinite, in solutions containing various organic acids, at temperatures of 30-90°C. Theoretical investigations are testing mechanistic connections between metal-anion complexation, anion adsorption, and mineral growth with the new experimental data. The influence of surface-site chemistry and bonding are being investigated, in an attempt to establish general crystal-chemical rules for predicting the extent of organically-controlled reactions during diagenesis.

Keywords: Surface Reactions, Aluminosilicate Minerals, Adsorption Mechanisms

155. **TRANSITION METAL CATALYSIS IN THE GENERATION OF PETROLEUM AND NATURAL GAS**
$104,538
DOE Contact: Paula M. Davidson, (301) 903-5822
Rice University Contact: Frank D. Mango, (713) 527-4880

Light hydrocarbons in petroleum, including natural gas (C_1-C_4), are conventionally viewed as products of progressive thermal breakdown of kerogen and oil. Alternatively, transition metals, activated under the reducing conditions of diagenesis, can be proposed as catalysts in the generation of light hydrocarbons. Transition metal-rich kerogenous sedimentary rocks were reacted under reducing conditions at temperatures for which the substrates alone, *N*-octadecene + hydrogen, are stable indefinitely. Catalytic activity was measured to be on the order of 10^{-7} g CH_4/d/g kerogen, suggesting robust catalytic activity over geologic time at moderate sedimentary temperatures.

Keywords: Transition Metals, Catalysis, Petroleum

156. **MINERAL DISSOLUTION AND PRECIPITATION KINETICS: A COMBINED ATOMIC-SCALE AND MACRO-SCALE INVESTIGATION**
$130,632
DOE Contact: P. M. Davidson, (301)903-5822
University of Wyoming Contact: Carrick M. Eggleston, (307)766-6769
Lawrence Livermore National Laboratory Contact: Kevin G. Knauss, (510) 422-1372

The project combines atomic-scale and macro-scale approaches for investigating mineral-fluid interactions, in order to provide improved understanding of mineral dissolution and precipitation processes. With the development of a high temperature flow-through atomic force microscope (AFM), atomic-scale kinetic experiments will be possible under geologically relevant conditions for important oxide and aluminosilicate minerals. Macroscopic measurements of dissolution/precipitation rates, activation energies, and rates of step motion across surfaces, performed under identical conditions, will provide the basis for addressing open questions concerning the macroscopic rate laws and microscopic interpretations, in terms of dissolution and precipitation mechanisms, and the nature of the reactive interface.

Keywords: Atomic Force Microscopy, Silicate Minerals, Dissolution and Precipitation Mechanisms

MATERIALS STRUCTURE AND COMPOSITION

157. **REACTION MECHANISMS OF CLAY MINERALS AND ORGANIC DIAGENESIS: AN HRTEM/AEM STUDY**
$132,386
DOE Contact: P. M. Davidson, (301) 903-5822
Arizona State University Contact: P. R. Buseck, (602) 965-3945

The research is to investigate the structures of fine-scale diagenetic material using high-resolution transmission electron microscopy/analytical electron microprobe (HRTEM/AEM) techniques which will facilitate *in situ* identification and evaluation of reaction mechanisms. As a basis for kinetic models this information is used to predict basinal diagenetic patterns for resource exploration. Structural analyses of intergrown product and reactant from three principal diagenetic reactions operative in the formation of hydrocarbon reservoirs are proposed: (1) berthierine to chamosite, (2) smectite to illite, and (3) maturation of kerogen to form oil and gas.

Keywords: Diagenetic Reactions, High-Resolution Transmission Electron Microscopy, Kerogen, Smectite, Illite, Berthierine, Chamosite

158. **INFRARED SPECTROSCOPY AND HYDROGEN ISOTOPE GEOCHEMISTRY OF HYDROUS SILICATE GLASSES**
$139,826
DOE Contact: P. M. Davidson, (301) 903-5822
Caltech Contacts: S. Epstein, (818) 356-6100 and E. Stolper, (818) 356-6504

The focus of this project is the combined application of infrared (IR) spectroscopy and stable isotope geochemistry to the study of dissolved components in silicate melts and glasses. Different species of dissolved water and carbon dioxide (e.g., molecules of H_2O and hydroxyl groups, molecules of CO_2 and carbonate ion complexes) have been analyzed to understand volatile transfer reactions in liquids and glasses. The partitioning of H isotopes between vapor and hydroxyl groups and molecules of H_2O dissolved in rhyolitic melts was measured. Concentrations of H_2O and CO_2 in volcanic glasses and CO_2 in rhyolitic liquid were measured at pressures up to 1500 bars. The fractionation of O isotopes between CO_2 vapor and rhyolitic glass and melt was measured. The kinetics of OH-forming reactions in silicate glasses were studied. Diffusion of water in basaltic melts and of water and CO_2 in rhyolitic glasses and melts was studied. Results were used to understand oxygen "self-diffusion" in silicate minerals and glasses and enhanced oxygen diffusion under hydrothermal conditions.

Keywords: Infrared Spectroscopy, Silicate Minerals, Glasses, Silicate Liquids, Speciation

159. **BIOMINERALIZATION: SYSTEMATICS OF ORGANIC-DIRECTED CONTROLS ON CARBONATE GROWTH MORPHOLOGIES AND KINETICS DETERMINED BY *IN SITU* ATOMIC FORCE MICROSCOPY**
$0
DOE Contact: P. M. Davidson, (301) 903-5822
Georgia Inst. of Technology Contact: P. Dove, (404) 894-6043

The research is to investigate biomineralization mechanisms of dissolution and precipitation reactions of the two common calcium carbonate polymorphs, calcite and (metastable) aragonite. Experiments are proposed to monitor surface reaction morphology and kinetics in the presence of isolated simple acidic and basic amino acids, that are candidates for directing growth in natural systems. In order to characterize dynamic nanoscale growth morphologies and mechanisms, atomic force microscopy (AFM) observations are proposed under in situ conditions. The combination of mechanism and rate determinations are important for understanding and predicting controls by organic molecules on natural precipitation and dissolution of calcite and aragonite, and provide new constraints on models of bonding and reactivity at the nanoscale in organized structures.

Keywords: Biomineralization, Calcium Carbonate, Atomic Force Microscopy, Surface Reactions

160. **REACTIONS AND TRANSPORT OF TOXIC METALS IN ROCK-FORMING SILICATES AT 25°C**
$200,000
DOE Contact: P. M. Davidson, (301) 903-5822
Johns Hopkins Contact: D. R. Veblen, (410) 516-8487
Lehigh University Contact: E. Ilton, (610) 758-5834

Heterogeneous electron-cation transfer reactions between aqueous metals and silicates can be responsible for the retention or mobilization of multivalent cations in the near-surface environment. Reaction mechanisms are investigated as a basis for models of aqueous metal-mineral transport processes applicable to a wide range of problems, from toxic metal migration in aquifers to scavenging of heavy metals from industrial solutions. Specific reactions to be investigated are aqueous Cr(III), Cr(VI), Cd(II), Se(VI), Co(II) solutions with specified surfaces of representative phyllosilicates biotite, and chain silicates pyroxene and amphiboles. As an outgrowth of this investigation, a widely applicable analytic tool is to be developed for measuring Fe(II)/Fe(III) concentrations of small areas (approximately 25 X 50 micron) of silicates in thin sections with X-ray photoelectron spectroscopy (XPS).

Keywords: Surface Reactions, High-Resolution Transmission Electron Microscopy, Phyllosilicates, Chain Silicates

161. **THE CRYSTAL CHEMISTRY AND STRUCTURAL ANALYSIS OF URANIUM OXIDE HYDRATES**
$100,000
DOE Contact: P. M. Davidson, (301) 903-5822
University of New Mexico Contacts: D. Miller and R. C. Ewing, (505) 277-4163

Systematic crystal chemical relationships among uranium oxide hydroxide phases which are initial corrosion products of uraninite ore and spent nuclear fuel, are investigated to help constrain systematic models for crystal structure topologies. Current work involves the determination of crystal structures for identified key missing phases, such as ianthinite and schoepite, which contain oxidized U^{6+} and are among corrosion products of UO_2 in near-surface, oxidizing environments. Research objectives are to use the new data on structural topologies to interpret and predict speciation and thermodynamic stability relations among uranium oxide hydrates.

Keywords: Uranium Oxide Hydrates, Crystal Chemistry, Structural Topology

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

162. **OXYGEN AND CATION DIFFUSION IN OXIDE MATERIALS**
$224,179
DOE Contact: P. M. Davidson, (301)903-5822
LLNL Contact: F. J. Ryerson, (510)422-6170
University of California at Los Angeles Contact: K. D. McKeegan, (310) 825-3580

The objective of this work is to measure the diffusion parameters for various cations and oxygen in important rock-forming minerals to constrain both geochemical transport processes and diffusive mechanisms affecting physical properties such as creep and electrical conductivity. Oxygen self-diffusion coefficients have been measured for three natural clinopyroxenes, a natural anorthite, a synthetic magnesium aluminate spinel, and a synthetic akermanite over oxygen fugacities ranging from the Ni-NiO to Fe-FeO buffers. The oxygen self-diffusion coefficients of the three clinopyroxenes are indistinguishable. At a given temperature, oxygen diffuses about 100 times more slowly in diopside than indicated by previous bulk-exchange experiments. New data for anorthite, spinel, and akermanite agree well with prior results obtained by gas-solid exchange and depth profiling methods at different oxygen fugacities, indicating that diffusion of oxygen in these nominally iron-free minerals is not greatly affected by fO_2.

Keywords: Diffusion, Minerals, Plastic Deformation

163. **STRUCTURE AND REACTIVITY OF FERRIC OXIDE AND OXYHYDROXIDE SURFACES: QUANTUM CHEMISTRY AND MOLECULAR DYNAMICS**
$200,000
DOE Contact: P. M. Davidson, (301) 903-5822
PNL Contacts: Jim Rustad and Andrew Felmy, (509)376-1134

The research is a theoretical investigation of the surface structure and reactivity of proton binding sites of ferric oxides and hydroxides. The surfaces of these common minerals are known to bind metals, oxy-anions, and organic chelates through mechanisms that are as yet poorly understood. The approach combines crystalline Hartree-Fock calculations for the ferric (hydr)oxides with a molecular dynamics (MD) model for water currently being developed by in collaboration with J. W. Halley of the University of Minnesota, in order to evaluate: (1) structures and relative stabilities of various ferric (hydr)oxide surfaces; (2) the most reactive sites for proton adsorption, indicated by relative proton affinities in vacuo; (3) solvation corrections to relative surface energies and relative proton binding energies; (4) improvements in thermodynamic models of proton adsorption resulting from better predictions of surface structure, site types, and proton binding energies.

Keywords: Proton Adsorption, Surface Structure, Surface Reactivity, Ferric Oxides, Ferric Hyrdoxides

164. **CATION DIFFUSION RATES IN SELECTED SILICATE MINERALS**
$130,000
DOE Contact: P. M. Davidson, (301) 903-5822
Sandia National Laboratory Contacts: Randall T. Cygan, (505) 844-7216 and H. R. Westrich, (505) 844-9092

Objectives of this research are to determine experimental cation diffusion coefficients for garnet and pyroxene minerals at temperatures less than 1000°C for evaluating disequilibrium behavior in geological, nuclear waste, energy, and materials applications. A new thin-film technique for preparation of diffusion couples was developed in order to measure the relatively slow diffusion of Mg^{2+}, Mn^{2+}, and Ca^{2+} in garnets and pyroxenes. Depth profiles of tracer isotopes are then evaluated using an ion microprobe. Comparison of the diffusion coefficients determined under various oxygen fugacities provides information about the diffusion mechanism and the defect structure of the mineral sample. Results suggest a slower mechanism for magnesium diffusion in pyrope for relatively reducing conditions.

Keywords: Cation Diffusion, Garnets, Pyroxenes, Silicate Minerals, Diffusion Mechanism, Defect Structure

165. **GRAIN BOUNDARY TRANSPORT AND RELATED PROCESSES IN NATURAL FINE-GRAINED AGGREGATES**
$152,460
DOE Contact: P. M. Davidson, (301)903-5822
Brown University Contacts: R. A. Yund and J. R. Farver, (401) 863-1931

The objective of this study is the direct measure of diffusional transport rates in rocks and how the rates vary with mineralogy and microstructure, as well as temperature and pressure. The results provide much needed data on the nature of grain boundaries in rocks and the rate of transport of chemical components through rocks. Grain boundary diffusion of oxygen and cations in monomineralic aggregates of feldspar and of calcite, and aggregates of feldspar plus quartz were determined with the ion microprobe (SIMS). Calcium grain boundary diffusion rates in Ca-rich feldspar aggregates are several orders of magnitude slower than oxygen, and than potassium in K-rich feldspar. This suggests that differences in size and formal charge of chemical species may play an important role in their relative grain boundary diffusion rates. TEM analysis of microstructures suggests that the equilibrium distribution of water in feldspar aggregates is that of isolated pockets. Studies continue in order to evaluate the role of pressure and nonhydrostatic stresses on fluid-feldspar interfacial energies and microstructures.

Keywords: Diffusion, Rocks, Quartz, Feldspar, Microstructures

166. **NEW METHOD FOR DETERMINING THERMODYNAMIC PROPERTIES OF CARBONATE SOLID-SOLUTION MINERALS**
$150,552
DOE Contact: P. M. Davidson, (301)803-5822
UC Davis Contact: P. A. Rock and W. E. Casey, (916) 752-0940

Incorporation of metals into calcium carbonate minerals is an important pathway for elimination of potentially toxic metals from natural waters. The thermodynamic properties of the resulting solution are, however, poorly known because of difficulties with the solubility measurements. This project uses a new method of measurement which avoids some of these difficulties. The new method is an electrochemical double cell including carbonates and no liquid junction. The cell is an advance over conventional techniques because: (1) reversibility can be directly established; (2) models of solute speciation are not required; (3) the measurements do not perturb the chemistry significantly.

Keywords: Carbonate Minerals, Solubility, Electrochemical Cell

167. **MICROMECHANICS OF FAILURE IN BRITTLE GEOMATERIALS**
$181,098
DOE Contact: P. M. Davidson, (301) 903-5822
SUNY, Stony Brook Contact: Teng-Fong Wong, (516) 632-8240
SNL Contact: Joanne Fredrich, (505) 846-0965

Differences in the onset of brittle failure in low-porosity and high-porosity rocks depend on the cementation, initial damage state and deformation history. However, efforts to predict failure are hindered by the inability to account for initial crack density and ductile intergranular phases. For example, although cementation increases brittle strength and reduces porosity, the toughening mechanism is not well understood. This project aims to resolve this question with a systematic study of microstructures induced in experimentally deformed samples (both pre-and post-failure) of: (1) high-porosity carbonate rocks, in which plastic grain deformation and plastic pore collapse are thought to be important; (2) sandstones of higher porosity but varying degree of cementation; (3) low-porosity crystalline rocks (as a test of models on rocks with distinct mechanical properties).

Keywords: Brittle Failure, Plastic Deformation, Experimental Rock Deformation, Cementation

168. **THREE-DIMENSIONAL IMAGING OF DRILL CORE SAMPLES USING SYNCHROTRON-COMPUTED MICROTOMOGRAPHY**
$150,000
DOE Contact: P. M. Davidson, (301) 903-5822
BNL Contact: Keith Jones, (516) 282-4588
SUNY, Stony Brook Contact: W. B. Lindquist, (516) 632-8361

Synchrotron radiation makes feasible the use of high resolution computed microtomography (CMT) for non-destructive measurements of the structure of different types of drill core samples. The goal of this work is to produce three-dimensional images of rock drill core samples with spatial resolution of 1 micron. CMT images are postprocessed (filtered) to provide specific grain/pore identification to each voxel in the image The pore topology is analyzed statistically to yield information on disconnected pore volumes, throat areas, pore connectivity and tortuosity. Current effort is on development of software to analyze the 3-dimensional connectivity and shape of the pore space using the medial axis theorem from computational geometry.

Keywords: Synchrotron Radiation, Computed Microtomography, Pore Structure, Drill Cores

169. **THERMODYNAMICS OF MINERALS STABLE NEAR THE EARTH'S SURFACE**
$150,000
DOE Contact: P. M. Davidson, (301) 903-5822
Princeton University: A. Navrotsky, (609) 258-4674

The purpose of this work is to expand our data base and understanding of the thermochemistry of minerals and related materials through a program of high temperature solution calorimetric studies. The technique of oxide melt calorimetry (in molten $2PbO{\cdot}B_2O_3$) has been extended to volatile-bearing phases. Measured mixing enthalpies of amphibole solid solutions are insensitive to OH-F substitution, but depend strongly on alkali ion substitution in the large A-site. Measured mixing enthalpies of open-framework zeolites are insensitive to species incorporation in the cavities, suggesting that there are few limitations on the variety of (metastable) structures that can be synthesized. Measured mixing enthalpies of damaged zircons are on the order of twice the heat of formation from component oxides, consistent with damage on the scale of near-neighbors and with greatly increased solubility in aqueous fluids.

Keywords: Thermochemistry, Solution Calorimetry, Amphiboles, Micas, Zircons

170. **THEORETICAL STUDIES OF THE ADSORPTION OF GOLD COMPLEXES AND FLOTATION COLLECTORS ONTO SULFIDE MINERAL SURFACES**
$27,547
DOE Contact: P. M. Davidson, (301) 903-5822
University of Maryland Contact: John Tossell, (301) 314-1868

The project involves quantum mechanical (Hartree Fock) calculations of relative stabilities of species participating in dissolution and precipitation of gold on sulfide minerals. Although the solubility and surface adsorption of aqueous Au species on sulfide minerals are important agents of ore deposition, current understanding is limited by lack of information on surface complexation sites and speciation. Calculated site geometries and stabilities will be used to evaluate reactivity of various As and Sb sulfide mineral surfaces, addressing questions such as how structural differences among amorphous and crystalline forms of As_2S_3 influence interactions with surface water and Au complexes. Flotation processes to concentrate As_2 from ore rely on selective adsorption of oxysulfide collector molecules on Au-bearing sulfide minerals. Calculations of relative energies of molecular orbitals of various C-containing sulfide collectors (xanthates and/or carbamates) and $P(OH)_2$ complexes with $Au+/Au_2$ and Au(SH) will help to identify candidate collector molecules with improved efficiency.

Keywords: Surface Complexation, Gold Sulfides, Metal Transport

171. **SHEAR STRAIN LOCALIZATION AND FRACTURE EVOLUTION IN ROCKS**
$0
DOE Contact: P. M. Davidson, (301) 903-5822
Northwestern University Contact: J. W. Rudnicki, (708) 491-3411

Prediction of the causative stresses, location, orientation, thickness, and spacing of fractures in fault zones is important to energy production, waste disposal, and mineral technologies. This study examines the relation of fractures to the macroscopic constitutive description and microscale mechanisms of deformation by testing a standard theory of localization that describes faulting as an instability of the constitutive description of homogeneous deformation. A new, more realistic nonlinear constitutive model, based on the growth and interaction of microcracks which produces increased bulk compliance, is being developed and calibrated with axisymmetric compression tests. Numerical studies (at SNL) will evaluate the complications of realistic geometries and boundary conditions. Preliminary results suggest that the response to an abrupt change in the pattern of deformation is completely nonlinear and cannot be approximated accurately by incrementally linear models, as is often done. This nonlinear response may therefore be critical to the evolution of typical fault zones.

Keywords: Shear Strain Localization, Fracture Evolution, Constitutive Description, Nonlinear Behavior

172. **TRANSPORT PHENOMENA IN FLUID-BEARING ROCKS**
$146,273
DOE Contact: P. M. Davidson, (301) 903-5822
Renssalaer Polytechnic Institute Contact: E. B. Watson (518) 276-6475

The research involves two parts: (1) determining the solubility and diffusivity of selected rock-forming minerals and mineral assemblages in deep C-O-H fluids, and (2) measuring the permeability of fluid-bearing synthetic rocks. A new procedure is being developed for measuring mineral solubilities and component diffusivities in fluids at pressures above 1 GPa, by measuring the total mass of transported component across a thermal gradient in dumbbell-shaped capsules at constant P (>1 GPa). Diffusivities are obtained from independent measurements of the component flux through different T gradients. In the second portion of the investigation, rocks synthesized at high (P > 1 GPa) pressures in the presence of differing fluid compositions and consequently porosity structure, will be analyzed at ambient conditions to determine permeability using dihedral angle measurements and bulk fluid (air) diffusion through the samples. Direct imaging of the pore structure will also be attempted with Scanning Electron Microscopy and synchrotron X-ray tomography.

Keywords: Diffusivity, Solubility, C-O-H Fluids, Porosity Structure, Rock Permeability

173. **CATION CHEMISORPTION AT OXIDE SURFACES AND OXIDE-WATER INTERFACES: X-RAY SPECTROSCOPIC STUDIES AND MODELING**
$0
DOE Contact: P. M. Davidson, (301) 903-5822
Stanford University Contacts: G. E. Brown and G. A. Parks, (415) 723-9168

The research focuses on reactions and reaction mechanisms between aqueous metal ions and oxide surfaces representative of those found in the earth's crust as an aid to developing large-scale models of contaminant transport. Objectives are to: (1) characterize reactions by direct sorption measurements, in-situ synchrotron-based X-ray absorption spectroscopy (XAS) of atomic environments at solid-water interfaces, and UV/Vis/IR spectroscopy; (2) investigate how these properties are affected by the solid surface and fluid composition; and (3) develop molecular-scale and macroscopic models for the sorption process. The reactions involve aqueous Co(II) and Pb(II) with Al_2O_3 (corundum), Fe_2O_3, and TiO_2, and the effect of organic liquids. New measurements of Pb(II) sorption on powdered corundum indicate sorption of polymeric species, suggesting that substrate structure is influencing the surface Pb(II) complexation. Comparative studies of the role of organic complexation on the sorption of Cu(II) on the surface of amorphous SiO_2 and on powdered corundum are aimed at specifying surface complexation mechanisms.

Keywords: Surface Complexation, Interface Reactions, Synchrotron X-ray Absorption Spectroscopy

174. **DISSOLUTION RATES AND SURFACE CHEMISTRY OF FELDSPAR GLASS AND CRYSTAL**
$117,302
DOE Contact: P. M. Davidson, (301) 903-5822
Penn State Contact: S. Brantley, (814) 863-1739

Dissolution rates and mechanisms of the most common crustal mineral group, the feldspars, (Na,K,Ca) $(Al,Si)AlSi_2O_8$, are key factors in environmental simulations of coupled fluid flow, effective water-rock surficial area, and fluid residence times. New dissolution experiments and characterization of these silicate mineral and glass surfaces and solutions are underway in order to help resolve discrepancies between existing laboratory measurements that are much faster than dissolution rates observed in the field for feldspars in soils, aquifers and small watersheds. Characterization of the laboratory-reacted solids and naturally weathered feldspars by IR and neutron methods for water content, and XPS and mass spectrometric methods for composition-depth profiling of leaching and surface adsorption complemented with surface analysis by field-emission SEM and AFM methods, will be used to constrain rate-controlling mechanisms of dissolution. Mechanistic information provided with a variety of microanalytic methods that can encompass mechanisms of dissolution from glass to crystal and from laboratory to field environments will help to determine which of several competing dissolution models best describes the natural weathering process.

Keywords: Silicate Minerals, Dissolution Rates, Dissolution Mechanism, Surface Reactions, Surface Characterization

OFFICE OF COMPUTATIONAL AND TECHNOLOGY RESEARCH

DIVISION OF ADVANCED ENERGY PROJECTS AND TECHNOLOGY RESEARCH

LABORATORY TECHNOLOGY RESEARCH (LTR) PROGRAM

The LTR program is managed by the AEPLTR Division of the Office of Computational and Technology Research within the Office of Energy Research. The program supports research primarily at the five ER multi-program national laboratories: Argonne, Brookhaven, Lawrence Berkeley, Oak Ridge and Pacific Northwest.

The LTR program links advances in basic research at the DOE laboratories to applied technologies of interest to DOE mission areas through high-risk, multidisciplinary research collaborations with private industry. The program funds the laboratories while the industry partners support their own participation at a level equal to the LTR funding.

The LTR program builds upon the results of ER basic research and other DOE research programs in collaboration with industry partners to enhance mission-oriented technolgoies at the laboratories while making technology available to industry for its use. The projects are selected in competitive peer reviews of solicited proposals submitted by the laboratories in conjunction with their partners.

The multi-year projects supported by LTR at the five multi-disciplinary ER laboratories are presented in the following discussion.

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

175. LUMELOID, A NEW SOLAR ENERGY CONVERSION MATERIAL (ANL94-42)

$100,000
DOE Contact: Walter M. Polansky, (301) 903-5995
ANL Contact: Michael Wasielewski, Chemistry, (630) 252-3538

The Argonne National Laboratory (ANL) is carrying out a research project to develop photoactive polymer composite materials to directly convert solar energy into electricity. This collaboration utilizes ANL expertise in developing photoactive materials in combination with ARDI film technology to generate new material composites that could have a significant impact on cheap and efficient power generation from solar energy.

Keywords: Polymers, Composites, Solar Energy Conversion

176. COLD CATHODE ELECTRON EMISSION FROM DIAMOND AND DIAMOND-LIKE CARBON THIN FILMS FOR FLAT PANEL COMPUTER DISPLAYS (ANL95-02)

$140,000
DOE Contact: Walter M. Polansky, (301) 903-5995
ANL Contact: Alan Krauss, MSD/CHM, (630) 252-3520

Cold cathode electron emission has been observed from a number of diamond and diamond-like carbon thin films. It is expected that this phenomenon can be used for the development of high visibility displays for critical applications such as avionics, high reliability microelectronics applications for operation in harsh environments where maintenance is not feasible, and flat panel computer displays. The development of devices like flat panel computer displays which use cold cathode electron emission has been hampered by a lack of basic understanding of the emission process. A method has been developed at Argonne National Laboratory for the growth of diamond films in the near-absence of atomic hydrogen, using Ar-C_{60} or Ar-CH_4 plasmas. This method produces films which respond differently to variations in growth conditions compared with films grown in large quantities of hydrogen. The differences manifest themselves in the manner in which the nucleation density, grain size, grain boundary width, surface roughness, crystallographic orientation and the extent and localization of regions of sp^2 and sp^3 electronic bonding character vary with the hydrogen concentration in the plasma. We have been able to relate several of these properties to the effective work function, turn-on voltage and emission site density by comparing the electron emission behavior and physical properties of conventional micro-and nano-crystalline, and low-hydrogen nanocrystalline diamond films.

Keywords: Diamond, Diamond-like, Coatings, Thin Films, Computer Displays

177. **GIANT MAGNETORESISTANCE WIRE SENSOR (ANL95-07)**
$150,000
DOE Contact: Walter M. Polansky, (301) 903-5995
ANL Contact: Samuel Bader, Materials Science, (630) 252-4960

Giant magnetoresistance (GMR) materials are composite metals whose resistance changes in the presence of magnetic fields. These materials are up to one hundred times more sensitive to magnetic fields than previously known systems. Currently the GMR materials are made by thin-film processing techniques thereby making their cost prohibitive for many applications. The goal of this project is to develop giant magnetoresistance sensors by inexpensive bulk processing techniques such as wire drawing, and to make prototype sensors that could be used in a variety of applications.

Keywords: Composites, Electrical, Magnetics, Sensors

178. **COMPOSITE METAL-HYDROGEN ELECTRODES FOR METAL-HYDROGEN BATTERIES (BNL94-06)**
$115,000
DOE Contact: Walter M. Polansky, (301) 903-5995
BNL Contact: Myron Strongin, Physics Department, (516) 344-3763

The project focuses on the fabrication and characterization of nano-scale bimetallic multilayered films and a feasibility study of their use as hydrogen-containing negative electrodes (anodes) in nickel-metal hydride (NiMH) batteries. If the feasibility of using these new materials is established, it is anticipated that the project will contribute to the advancement of NiMH battery technology and provide batteries with more rapid charging characteristics, greater energy efficiency or larger energy storage capacity.

Keywords: Composite Electrodes, Metal-Hydrogen Electrodes, Batteries

179. **DEVELOPMENT OF CdTe/CdZnTe MATERIALS FOR RADIATION DETECTORS (BNL94-09)**
$115,000
DOE Contact: Walter M. Polansky, (301) 903-5995
BNL Contact: Csaba Szeles, Physics, (516) 344-3710

The objective of this project is to broaden the potential use of Cadmium Zinc Telluride (CdZnTe) materials as room-temperature solid-state radiation detectors. Achieving this goal requires improvement of the existing material-growth and processing techniques in order to enhance the production yield and energy resolution of CdZnTe crystals limited by the unpredictability of the as-grown material. This unpredictability is largely due to the uncontrolled incorporation of electrically active native and impurity-related defects in the bulk and at the surface of the crystals and defects at the semiconductor-metal interface. Production of better crystals demands improved understanding of the nature of lattice defects, their influence on the detector performance and their formation and compensation mechanism during the crystal growth and processing. The availability of inexpensive, high-efficiency, room-temperature gamma-ray detectors is of great commercialization potential. It stimulates instrument and device manufacturers to develop new products and retrofit old applications using conventional NaI(Tl) and HPGe detectors. The total addressable market for CdZnTe materials and the new instruments and devices that integrate CdZnTe as a primary gamma-ray detector is in excess of 40 million dollars annually. DOE has extensive programs which use X-ray, gamma-ray and particle detectors. Improved, low-cost, room-temperature radiation detectors are important for a number of key DOE programs such as nuclear safety and safeguards, field assays, X-ray and gamma-detectors for next generation light sources, solar cells, X-ray and gamma-ray satellite surveillance etc.

Keywords: CdZnTe, Radiation, X-ray, Gamma Detectors

180. **CORROSION RESISTANCE OF NEW ALLOYS FOR BIOMEDICAL APPLICATIONS (BNL94-20)**
$25,000
DOE Contact: Walter M. Polansky, (301) 903-5995
BNL Contact: Hugh Isaacs, Applied Science, (516) 344-4516

The development of new materials for prosthetic devices and other biomedical applications is currently underway. The objective of this project is to provide a detailed understanding of alloy corrosion in bio-systems and the role of the individual alloying additions. Ultimately an understanding of the interactions between alloy composition and the electrochemical response of alloys with optimum mechanical properties and biocompatibility will be developed. In situ XANES measurements in simulated bio-fluid (Ringer's solution) and under crevice conditions (concentrated chloride solution) will provide information on the chemical behavior of the alloys during corrosion. A detailed study of oxide formation will be carried out using XANES, surface analytical techniques and in situ AFM.

Keywords: Corrosion Resistance, Biomedical, Applications, Alloys

181. **NOVEL BIOCOMPATIBLE "SMART" CONTACT LENS MATERIAL (LBNL94-28)**
$75,000
DOE Contact: Walter M. Polansky, (301) 903-5995
LBNL Contact: Carolyn Bertozzi, Materials Sciences Division, (510) 643-1682

Vision is by far the most important of the human senses and better ophthalmological care products are continuously being sought. For example, current synthetic contact lens materials have limited tolerance by the population. The project goal is to develop improved materials that will increase the quality of life not only for current wearers but also for those whose physiology cannot tolerate existing materials. In our design of new contact lens materials, we utilize the lessons we have learned in nature. Our approach is to modify materials with favorable lens properties so that they more closely resemble biological tissue, and are therefore tolerated well by the eye. The knowledge gained here is expected to further the understanding of how materials behave in a physiological environment and benefit biomedical implant devices development in general. The work represents a significant advance in the development of new biocompatible materials. The first phase in the development of new contact lens materials is the design of biocompatible monomers for incorporation into hydrogel polymers. In order to create lenses that best mimic biological tissue, we focused on carbohydrate molecules which comprise the coating of most living cells. Our strategy, therefore, is to synthesize polymerizable monomers possessing cell surface-like carbohydrates, and to incorporate them into lenses with better biocompatibility properties.

Keywords: Biocompatible, Smart Contact Lens, Materials, Monomers, Hydrogel Polymers

182. **ALLOY DESIGN OF NEODYMIUM ($Nd_2Fe_{14}B$) PERMANENT MAGNETS (ORL94-15)**
$282,000
DOE Contact: Walter M. Polansky, (301) 903-5995
ORNL Contact: Joseph Horton, Metals and Ceramics, (423) 574-5575

The objective of this project is to improve the room temperature fracture toughness of the neodymium permanent magnet without decreasing its magnetic properties. This will improve machinability, allow closer tolerances, use as a structural element and more rapid and further market penetration for uses such as electric motors.

Keywords: Neodymium Magnets, Alloy Design, Fracture Toughness, Electric Motors

183. **DEVELOPMENT OF ALUMINUM BRIDGE DECK SYSTEM (ORL94-56)**
$100,000
DOE Contact: Walter M. Polansky, (301) 903-5995
ORNL Contact: H. Wayne Hayden, Metals & Ceramics, (423) 574-6936

The purpose of this project is to investigate refinement of the aluminum bridge deck panel system using aluminum multi-void extrusions joined together to make panel sections. The desired results could be of use for the upgrading of deficient bridges throughout the U.S. with the use of aluminum bridge decks, and to use aluminum decks on new bridges.

Keywords: Aluminum Bridge Decks, Cost Effective, Lightweight Systems, Consortium

184. NEW THERMOELECTRIC MATERIALS FOR SOLID STATE REFRIGERATION (ORL95-10)
$180,000
DOE Contact: Walter M. Polansky, (301) 903-5995
ORNL Contact: Brian Sales, Solid State Division, (423) 576-7646

The goal of this project is to develop new materials that will significantly improve the performance of thermoelectric devices for solid state refrigeration and air conditioning. Thermoelectric refrigerators involve no moving parts, use no greenhouse gases, and are extremely reliable. ORNL will synthesize candidate thermoelectric materials along several paths including filled and unfilled materials with the skutterudite structure and unusual "kondo-like" alloys.

Keywords: Thermoelectric Devices, Refrigeration, Air Conditioning, Alloys

185. MANUFACTURING OF Ni-BASE SUPERALLOYS WITH IMPROVED HIGH-TEMPERATURE PERFORMANCE (ORL95-05)
$150,000
DOE Contact: Walter M. Polansky, (301) 903-5995
ORNL Contact: C. Liu, Metals and Ceramics Division, (423) 574-4459

The objective of this research project is to enhance the manufacturing of high-temperature nickel-base superalloys with improved performance through the control of vital minor elements in the parts-per-million range without significantly increasing production cost . It is anticipated that the control of these vital elements would extend the creep rupture life of superalloy structural members by more than an order of magnitude. Nickel-base superalloys are state-of-the-art materials for high-temperature structural applications in advanced engines, petrochemical, other energy conversion systems.

Keywords: Ni-base Superalloys, High-Temperatures, Manufacturing

186. POLYMER MULTILAYER (PML) FILM APPLICATIONS IN OPTICS, ELECTROLYTES, AND GLAZINGS (PNNL94-06)
$65,000
DOE Contact: Walter M. Polansky, (301) 903-5995
PNNL Contact: John Affinito, Materials and Chemical Sciences, (509) 375-6942

The work undertaken in this research is in response to the requirement of a number of industries for a much higher rate, and much lower cost, process for vacuum deposition of dielectric and/or deposition techniques. The Polymer Multi-Layer (PML) deposition technology being developed at PNNL, can deposit fully cured polymer films, in a roll-to-roll web coating system, at line speeds in excess of 600 linear meters per minute. While the technology developed under this research can potentially be applied in many applications, in this project, four application areas are being explored. These are: (1) deposition, on flexible polyester substrate, of; enhanced and protected polymer/Ag/ polymer and polymer/Al/ polymer reflectors; (2) all polymer (polymer1/ polymer2)^N, Quarter Wave Optical Thickness (QWOT) multilayer reflection filters; (3) polymer/ silver/polymer "Heat Mirror" structures; and (4) thin film battery structures utilizing polymer-only electrolyte layers.

Keywords: Polymer Multilayer Films, Optics, Electrolytes and Glazings, Film Deposition

187. DEVELOPMENT OF MIXED METAL OXIDES (PNNL94-28)
$25,000
DOE Contact: Walter M. Polansky, (301) 903-5995
PNNL Contact: Larry Pederson, Materials and Chemical Sciences, (509) 375-2731

This research is directed towards the development of unique lithiated metal oxides for use in secondary batteries. The oxides will be produced using PNNL's glycine nitrate process and will involve varying the compositions of the materials to optimize their desired properties. Lithiated manganese oxides are expected to be used in future lithium ion systems and a lithium polymer system (which is becoming commercially available with a vanadium oxide cathode). The lithium polymer system is expected to be used as a power source for electric vehicles later in this decade.

Keywords: Mixed Metal Oxides, Lithiated Metal Oxides, Lithiated Mn Oxides, Secondary Batteries, Polymer Systems

188. **DEVELOPMENT OF TAPE CALENDARING TECHNOLOGY FOR SEPARATION MEMBRANES (PNNL95-04)**
$40,000
DOE Contact: Walter M. Polansky, (301) 903-5995
PNNL Contact: Timothy Armstrong, Materials & Chemical Sciences, (509) 375-3938

The purpose of this research is to develop tape calendering technology to produce mixed conducting and oxygen ionically conducting oxide membranes for use as air separation and oxygen production devices. Tape calendering technology shows exceptional promise as a means to manufacture complex ceramic structures on a large scale and at low cost. This project could provide key technology that would help to produce large quantities of oxygen at a significantly lower cost than current cryogenic methods. Tape calendering combines oxide powders, binder, and plasticizer in a high-intensity mixer. The binder-plasticizer system can be softened by externally heating the mixing chamber, using only internal heating resulting from frictional forces generated within the mixing chamber, or combinations of the two. The softened binder system mixes with the ceramic powder to form a plastic-like mass. The mass is calendered into a thin, flat tape using a two-roll mill with counter rotating rolls. Tape thickness is controlled by the spacing of the two rolls.

Keywords: Tape Calendering of Oxide Membranes, Separation Membranes, Air Separation, Oxygen Production, Complex Ceramic Structures

189. **INNOVATIVE MULTILAYER THERMAL BARRIER COATINGS FOR GAS TURBINE ENGINES (PNNL95-07)**
$275,000
DOE Contact: Walter M. Polansky, (301) 903-5995
PNNL Contact: Edward Courtright, Materials& Chemical Sciences, (509)375-6926

The objective of this project is to determine the feasibility of producing innovative multilayer thermal barrier coatings. The fundamental issues associated with maximizing infrared reflectivity and phonon scattering, and the thermodynamic stability issues which affect durability, reliability, and life-cycle performance are being investigated. In the first phase of the program, the feasibility of producing higher performance thermal barrier coatings with multilayered systems will be demonstrated. In the second phase of the program, actual components will be coated and tested under simulated engine conditions, e.g., burner rigs or in actual land-based gas turbine engines

Keywords: Thermal Barrier Coatings, Multilayer Coatings, Gas Turbine Engines, Thermal Barriers

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

190. **APPLICATION OF HIGH PERFORMANCE COMPUTING TO AUTOMOTIVE DESIGN AND MANUFACTURING (ANL94-54)**
$250,000
DOE Contact: Walter M. Polansky, (301) 903-5995
ANL Contact: David Weber, Reactor Engineering Division, (630) 252-8175

This research focuses on the application of high-performance computing to automotive design and manufacturing. The major thrust of the work is to develop easy-to-use computer codes for new high performance computing (HPC) platforms. Argonne National Laboratory is focusing on two areas: computational fluid dynamics and composite material modeling. The Computational Fluid Dynamics (CFD) task will develop "next generation" computational tools for the analysis of CFD phenomena. These tools, including improved physical models and taking advantage of advanced parallel computing architectures, will allow manufacturers to design improved systems and shorten the design time. The Composite Materials Modeling Task will develop predictive numerical analysis tools. This research will: (1) permit the reliable incorporation of lightweight fiberglass reinforced composites into the design of more fuel efficient passenger automobiles without compromising passenger safety, (2) decrease design and manufacturing times and cost, and (3) result in a decrease in domestic fuel consumption. DOE will benefit by adding advanced numerical methods for composite materials to its current suite of state-of-the-art computational tools. This new capability can then be used for other DOE projects that require modeling of composite materials.

Keywords: Composites, Modeling, Analyses

191. **MICROFABRICATION OF A MULTI-AXIS MICROACCELEROMETER USING HIGH ASPECT RATIO MICROFABRICATION (HARM) AND SILICON MICROMACHINING (BNL94-02)**
$250,000
DOE Contact: Walter M. Polansky, (301) 903-5995
BNL Contact: John Warren, Instrumentation, (516) 344-4203

The primary goal of this project is to use high aspect ratio microfabrication to bulk fabricate all of the components of a multi-axis accelerometer. The inherent accuracy of the microfabrication process (based on lithography) should also lead to improvements in performance. The completed micro-accelerometer will have many applications in aviation, auto navigation, active automotive suspension system control, drill bit navigation, and airbag deployment. The high aspect ratio microfabrication process has many scientific applications and is currently being used in the Instrumentation Division at BNL to construct prototype position-sensitive X-ray detector arrays that have many applications in high energy physics. Knowledge gained from microfabrication methods is directly applicable to these on-going efforts.

Keywords: Microfabrication, Accelerometer, X-ray Detector

192. **NONDESTRUCTIVE X-RAY SCATTERING CHARACTERIZATION OF HIGH TEMPERATURE SUPERCONDUCTING WIRES (BNL95-10)**
$140,000
DOE Contact: Walter M. Polansky, (301) 903-5995
BNL Contact: Thomas Thurston, Physics, (516) 344-5534

Prototypes of generators, transformers, transmission cables, and current limiters which utilize wires made of high-temperature superconducting materials are just beginning to be built. Although the ultimate purposes of these electric power devices vary, all of them offer the potential for substantial energy savings, since there is no loss of energy in the form of heat generated by electrical resistance. DOE has programs to develop technologies for electric power applications of high temperature superconductors. All of the electric power applications of high-temperature superconductors described above require long lengths (at least ~100 meters) of wire with large current carrying capacities. Unfortunately, there are a variety of effects that can limit the current carrying capacity of the wires, with the consequence that today's wires have capacities which are at least 10 times smaller than the maximum theoretical capacity. The purpose of this research is to characterize the structure of the superconducting material within wires in order to understand the causes of poor current carrying capacity, and to suggest alternative processing procedures which can minimize or eliminate the effects which cause poor wire performance. The methods which Brookhaven is using to characterize the wires utilize intense beams of X-rays generated at Brookhaven's National Synchrotron Light Source. Work performed earlier showed that the current carrying capacity is affected by the presence of certain impurity phases, and by poor texturing of the superconducting material within the wires. Both of these deleterious effects can be readily measured only with the intense X-ray beams available at facilities like the National Synchrotron Light Source. Work currently in progress involves direct X-ray monitoring of superconducting wire processing in a "mini-factory" which has been set up at Brookhaven. This work has already suggested modifications increase the current carrying capacity of wires. BNL has started to apply the techniques developed to characterize these wires on other problems of interest to the DOE, such as characterizing the properties of battery electrode materials and permanent magnets.

Keywords: Superconducting Wires, Prototypes, Characterization, High-Temperature

193. **THIN FILM LITHIUM BATTERIES (BNL95-11)**
$90,000
DOE Contact: Walter M. Polansky, (301) 903-5995
BNL Contact: James McBreen, Applied Science, (516) 344-4513

This research is focused on the development and testing of polymer electrolytes for primary thin film lithium batteries. A cell design, based on thin electrodes, with the cell enclosed in a thin heat sealed foil-laminate pouch like that used in the food industry (e. g. coffee) has been developed by an industry source. While this design is attractive for thin film batteries, and is adequate for prevention of ingress of water vapor or air, it presents many technical challenges. The foil laminate gives no mechanical support to ensure intimate contact between the electrodes and the electrolyte. Bulging of the pouch and its contents can result in large increases in the resistance losses in the cell. These problems were solved by the development of a new low cost polymer electrolyte, with good conductivity, and excellent adhesion to the electrodes.

Keywords: Thin Films, Lithium, Batteries

194. **NEW CATALYSTS FOR DIRECT METHANOL OXIDATION FUEL CELLS (BNL95-14)**
$15,000
DOE Contact: Walter M. Polansky, (301) 903-5995
BNL Contact: Radoslav Adzic, Applied Science, (516) 344-4522

A search for an active metal oxide-metal electrocatalysts for methanol oxidation has been performed with platinum electrocatalyst supported on several types of metal oxides. Synthesis and the electrochemical and/or spectroscopic characterizations were carried out. A very active electrocatalyst was obtained with Pt supported on Ru oxide. Reaction intermediates and products for some systems were characterized by in situ Transform Infrared Spectroscopy (FTIR).

Keywords: Electrocatalysts, Methanol Oxidation, Fuels Cells

195. **RECHARGEABLE ZINC/AIR BATTERIES FOR CONSUMER APPLICATIONS (LBNL94-43)**
$15,000
DOE Contact: Walter M. Polansky, (301) 903-5995
LBNL Contact: Elton Cairns, Energy & Environment Division, (510) 486-5028

The Zn/air battery is an especially appealing technology for use in consumer batteries because of its high specific energy, low cost and environmentally benign components. The zinc-air technology is greatly under-utilized because of the generally low power available from the cell. The power limitations stem primarily from the air electrode as a result of the slow kinetics of the electrochemical reduction of oxygen from air. Complete utilization of the zinc loading can also be a problem at high power drains. The focus of this project has been to address these two limitations in order to extend the possible markets for the zinc/air primary battery technology. The first year of this project has been concerned with the application of novel electrocatalysts to the air electrode structure to improve the high-power performance of this electrode. The second year will focus on the study and modification of the zinc electrode formulation in order to optimize zinc utilization at high power. Four electrocatalyst systems are under study at LBNL. The electrocatalysts are added to a state-of-the-art air electrode and performance is evaluated in the three-electrode configuration in the absence of zinc. Two candidates appear promising and will be incorporated into full zinc-air cells for testing.

Keywords: Zn/Air Batteries, Electrochemistry, Electrocatalysts, Electrodes

196. **MICROMAGNETIC STRUCTURES (LBNL95-12)**
$71,000
DOE Contact: Walter M. Polansky, (301) 903-5995
LBNL Contact: Neville Smith, Accelerator and Fusion, (510) 486-5423

This goal of this project is to produce a powerful and unique tool for microscopic imaging of magnetic materials (a tool which will take full advantage of the capabilities of the ALS), and to use this tool to develop new magnetic materials for high density information storage. The microscope is based on a full field photoelectron emission technique, and magnetic information is extracted using a synchrotron radiation spectroscopy known as X-ray Magnetic Circular Dichroism. The microscope will have elemental and chemical selectivity, combined with surface sensitivity, and the ability to measure surface magnetic moments. This combination of features is unique in the array of tools currently used to study magnetic materials. The project uses LBNL's expertise in design and operation of synchrotron instrumentation, beamlines, and experimental end stations in the production of artificially engineered magnetic microstructures.

Keywords: Micromagnetics, Information Storage, Magnetic Imaging, Photoelectron Emissions

197. **DEVELOPMENT OF ZINC/NICKEL OXIDE BATTERIES FOR ELECTRIC VEHICLE APPLICATIONS (LBNL95-27)**
$90,000
DOE Contact: Walter M. Polansky, (301) 903-5995
LBNL Contact: Frank McLarnon, Energy Conversion and Storage, (510) 486-4636

The goal of this project is to develop a light-weight, rechargeable battery for electric vehicles. This battery uses an alkaline electrolyte, a zinc negative electrode and a nickel oxide positive electrode. It has two major advantages over competing types such as cadmium/ nickel oxide (nickel-cadmium) and metal-hydride/nickel oxide (nickel-metal hydride): it delivers more energy per unit battery mass and costs less to produce. LBNL has developed a novel electrolyte for the zinc/nickel oxide battery that extends its useful life to several hundred charge-discharge cycles. Additional improvements to lower the battery mass and to increase the ability of the electrolyte to wet the electrodes are being investigated. If these efforts are successful, full-size electric vehicle batteries will be built for testing. A superior zinc/nickel oxide battery could be the key to inexpensive and durable electric vehicles which will reduce air pollution and petroleum imports while creating a new growth industry.

Keywords: Zn/Ni Batteries, Electric Vehicles, Alkaline Electrolytes, Zn and Ni Electrodes

198. **CATALYTIC CONVERSION OF CHLORO-FLUOROCARBONS OVER PALLADIUM-CARBON CATALYSTS (LBNL95-45)**
$104,000
DOE Contact: Walter M. Polansky, (301) 903-5995
LBNL Contact: Gabor Somorjai, Materials Sciences, (510) 486-4831

Chlorofluorocarbons must be substituted as refrigerants and chemicals because of their adverse health effects (ozone depletion and other effects). The hydrodechlorination (HDCl) of $C_2F_4C_{12}$ is a technology that uses palladium catalyst supported on carbon. This research investigates the structure and bonding of reactants and products on palladium crystal surfaces that are also used as model catalysts. The elementary steps of the reaction and its mechanism are explored this way. The causes of catalyst deactivation is being studied, along with the use of promoters to inhibit it. The roles of the carbon support and the palladium-carbon interface are also of interest as they influence the catalytic reaction rate and selectivity.

Keywords: Chlorofluorocarbons, Pd Catalysts, Hydrodechlorination, Reaction Mechanisms

199. **DEVELOPMENT OF A THIN-FILM BATTERY POWERED HAZARD CARD AND OTHER MICROELECTRONIC DEVICES (ORL94-39)**
$70,000
DOE Contact: Walter M. Polansky, (301) 903-5995
ORNL Contact: John Bates, Solid State, (423) 574-6280

The goals of this research project are to investigate the feasibility of powering integrated circuit chips and compact microelectronic-based devices with thin-film, rechargeable batteries that can withstand temperatures of up to 200°C, and to determine and eliminate obstacles to their manufacturability. Since they have high energies per unit of volume and mass and because they are rechargeable, thin film lithium batteries have potentially many applications as small power supplies in consumer and medical microelectronic products. This research into battery technology will enable the reduction in size and improvement in performance of existing microelectronic devices.

Keywords: Thin-Film Batteries, Microelectronics, Electronic Devices

200. **ION IMPLANTATION PROCESSING TECHNOLOGIES (ORL94-72)**
$100,000
DOE Contact: Walter M. Polansky, (301) 903-5995
ORNL Contact: Tony Haynes, Solid State, (423) 574-2858

The objective of this project is to cooperate in ion implantation research and related processing of semiconductors to accelerate the development cycle for three critical technologies required for the manufacturing of the next generation of microelectronic integrated circuits (ICs). These include: (1) gettering of impurities, where the goal is to identify and evaluate implantation-based schemes for generating stable gettering sites for deleterious impurities within silicon wafers; (2) dielectrics, where the aim is to develop and test thin dielectric films for compatibility with shallow junction formation; and (3) metallization, where the challenge is to eliminate stress-induced metal failures. In this research, the feasibility of using ion-implantation-based approaches for solving these problems during manufacturing will be evaluated.

Keywords: Ion Implantation, Integrated Circuits, Semiconductor Manufacturing

201. **RAPID PROTOTYPING OF CERAMICS (ORL94-95)**
$ 150,000
DOE Contact: Walter M. Polansky, (301) 903-5995
ORNL Contact: Robert Lauf, Engineering Technology Division, (423) 241-2102

The goal of this project is to develop fundamental knowledge and apply that knowledge to the technology of rapid product realization for structural ceramic components. A major part of the effort is directed to modifying solid freeform fabrication techniques to produce sinterable ceramic green bodies rather than plastic models. The program also recognizes the crucial role of advanced computational techniques for creating and manipulating the large data files needed to adequately represent complex three-dimensional components with the necessary resolution.

Keywords: Freeform Fabrication, Rapid Manufacturing, Ceramics

202. **RAPID PROTOTYPING OF BIOCERAMICS FOR IMPLANTS (ORL95-12)**
$105,000
DOE Contact: Walter M. Polansky, (301) 903-5995
ORNL Contact: Ogbemi Omatete, Metals and Ceramics Division, (423) 576-7199

The goal of this research is to combine the ORNL gelcasting process and an injection stereolithography process to make a rapid manufacturing system suitable for the fabrication of limited-production ceramic components for implants and prostheses. This project will complement a related effort led by Argonne National Laboratory in the conversion of CAT/MRI data sets into a format suitable for rapid freeform fabrication processes.

Keywords: Ceramics, Gelcasting Process, Rapid Manufacturing, Freeform Fabrication

INSTRUMENTATION AND FACILITIES

203. **MICRO-SPECTROSCOPY FACILITY FOR NEW INFRARED IMAGING MATERIALS (BNL94-60)**
$25,000
DOE Contact: Walter M. Polansky, (301) 903-5995
BNL Contact: Gwyn Williams, NSLS, (516) 344-7529

Brookhaven National Laboratory is developing a custom synchrotron beamline facility for characterizing infrared sensor technology materials. New materials for high performance and/or low cost infrared imaging systems will be developed and tested. The testing involves infrared microspectroscopy using infrared synchrotron radiation as the source for the microscope. Synchrotron radiation is 1000 times brighter than conventional thermal infrared sources, making this a unique facility.

Keywords: Micro-spectroscopy, Infrared, Imaging Materials, Synchrotron Beamline

204. **DEVELOPMENT OF ENVIRONMENTALLY CONSCIOUS MACHINING FLUIDS (ORL94-91)**
$445,000
DOE Contact: Walter M. Polansky, (301) 903-5995
ORNL Contact: Thomas Morris, Metals and Ceramics, (423) 241-2796

The objective of this project is to develop required cutting fluids for ceramic and other advanced materials that are more environmentally benign and will reduce or eliminate the environmental problems associated with management and disposal of these cutting fluids. The specific goal of the project is to develop a method to degrade synthetic cutting fluids and reduce their total organic carbon (TOC) content and chemical oxygen demand (COD) to allow for final disposal in municipal sewage treatment facilities. Water-based industrial fluids can have excessively high TOC (ca. >15,000 PPM), thus making their treatment especially challenging.

Keywords: Cutting Fluids, Ceramics, Machining, Environmental

205. **NOVEL METHODS FOR FABRICATION COST REDUCTION OF PRESSURE INFILTRATION CAST METAL MATRIX COMPOSITE COMPONENTS (ORL95-01)**
$200,000
DOE Contact: Walter M. Polansky, (301) 903-5995
ORNL Contact: James Hansen, Engineering Technology Division, (423) 241-2102

The goal of this project is to develop pressure infiltration casting as a method to manufacture high quality metal matrix composite castings at high production rates. The manufacturing demonstration component of the project is a lightweight (60 percent reduction or 20 pound weight savings versus cast iron calipers), high modulus, particulate reinforced aluminum brake caliper.

Keywords: Pressure Infiltration Casting, Manufacture, Metal Matrix Composites

206. **ULTRA-PRECISION AUTOMATED MEASUREMENT FOR MANUFACTURING (ORL95-08)**
$80,000
DOE Contact: Walter M. Polansky, (301) 903-5995
ORNL Contact: C.Thomas, Fusion Energy Division, (423) 574-1155

Project goal is to demonstrate a new level of automated process control, noncontact measurement technology for the United States manufacturing sector. The immediate goal is proof of concept for intelligent automated electronic interferometry inspection of digital microchips with a resolution better than the lithographic mask resolution (e.g., a transverse resolution of 200 nanometers and a longitudinal resolution of 20 nanometers). This will allow automated 3-dimensional inspection of the chips between processing steps to insure success of the processing at each step; immediately identify process failures; save time, money, and energy; improve quality and yield by eliminating defective chips early in the processing; and immediately identify process failures. The intention is to provide a totally automated, rapid, on-line inspection capability to automatically detect and sort defective chips or call for human intervention. This technology can be extended to inspection and process control for all kinds of precision components, particularly for the automotive, electronics, and defense industries. Some examples of additional uses include: automated inspection of precision machined parts; automated inspection of heads and platters for hard disk drives (where some tolerances are starting to approach the sub-micron level); and automated noncontact inspection of aircraft wing sections and automotive body panels on a more macroscopic level.

Keywords: Ultra-Precision Measurements, Automated Process Control, Manufacturing, Inspection

207. **NEURAL NETWORK MODEL (ORL95-90)**
$150,000
DOE Contact: Walter M. Polansky, (301) 903-5995
ORNL Contact: Gerald Ludtka, (423) 574-5098

The goal of this project is to significantly reduce the required number of iterations in the sheet metal forming die design process, a process typically involving extensive and costly physical prototyping. The project employs a collection of emerging computational technologies such as digital simulations of deformation processes, neural networks, high-performance computing, and 3-dimensional optical metrology in order to achieve accurate and timely computations during the design process as well as during the control of the stamping process so as to eliminate a large fraction of the presently required design iterations.

Keywords: Neural Networks, Die Design, Sheet Metal Forming, Optical Metrology, Stamping Process

208. **MODELING AND SIMULATION OF ADVANCED SHEET METAL FORMING (PNNL94-38)**
$340,000
DOE Contact: Walter M. Polansky, (301) 903-5995
PNNL Contact: Mark Smith, Materials & Chemical Sciences, (509) 376-2847

This project will enhance numerical modeling and simulation of advanced sheet metal forming processes, allowing rapid elevated temperature processing of lightweight aluminum alloy sheet. In this project, improved material deformation models and predictive codes for advanced forming processes will be developed. Development of the new capabilities will allow the manufacturing industries to optimize the component and tooling designs and improve the forming processes without costly trial and error development of the advanced forming technology. Implementation of this modeling and forming technology will enhance the competitiveness of U.S. industry.

Keywords: Advanced Sheet Metal Forming, Modeling and Simulation, Lightweight Al Alloy Sheets, Manufacturing, Competitiveness of U.S. Industry

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

209. **IN-LINE ALUMINUM SENSORS (ORL95-04)**
$90,000
DOE Contact: Walter M. Polansky, (301) 903-5995
ORNL Contact: Jack Young, Chemical & Analytical Sciences, (423) 574-5241

The objective of this project is to develop in-line sensors for commercial aluminum electrolysis cell operation. The sensors to be developed will be of a Raman spectral type. The research goal is to develop technology which will allow measurement of soluble alumina, bath ratio and bath temperature. These in-line measurements will be inputs to new process control algorithms that can then be developed to improve the efficiency of aluminum electrolysis operations thereby reducing energy consumption. Such energy saving is in line with the goals of DOE. The improved control algorithm will also lead to a reduction in the anode effect which results in wasted energy and fluorocarbon emission. Reduction of potentially hazardous environmental gases is also a goal of DOE. Along with the development of these sensors, the basic chemistry of the melts will be studied to gain knowledge of speciation and effect of impurities on the process efficiency. A critical parallel study will be carried out to develop sheath materials that will have a useful lifetime (6 months) in cryolite melts. With such sheath materials, the long-term measurement of temperature by standard techniques can also be accomplished.

Keywords: Aluminum Electrolysis Cell, In-Line Sensors, Manufacture

210. **THE ROLE OF YTTRIUM IN IMPROVING THE OXIDATION RESISTANCE IN ADVANCED SINGLE CRYSTAL NICKEL-BASED SUPERALLOYS FOR TURBINE APPLICATIONS (ORL95-07)**
$45,000
DOE Contact: Walter M. Polansky, (301) 903-5995
ORNL Contact: Kathleen Alexander, Metals and Ceramics Division, (423) 574-0631

The focus of this project is to examine the role of yttrium and other alloying elements on the microstructure and oxidation performance of improved single crystal nickel-based superalloys for advanced turbine applications. Anticipated improvements from these new alloys include enhanced durability and performance at the high temperatures required to improve energy efficiency. Specific technical goals include: (1) identifying the partitioning behavior of the elemental additions in these superalloys before and after burner rig and engine tests and the effect on the misfit energy between the phases in the alloys; (2) examining the oxidation performance of these newly-developed alloys; and, (3) relating the microstructural observations to the observed performance.

Keywords: Turbines, Ni-Based Superalloys, Oxidation, Yttrium Alloying, Microstructure

211. **PROCESSING/PROPERTY RELATIONSHIPS IN CENTRIFUGALLY CAST AL-METAL MATRIX COMPOSITES (MMC) (PNNL94-02)**
$80,000
DOE Contact: Walter M. Polansky, (301) 903-5995
PNNL Contact: Ed Courtright, Material Sciences, (509) 375-6926

The goal of this project is to develop cost-effective selectively reinforced metal matrix processing technology. Light alloy metal matrix composites reinforced with silicon carbide or alumina particulates can replace steel in many automobile applications, and the corresponding reduction in vehicle weight translates to a proportional increase in gas mileage. This project concentrates on understanding the microstructure of centrifugally cast MMC's because the process offers the unique capability to distribute the particle phase in regions or zones where the reinforcements will have the greatest benefit. Emphasis will be placed on understanding processing/property relationships and in determining how these can be controlled to optimize selectively reinforced composite structures.

Keywords: Metal Matrix Processing, Centrifugal Casting, Al-Metal Composites

212. **BIOACTIVE AND POROUS METAL COATINGS FOR IMPROVED TISSUE REGENERATION (PNNL95-23)**
$155,000
DOE Contact: Walter M. Polansky, (301) 903-5995
PNNL Contact: Allison Campbell, Materials & Chemical Sciences, (509) 375-2180

The goal of this project is to combine complementary technologies and conduct a testing program which would provide information necessary to develop novel health-related technology devices. If the laboratory research demonstrates that metals or alloys can be reproducibly and uniformly coated using PNNL's unique technology and the biologically suitable metallic or alloy devices coated with the technology are shown to have improved performance in selected animal studies and clinical trials, then the potential products will target a growing market currently estimated to be between $1.2 to $1.5 billion annually.

Keywords: Biologically Suitable Metallic Devices, Tissue Regeneration, Health-Related Technology Devices

ADVANCED ENERGY PROJECTS PROGRAM

The Division of Advanced Energy Projects (AEP) provides support to explore the feasibility of novel, energy-related concepts that evolve from advances in basic research. These concepts are typically at an early stage of scientific development and, therefore, are premature for consideration by applied research or technology development programs. The AEP also supports high-risk, exploratory concepts that do not readily fit into a program area but could lead to applications that may span several disciplines or technical areas.

The Division provides a mechanism for exploring the conversion of basic research results into applications that could impact the Nation's energy economy. AEP does not support ongoing, evolutionary research or large scale demonstration projects. Technical topics include physical, chemical, materials, engineering, and biotechnologies. Projects can involve interdisciplinary approaches to solve energy-related problems. The DOE Contact for this program is Walter M. Polansky, (301) 903-5995.

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

213. **MAGNETIC REFRIGERATION FOR SUB-ROOM TEMPERATURE COOLING**
$310,000
DOE Contact: Walter Polansky, (301) 903-5995
Ames Laboratory Contact: Karl A. Gschneidner, Jr., (515) 294-7931

The design of a new type of near-room temperature magnetic refrigerator and the demonstration of its technical feasibility as an alternative refrigeration technology for energy-intensive industrial and commercial refrigeration systems is under development. Large-scale (>30 kW) chlorofluorocarbon (CFC) vapor cycle refrigeration units in commercial facilities, such as deep-freezers in meat packing plants and display case chillers in supermarkets, represent a significant portion of the total U.S. electrical energy demand. The efficiency of existing refrigerators is considerably less than that of the ideal Carnot efficiency because of intrinsic limitations of the currently used vapor cycle process, especially in the compression and Joule-Thomson expansion parts of the cycle. In contrast, the magnetic refrigeration cycle has a very high intrinsic efficiency; the efficiency appears to be limited by factors susceptible to control, such as non-ideal materials properties, parasitic heat transfer, and flow losses. Replacement of vapor cycle refrigerators with magnetic refrigerators offers a significant potential energy savings. In addition, magnetic refrigerators do not require any ozone-damaging CFCs or other volatile fluids that have a significant greenhouse effect, so their widespread use would reduce potential environmental hazards. The elimination of CFCs is also in compliance with federally mandated programs to reduce the risk to the ozone layer. There are two major aspects of this project. The first is a materials development task, which will be carried out by the Ames Laboratory in Ames, Iowa. The second task involves the engineering aspects of designing, constructing, and demonstrating a sub-room temperature active magnetic regenerator magnetic refrigerator, which will be carried out at the Technology Center of the Astronautics Corporation of America, in Madison, Wisconsin.

Keywords: Magnetic Refrigeration, Alternative Refrigeration Technology

214. **COMPOSITE MAGNETOSTRICTIVE MATERIALS FOR ADVANCED AUTOMOTIVE MAGNETOMECHANICAL SENSORS**
$101,000
DOE Contact: Walter Polansky, (301) 903-5995
Ames Laboratory Contact: David C. Jiles, (515) 294-9685

There is a well established need for torque sensors for a variety of applications in automobiles. Such sensors can be used for electronic control of the vehicle by monitoring steering and drive train torques. In this project, new highly magnetostrictive materials are being investigated for use in advanced steering systems. Such sensors will eliminate the need for maintaining a pressurized hydraulic power steering system and will improve fuel efficiency by 5 percent. These sensors will need to meet stringent specifications such as the ability to operate over a range of temperatures between minus 40 C and plus 85 C, be able to survive unexpected mechanical shocks of up to 500 N and operate under continual vibrational forces of 150 N. In addition, the sensors must be able to sustain overload torques of 135 N.m without malfunctioning or significantly changing sensitivity over the normal operating range of +/- 10 N.m. Analysis of the relationship between the magnetomechanical effect (the change in magnetization with stress) and the magnetostriction (particularly the rate of change of strain with magnetic field) has shown that highly magnetostrictive materials with low anisotropy, and hence high permeability, form the most promosing class of materials from which to develop such high performance sensors. This project is therefore investigating the fabrication of composite materials consisting of the highly magnetostrictive material Terfenol-D in a high-strength matrix material, in order to meet the performance specifications for these torque sensors.

Keywords: Magnetostrictive Materials, Torque Sensors, Terfenol-D

215. **ENERGY RELATED APPLICATIONS OF SELECTIVE LINE EMITTERS**
$254,000
DOE Contact: Walter Polansky, (301) 903-5995
Auburn University Contact: M. Frank Rose, (334) 844-5894

Infrared heat sources are used extensively for many processes in industry. From initial work, it appears feasible to develop intense infrared sources based upon electronic transitions in compounds of the rare earths which tend to radiate efficiently at discrete wavelengths rather than a continuum. This work is aimed at conducting the basic and exploratory research which will allow the development of high intensity, discrete frequency infrared sources which are custom tailored to specific industrial processes. This will be accomplished by investigating and characterizing the emissive properties of the rare earths in inert forms such as oxides, borides, carbides, or nitrides. The Center for the Rare Earth Elements at the DOE Ames Research Laboratory will be used as the source of information for selection of suitable rare earth elements and compounds. Fibrous inert compounds of the rare earths will be formed as necessary. Oxide fibers can be formed by soaking activated carbon fibers in a suitable liquid compound of the rare earth, such as a nitrate of the material. Since activated carbon fibers can be greater than 70 percent porous, a substantial fraction of the liquid can be absorbed for suitable processing. The composite materials are formed into a paper with minor additions of cellulose using standard paper making technology. Subsequent heating in a reducing atmosphere removes the cellulose and carbon, and forms essentially a pure metallic shell, mimicking the size of the activated carbon precursor. The final dimensions of the rare earth oxide fiber are determined by the initial dimensions of the precursor material. Successful samples will also be characterized for strength, flexibility, and lifetime at temperature. Large area radiators for specific frequencies will be constructed and evaluated with the cooperation of an industrial affiliate.

Keywords: Infrared Energy Delivery Sources, Rare Earth Selective Line Emitters, Industrial Processes

216. **A NOVEL TANDEM HOMOJUNCTION SOLAR CELL: AN ADVANCED TECHNOLOGY FOR HIGH EFFICIENCY PHOTOVOLTAICS**
$268,000
DOE Contact: Walter Polansky, (301) 903-5995
Colorado State University Contact: Bruce Parkinson, (970) 491-0504

A material for the construction of a solar cell must meet a number of criteria to be suitable for large scale photovoltaic applications. It must be made up of abundant elements, which are environmentally benign, and when combined into a crystal have suitable electronic properties. The required electronic properties include a bandgap in the 1.1-1.8 eV range, high absorption coefficients to minimize the amount of material required, and high mobilities of photogenerated carriers to facilitate the collection of these carriers. The semiconductor, ZnSnP(2), meets all of the above requirements. It is isoelectronic with the III-V alloy InGaP(2), but has the advantage, for photovoltaic applications, of not containing expensive and rare group III elements. In addition, this material does not contain toxic heavy metals such as are found in CdTe and CuInSe(2)/CdS thin film solar cells. The absorption coefficient for this material is also very high. The bandgap of ZnSnP(2) has the additional interesting and useful property of ranging from 1.24 to 1.66 eV, depending on the preparation conditions. Bulk crystal growth techniques have not yielded high mobility ZnSnP(2) but there is no *a priori* reason that the electronic properties of these materials cannot be as good as III-V materials, since very high mobilities were only achieved in III-V's after the development of modern epitaxial growth techniques. State-of-the-art metal-organic molecular beam epitaxy (MOMBE) will be used to grow epitaxial layers of ZnSnP(2) on lattice matched GaAs substrates. Studies of the order-disorder transition in the metal sublattice, using both optical and electrical techniques and especially solid state NMR to examine atomic scale local environments, will be conducted in order to find the conditions for preparing materials with various bandgap energies and to understand the basic chemistry and physics associated with this interesting order/disorder phase transition. When the conditions can be established for preparing a material of a given bandgap, a "tandem homojunction" solar cell will be fabricated by variation of growth conditions in the MOMBE chamber in the appropriate way. This device should show significant efficiency advantages over a single material device or tandem heterojunction devices where lattice mismatch produces recombination promoting interface states.

Keywords: Solar Cells, Photovoltaics, MOMBE, Metal-Organic Molecular Beam Epitaxy

217. **TWO-DIMENSIONAL SYNTHESIS: ULTRATHIN POROUS MEMBRANES**
$300,000
DOE Contact: Walter Polansky, (301) 903-5995
University of Colorado Contact: Josef Michl, (303) 492-6519

The objective of this research program is to synthesize and characterize an ultrathin fishnet-like sheet, suitable for application in molecular separations. This will be a new kind of heat-resistant organic-inorganic solid with a regular repeating two-dimensional structure, containing openings of a predetermined size. The first step will be the synthesis of a tentacle-carrying pillar-like monomer with three arms opposite to the tentacled end. Next, its molecules will be constrained by strong adsorption of the tentacles to a liquid-liquid interface, oriented with the pillar perpendicular to the surface and the arms parallel to it, at a distance of a little less that 10 angstroms. In the subsequent step, the arms of the monomer molecules will be cross-linked in two dimensions into a sheet composed of a regular covalent hexagonal lattice parallel to the surface. The polymerization will be monitored *in situ*. The lateral dimensions of the sheet will be maximized by a search for optimum reaction conditions. Neighboring sheet segments will be stitched together with relatively flexible threads to yield a large macroscopic piece of ultrathin membrane. The tentacles will then be clipped off, permitting desorption and removal of the net-like membrane from the surface. The construction will be completed by additional cross-linking to form a second hexagonal lattice on the side that previously carried the tentacles. The two hexagonal nets will thus be bonded into a single sheet through pillars located at well separated trigonal connector centers. The sheet will be about 15 to 20 angstroms thick, and will contain openings with a diameter of about 20 angstroms. The structure will be characterized by the techniques of surface science and its separatory properties will be tested. This will complete the proof-of-concept part of the project. The experience gained in the project will be used to design a second generation membrane for an actual industrial separation process, taking advantage of the flexibility available in the choice of the size of the openings, which can be chosen anywhere from nearly zero to about 40 to 50 angstroms in diameter, and in the choice of chemical functionalities at the rim of the openings.

Keywords: Membranes, Molecular Separations, Separation Processes, Ultrathin Membranes

218. **BLUE-EMITTING DEVICES BASED ON GALLIUM NITRIDE**
$332,000
DOE Contact: Walter Polansky, (301) 903-5995
Lawrence Berkeley National Laboratory Contact: Michael D. Rubin, (510) 486-7124

The purpose of this project is to convert the recent breakthroughs in growth of gallium nitride (GaN) into practical ultraviolet and blue light emitting diodes and lasers. This technology is critical to national competitiveness in the development of the next generation of optoelectronic devices. Short-wavelength semiconductor devices based on GaN are needed for many important applications such as energy-efficient illumination, high-density optical data storage, flat-screen color displays, underwater communications, and high-temperature electronics. GaN is a III-V semiconductor with a direct bandgap of 3.4 eV in the ultraviolet. One of the principal technical problems that limits device applications has been achieving controllable properties with addition of Mg. The nitrogen concentration of the films was greatly increased, by using a reactive ion-beam process, thus eliminating the primary background defect concentration. Upon attaining threshold levels of conductivity and mobility, it was discovered that good quality material could be readily obtained by a variety of doping methods including ion implantation, diffusion and co-evaporation of Mg. The defect studies which guide the improvements in the growth process will be continued. This process, along with specialized ion beam technology, will be transferred to Hewlett-Packard where it will be reproduced in a large-scale commercial growth system. Simultaneously, fabrication of light-emitting devices will begin, using current materials, in cooperation with Hewlett-Packard.

Keywords: Gallium Nitride, Blue-Emitting Devices

219. **MAGNETICALLY ENHANCED THERMOELECTRIC COOLING**
$250,000
DOE Contact: Walter Polansky, (301) 903-5995
Los Alamos National Laboratory Contact: Albert Migliori, (505) 667-2515

Cryogenic solid-state refrigerators based on the Ettinghausen effect can provide vastly superior performance to Peltier devices, opening up new markets in electronics and in superconductor-, and medical applications. Surprisingly, this most effective of solid-state cryogenic refrigeration processes is not being studied at present. Yet it is much less restrictive in the possible materials that can be used, is simpler to construct (even noting that a small permanent magnet must produce a field at the device), and has already achieved lower temperatures than Peltier coolers, the only devices presently under investigation. Recent discoveries of new hybridization-gap semi-conductors and semi-metals, and the commercial availability of high-strength Nd(2)Fe(14)B permanent magnets, open the way for development of new ultra-high-performance, all solid-state Ettinghausen refrigerators. We propose here to initiate studies of such coolers using modern materials and to engineer the world's best solid-state cryocooler.

Keywords: Thermoelectric Cooling, Peltier Devices, Solid-State Refrigeration, Ettinhausen Effect

220. **PV-POWERED, ELECTROCHROMIC WINDOWS**
$330,000
DOE Contact: Walter Polansky, (301) 903-5995
National Renewable Energy Laboratory: David K. Benson, (303) 384-6462

This project will develop a retrofit window treatment for architectural windows. The window treatment will be a combination of thin-film photovoltaic cells and an electrochromic coating, both deposited onto a flexible polymer film. The coated polymer film will be applied to the interior surfaces of existing building windows and used to modulate the solar transmittance into the building thereby providing automatic solar-gain control and daylighting control functions which will reduce heating, cooling, and lighting energy usage in the building. The self-powered window obviates the need for costly electrical wiring. This kind of "smart" window covering has the potential to balance the performance of the window, giving it a net energy benefit. It has been predicted to be able to reduce the cooling power demand of a south-facing window in a climate such as southern California by about 40 percent and to have similar benefits in other locations. A large fraction of the billion square meters of existing building windows in the U.S. could benefit from this kind of treatment. At present, an estimated 1 to 1.5 percent of the total cooling energy need in buildings and 10 to 30 percent of the peak electric utility power demand is caused by windows amounting to about a 1500 MW increase in electric utility peak electric power demand each year due to new windows at a national operating cost of about $10 billion. New photovoltaic and electrochromic coating designs and new processes for their deposition onto flexible polymer substrates will be developed in this project.

Keywords: Electrochromic Windows, Smart Windows, PV-Powered Windows

221. **HOT CARRIER SOLAR CELLS**
$330,000
DOE Contact: Walter Polansky, (301) 903-5995
National Renewable Energy Laboratory Contact: Mark C. Hanna, (303) 384-6620

This project is focused on the development and understanding of a new kind of high efficiency solar cell, called a Hot Carrier Solar Cell (HCSC), which may have the potential to double the maximum efficiency of conventional solar cells. The ultimate thermodynamic conversion efficiency of an optimized HCSC is 66 percent, compared to 31 percent for an optimized conventional single bandgap solar cell. This project explores a new approach for increasing the efficiency of solar cells by attempting to utilize the excess kinetic energy of higher energy (hot) carriers generated by the absorption of high energy photons in the solar spectrum. Normally, the excess kinetic energy of hot carriers created by absorption of solar photons in photovoltaic cells is converted to heat and is thus unavailable for useful work. The HCSC employs a new type of semiconductor structure (called a superlattice) to absorb the solar photons and to inhibit hot carriers from cooling in the photovoltaic device. Bandgap engineering techniques will be used to control important physical properties of the superlattice, such as the hot carrier energy loss rate, hot carrier mobility, and the absorption threshold. Hot carriers from the superlattice region are collected in high bandgap contacts to produce a higher photovoltage. With this combination, the photocurrent and photovoltage of the cell can be separately controlled and optimized, unlike the conventional p-n photovoltaic cell where the photocurrent and photovoltage are coupled. The HCSC is fabricated from Group III-V semiconductor compounds and alloys grown by low pressure organometallic chemical vapor deposition. This project will synthesize HCSCs, measure their performance and properties, compare them to appropriate conventional solar cells, and develop a theoretical model for predicting the device characteristics of the HCSC.

Keywords: Hot Carrier Solar Cells, High Efficiency Energy Conversion

222. **ATOMIC AND NANOSCALE ENGINEERING OF THERMOPHOTOVOLTAIC SEMICONDUCTORS USING SCANNING PROBE MICROSCOPY TECHNIQUES**
$315,000
DOE Contact: Walter Polansky, (301) 903-5995
National Renewable Energy Laboratory
Contact: Lawrence L. Kazmerski, (303) 384-6600

This project uses scanning probe microscopies for the atomic-scale engineering of semiconductors leading to advances in understanding their improvement, and their use in energy-conversion thermophotovoltaic (TPV) structures and devices—cells designed to produce electricity from surfaces emitting radiation in the 1400 to 2000 K range. This program consists of three interrelated segments: (1) preparation of selected GaInAs and GaInAsP alloy surfaces having suitable compositions; (2) use of modern electronic structure theory to predict the properties of these semiconductor surfaces before and after atomic-scale engineering takes place and to provide guidance for the experiments; and, the central and primary activity, (3) evolution of the novel atomic processing microscope to image, process (including atom removal and placement), and characterize these semiconductors with the same nanoscale spatial resolutions and to produce nanometer-scale optimized TPV structures for the next generation of these energy conversion devices. These atomic-scale investigations involve the manipulation of atoms in order to study the fundamental defect properties that limit both materials properties and device performance. The program provides the first atomic engineering directed toward these III-V materials. It further provides fundamental information of the nature of defects, their electro-optical properties and the ability to electronically heal them with intrinsic and extrinsic atomic species. This project links events on the atomic scale to the current understanding of semiconductor surface and interface physics. The project provides first-time characterization of the electrooptical properties of TPV semiconductors in compositional ranges not previously investigated. This information is used to demonstrate optimized next-generation TPV structures that will lead to highly efficient cells for energy applications.

Keywords: Thermophotovoltaics, Atomic Force Microscopy

223. **PHOTOCHEMICAL SOLAR CELLS**
$150,000
DOE Contact: Walter Polansky, (301) 903-5995
National Renewable Energy Laboratory
Contact: Arthur J. Nozik, (303) 384-6603

Very high power conversion efficiencies (8-12 percent) for photochemical solar cells were reported in 1991. These solar cells consist of highly porous nanocrystalline films of TiO(2) (band gap=3.0 eV) that are sensitized to the visible region of the solar spectrum through adsorption of Ru-containing metal-organic dye complexes on the TiO(2) particle surface. This represents more than two orders of magnitude improvement in the power conversion efficiency of dye-sensitized semiconductor electrodes in a photochemical cell. A dye-sensitized photochemical solar cell system based on TiO(2) powders is very attractive from the point of view of potential low cost and high semiconductor photostability. This project is an integrated program of basic and applied development research that is funded jointly by three U.S. Department of Energy program offices: the Division of Chemical Sciences in the Office of Basic Energy Sciences, the Photovoltaic program in the Office of Utility Technology and Advanced Energy Projects. In addition to the molecular dye-sensitized TiO(2) system, research is also occurring to study other organic heterojunctions with wide bandgap semiconductors for photovoltaic applications. The AEP portion of the project is to develop a configuration where the system is able to efficiently split water into hydrogen and oxygen, rather than to produce electricity. An inexpensive source of solar-produced hydrogen would be greatly beneficial to the energy economy of the world, and would result in the use of hydrogen as a non-polluting substitute for many of the fuels currently in use.

Keywords: Photochemical Solar Cells, Hydrogen Production, Dye-Sensitive Semiconductors

224. **BIOMOLECULAR OPTOELECTRONIC DEVICES**
$370,000
DOE Contact: Walter Polansky, (301) 903-5995
Oak Ridge National Laboratory Contact: Elias Greenbaum, (423) 574-6835

The key purpose of this research is acceleration of practical device development based on original Oak Ridge National Laboratory proof-of-principle scientific discoveries which were supported by the Division of Chemical Sciences, Office of Basic Energy Sciences. It is motivated by knowledge of the intrinsic photophysical properties of the reaction centers of photosynthesis: nanometer dimensions, picosecond response times, and the ability to generate potential differences of about 1 volt upon absorption of a photon. The proposed research project is based on original discoveries in molecular electronics made at Oak Ridge National Laboratory. These include: (1) first demonstration of direct electrical contact with the electron transport chain of photosynthesis; (2) photoflash deposition of metallic platinum at the site of electron emergence from the Photosystem I reaction center of photosynthesis; (3) establishment of a novel platinization "welding" technique that allows construction of two-dimensional arrays of Photosystem I reaction centers on a metal surface; (4) first demonstration of a biomolecular diode in a single isolated photosynthetic reaction center; and (5) first demonstration of the compatibility of metallic platinum with the functionality of isolated Photosystem I reaction centers.

Keywords: Biomolecular Optoelectronic Devices, Molecular Electronics, Photosynthesis

225. **SEMICONDUCTOR BROADBAND LIGHT EMITTERS**
$382,000
DOE Contact: Walter Polansky, (301) 903-5995
Sandia National Laboratories Contact: Paul Gourley, (505) 844-5806

Semiconductors are compact, lightweight, operate in air, and are rugged. However, conventional semiconductor diodes emit light only into a narrow range of wavelengths. To obtain broadband emission, new structures are needed that utilize a wide range of alloy compositions available from modern semiconductor growth techniques. Fractal lattice and chirped quantum wells form a new class of materials which can provide broadband light emitters. The goal of this proposal is to develop such multi-alloy structures grown by metal organic vapor phase epitaxy and molecular beam epitaxy for efficient, broadband light emission. To develop broadband emitters, we will focus our efforts on this class of fractal and chirped quantum-wells structures utilizing InAlGaP alloys grown by metal-organic vapor phase epitaxy on GaAs substrates. The work will concentrate on three areas: materials design and growth, characterization and modelling, and device design and fabrication. The interplay of these three parallel efforts will lead to optimized device structures that emit broadband light with at least 300 meV bandwidth in the green to red regions and a few percent external quantum efficiency. Materials and design parameters will be understood through a wide variety of experimental and theoretical tools. To implement this new class of broadband emitters, we will design, grow and fabricate light-emitting diode structures, and measure electroluminescence spectra, current-voltage, and light-current characteristics.

Keywords: Broadband Light Emitters, Indium-Aluminum-Gallium-Phosphide, Fractal Lattice and Chirped Quantum Wells

226. **A THERMO-PHOTOVOLTAIC GENERATOR FOR USE IN A LIGHTWEIGHT ELECTRIC CAR**
$299,851
DOE Contact: Walter Polansky, (301) 903-5995
Western Washington University Contact: Michael R. Seal, (360) 650-3045

In an internal combustion engine, fuel is mixed with air and periodically exploded. Because the explosions are of very short duration, the fuel combustion is incomplete, leading to carbon monoxide and hydrocarbon exhaust emissions. More pollution results because the temperature at the peak of the explosion is very high leading to the creation of nitrous oxides. A quiet, lightweight, clean, electric power source will be built in which a fuel is continuously burned in a ceramic tube, the tube glows red hot, and photovoltaic cells receive the infrared from this emitter and convert it to electric power. In effect, "solar" cells are used with a small manmade "sun" created by burning natural gas. Because fuel is burned continuously without periodic explosions, the thermophotovoltaic unit is very clean, quiet, efficient, and lightweight. The first benchtop experiments have already shown that this generator is 50 times cleaner than an internal combustion engine. Such a thermophotovoltaic unit has only recently become feasible as a result of new gallium antimonide cells fabricated by the JX Crystals Company. These new cells are much more sensitive in the infrared range than traditional solar cells. These new infrared cells will be integrated with an efficient natural gas fired infrared source with sufficient power to charge onboard vehicle batteries. The thermophotovoltaic eight cylinder unit alone, will be able to maintain an automobile at a speed of 60 miles per hour on level ground. Additional power for hill climbing and performance will be provided by onboard batteries.

Keywords: Thermophotovoltaics, Electric Vehicles

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

227. **PHOTOREFRACTIVE LIQUID CRYSTALS: NEW MATERIALS FOR ENERGY-EFFICIENT IMAGING TECHNOLOGY**
$300,000
DOE Contact: Walter Polansky, (301) 903-5995
Argonne National Laboratory Contact: Gary P. Wiederrecht,, (630) 252-6963

This project will develop a new class of materials that will be used to produce energy-efficient image processing micro-devices. These materials will exploit the photorefractive effect, a light-induced change in the refractive index of a nonlinear optical material that results from photogeneration of a space charge field caused by directional charge transport over macroscopic distances within a solid. Both frequency and phase information contained in light that has passed through a distorting medium can be recovered noise-free using photorefractive materials. The only high quality photorefractive materials commercially available today are expensive single crystals of inorganic materials such as barium titanate. This project will develop a completely new approach that combines cheap, easily processed organic materials with a built-in method of achieving the solid state order necessary to achieve photorefractivity comparable to that seen in inorganic crystals. The new approach uses organic molecules that undergo a phase transition above ambient temperatures to a liquid crystalline phase. Self-ordering in the liquid crystalline phase, followed by cooling to an ordered molecular solid, will impart both good optical nonlinearity and directional photoconductivity to thin solid films of these materials. These solid films have the potential to possess greater photorefractive sensitivity and faster response times than any material developed to date. The liquid crystals will be based on easily oxidized, disc-shaped organic molecules that are known to have liquid crystalline phases. The specific materials will be derivatives of triphenylenes, coronenes, porphyrins, and phthalocyanines. These molecules can be used to achieve the macroscopic order and good photoinduced charge generation characteristics that are required of high quality photorefractive materials for application throughout the visible and near-infrared spectral regions. Intrinsically asymmetric, nonlinear optical molecules, e.g. a chiral p-nitroaniline derivative, will be attached to the disc-shaped molecules and oriented in the liquid crystalline phase so as to maximize the nonlinear susceptibility of the material. Optical studies on the resulting solids will be utilized to verify the existence of photorefractivity and to accurately characterize the materials. Several device applications will be demonstrated.

Keywords: Photorefractive Liquid Crystals, Image Processing, Nonlinear Optical Materials

228. **EVAPORATION THROUGH TUNGSTEN TO ACHIEVE HIGH-RATE VAPOR PHASE PROCESSING OF INTERMETALLICS**
$318,000
DOE Contact: Walter Polansky, (301) 903-5995
General Electric Company Contact: David W. Skelly, (518) 387-6534

The understanding of high-rate electron beam evaporation synthesis derived from this investigation will have significant impact on the ability to fabricate advanced designs of turbine blades, designs which cannot be produced by any state-of-the-art technology. Success in this program will make possible forming the complex cooling structure after the casting process, followed by a thin outer skin deposited by electron beam (EB) evaporation to create a double-wall. This structure combined with composite materials developed specifically for the EB process, will provide long term efficiency improvements and enhanced service life. High-rate EB evaporation processes are currently difficult to control for deposition of complex alloys and intermetallics: fluctuations in power level and beam position can lead to large fluctuations in deposition rate and deposit chemistry. Modification of current practice of EB processes has been found to enhance chemistry uniformity and deposition rates through the addition of tungsten to the evaporation pool to permit much higher pool temperatures and stable pool dynamics. The objective of this research is to define optimum operating conditions for achieving economic deposition of controlled-chemistry, controlled-thickness Ni-base superalloys, NbTi-base metallic materials, and high strength, high temperature intermetallic phases. The approach will be to: evaluate process stability during prolonged evaporation through a tungsten-rich liquid pool; measure the effect of tungsten concentration in the pool on the evaporation process; characterize the influence of electron beam scan rate and scan pattern on the deposit chemistry and deposition rate; characterize the influence of the source temperature profile on deposit chemistry and deposition rate; determine evaporation conditions for Ni-base alloys containing Ta and Mo; and extend the electron beam evaporation-through-tungsten processing to higher melting intermetallic phases and NbTi-base metals.

Keywords: Superalloys, Intermetallics, Electron Beam Processing, Turbine Blades

229. **SUPPORTED MOLTEN METAL CATALYSTS: DEVELOPMENT OF A NEW CLASS OF CATALYSTS**
$316,000
DOE Contact: Walter Polansky, (301) 903-5995
University of Iowa Contact: Ravindra Datta, (319) 335-1395

This project is concerned with the design and development of an entirely novel class of active and selective catalysts called supported molten-metal catalysts, or SMMC, with a view to eventually replace some of the existing precious metal heterogeneous catalysts used in the production of fuels and chemicals. SMMC is based on supporting ultra-thin films of the relatively low-melting, inexpensive, and abundant metals and semimetals, from groups Ia, IIb, IIIb, IVb, Vb, and VIb, of the periodic table, on porous refractory supports, much like supported microcrystallites of traditional solid catalysts. This technique, thus, provides orders of magnitude higher surface area than is obtainable in conventional reactors containing molten metals in pool form and also avoids corrosion. These have so far been the chief stumbling blocks in the use of molten metal catalysts despite their higher selectivity and lower susceptibility to deactivation. While the SMMC technique can be applied to a large variety of reactions, it is proposed to initially concentrate on dehydrogenation and reforming reactions due to their commercial significance. Thus, dehydrogenation of methylcyclohexane and decalin and reforming of methylcyclopentane are planned to be studied. These represent reactions of increasing complexity in catalytic reforming. The initial choice of catalyst are tellurium based catalysts including alloys, due to the very promising results obtained in preliminary screening experiments. Other catalytic formulations will also be tested. The activity, selectivity, and stability of the selected catalysts will be compared with the traditional Pt catalyst in differential packed-bed reactors. The commercial potential of the developed catalysts will be explored.

Keywords: Molten Metal Catalysts, SMMC, Dehydrogenation, Reforming

230. **ULTRASONIC AND DIELECTRIC NONINVASIVE DIAGNOSTICS FOR SINTERING OF CERAMIC COMPOSITES**
$290,000
DOE Contact: Walter Polansky, (301) 903-5995
Johns Hopkins University Contact: Moshe Rosen, (410) 516-8678

The potential advantages of using microwaves to process ceramics have been recognized for more than three decades. However, only during the last several years, the scientific and engineering communities have experienced an outburst of research in this area. Nevertheless, a profound understanding of how materials interact with microwaves during sintering is still lacking. Measurement of the dielectric and mechanical properties of a material during microwave processing in real-time can provide the necessary theoretical and experimental insight into understanding this interaction that can subsequently be applied for the optimization of microwave processing of materials. In the course of this project, *in situ*, nonintrusive diagnostics for microwave sintering of ceramic materials will be developed. The essence of the project is a specially designed system for ultrasonic and dielectric probes to be integrated within the microwave furnace. The ultrasonic data can be ultimately related to the densification process during sintering of ceramics, while the dielectric characteristics are connected to the absorption mechanism of the microwave energy by the ceramic material. Acquisition of such data during sintering will shed light on the sintering kinetics and its mechanism and, consequently, provide an understanding of the optimal sintering conditions needed to achieve maximum densification and the desired material properties. Furthermore, such data can be instrumental in developing predictive models for microwave sintering of ceramic materials.

Keywords: Microwave Sintering, Ceramics, Noninvasive Diagnostics

231. **COMPACT MEV ION IMPLANTER**
$298,000
DOE Contact: Walter Polansky, (301) 903-5995
Lawrence Berkeley National Laboratory
Contact: Simone Anders, (510) 486-6745

A new kind of MeV ion implanter will be developed, the distinguishing features of which will be its relatively small size and low cost. The heart of the device will be a novel kind of ion source by means of which high charge state ions will be produced, thereby allowing the production of high energy ion beams (1 MeV and above), using only modest accelerating voltages (one to several hundred kV). The ion source will be a repetitively pulsed vacuum spark source, and the implantation facility will thus also generate repetitively pulsed, large area, metal ion bea By virtue of the relatively low voltages employed the implanter will be much more compact and of much lower cost than present state-of-the-art facilities that employ singly charged ions and megavolt power supplies. From the perspective of new physics, a novel kind of ion source will be developed—vacuum arc ion sources have been developed but not vacuum spark ion sources, and it is in the latter that the highly stripped ions are to be found, yielding high energy at modest voltage. From the perspective of new technology, this is an entirely new approach to doing MeV ion implantation, making high energy surface modification techniques feasible for a vastly broader field of users than at present.

Keywords: Ion Source, Ion Implanter, Ion Beams, Surface Treatment

232. **COMBINATORIAL SYNTHESIS OF HIGH T_C SUPERCONDUCTORS**
$144,000
DOE Contact: Walter Polansky, (301) 903-5995
Lawrence Berkeley National Laboratory
Contact: X. D. Xiang, (510) 486-6640

Currently, there is a tremendous interest in materials such as high temperature superconductors, organic conductors, permanent magnets, nonlinear optical materials and zeolites. However, even through the properties of such materials have been extensively investigated, few general principles have emerged that allow one to predict the structures of new materials with enhanced properties. Consequently, the discovery of such materials remains a time consuming and rather unpredictable trial and error process made even more difficult by the increasing complexity of modern materials. The question arises whether there is a more efficient and systematic approach to search through the largely unexplored universe of ternary, quartenary, and higher order solid state compounds, in order to discover materials with novel electronic, optical, magnetic or mechanical properties. We propose to develop a new approach to materials discovery that will significantly increase the rate at which novel materials are discovered as well as increase our ability to correlate physical properties with structure. Specifically, we will develop the ability to rapidly synthesize and analyze large libraries, or collections, of solid state materials for specific electronic, magnetic, optical and structural properties. The aim of this project is twofold: (1) to develop the technology to the point where it can be used effectively for materials discovery; and (2) to apply the technology to the discovery of new superconducting materials.

Keywords: Combinatorial Synthesis, High Temperature Superconductors, High T_c Superconductors, Superconducting Materials

233. **THERMOELECTRIC QUANTUM WELLS**
$350,000
DOE Contact: Walter Polansky, (301) 903-5995
Lawrence Livermore National Laboratory
Contact: Joseph C. Farmer, (510) 423-6574

Solid state thermoelectric devices have no moving parts and can be used to convert heat directly into electricity. Such devices can also be used as chlorofluorocarbon (CFC)-free refrigerators, provided that an external voltage is applied. Unfortunately, thermoelectric devices are not as efficient as their mechanical counterparts. However, theoretical physicists at the Massachusetts Institute of Technology have recently used quantum mechanics to design a new class of thermoelectric materials that may improve the efficiency (figure of merit) of thermoelectric devices to a point where they are competitive with conventional internal combustion engines and CFC-based refrigerators. Process technology developed at Lawrence Livermore National Laboratory for the fabrication of x-ray optics is now being used to synthesize these new multilayer thermoelectric thin fil Multilayers are being made by alternately sputtering quantum well and barrier layers onto a moving substrate from dual magnetrons. A number of multilayer films, including high-temperature Si(0.8)Ge(0.2)/Si and low-temperature Bi(0.9)Sb(0.1)/ PbTe(0.8)Se(0.2), are being synthesized and evaluated. This research can lead to new materials and devices.

Keywords: Quantum Wells, Thermoelectric Devices

234. **POROUS CARBONS: CONTROLLING STRUCTURE, COMPOSITION AND PERFORMANCE**
$374,000
DOE Contact: Walter Polansky, (301) 903-5995
Lawrence Livermore National Laboratory Contact: Tri D. Tran, (510) 422-0152

This research examines the synthesis and processing conditions necessary to tailor the local structure and composition of porous carbons for potential applications in energy storage devices (i.e., batteries, capacitors). Carbon aerogels are being formed from resorcinol-formaldehyde and phenolic-furfural precursors. These porous carbons have low electrical resistivity, an ultrafine pore size distribution, high surface area (400 to 1100 square meters per gram, roughly the size of one or two basketball courts), and a solid matrix composed of interconnected particles or fibers. Preliminary data show that these materials are attractive electrodes for double layer capacitors. Carbon foams derived from the phase separation of polyacrylonitrile/ solvent mixtures are being investigated as lithium intercalation anodes for rechargeable lithium-ion batteries. These carbon foams differ from aerogels in that they have much larger pore sizes and one or two orders of magnitude lower surface area. High capacity and good cycleability are observed during lithium intercalation experiments. These materials can potentially lead to new batteries with energy densities that are approximately four times greater than conventional nickel-cadmium batteries. In summary, this research project investigates sol-gel polymerization of multifunctional organic monomers, the phase separation of polymer/solvent mixtures, the formation of porous composites, intrinsic chemical doping, and pyrolysis in controlled atmospheres. A variety of characterization tools are being used to study the structure and properties of porous carbons. The overall objective is to develop a fundamental understanding of how morphology, chemical composition, and local order affect the electrochemical performance of porous carbons. The potential payoff from this research is the development of new energy storage devices with superior performance.

Keywords: Porous Carbon, Aerogels, Energy Storage Devices, Sol-Gel

235. **FABRICATION AND CHARACTERIZATION OF MICRON SCALE FERROMAGNETIC FEATURES**
$101,000
DOE Contact: Walter Polansky, (301) 903-5995
University of Nebraska Contact: Peter A. Dowben, (402) 472-9838

This is a project to study micro scale features of ferromagnetic nickel, cobalt, cobalt-palladium alloys and cobalt-palladium heterostructures fabricated by "direct writing," i.e. by selective area deposition from organometallic compounds. There are two goals for this research program. First, by making magnetic features smaller and smaller, in a variety of different shapes, the project will elucidate the influence of defects on magnetization reversal and coercivity. Second, the project will determine if there is any coupling between small ferromagnetic features (approx. 1 micron), possibly substrate mediated, on the length scale of 1000 angstroms smaller. This research program is based upon conventional methods for imaging magnetic domains. Polarized light microscopy permits not only imaging micron scale features but also determination of the magnetic orientation and coercivity with some spacial resolution. A microscope will be used to make polar Kerr rotation measurements and obtain spatially-selective magnetic information. A unique capability for probing the electronic structure of our magnetic features at resonance: spin polarized inverse photoemission with both longitudinal and transverse spin polarization will also be used. Essential to this project is a new technique for fabricating micro-scale ferromagnetic features. Organometallic chemical vapor deposition techniques sufficient to deposit pure metal features with excellent spacial resolution have been developed at this laboratory. These techniques allow selective deposition of large uniform arrays of nickel, cobalt, cobalt-palladium alloys and cobalt-palladium heterostructures in features as small as 0.2 microns, and as thin as a few monolayers or as thick as 10 microns. Multilayers can be made by the successive deposition of different metals or alloys by the sequential photolysis of different organometallic source compounds. While unconventional in many respects, this program utilizes a technology that is compatible with the fabrication of metal features 100 angstroms across in one Scanning-Tunneling microscopy run. The approach is superior to techniques employing ion beams or conventional lithography and is inexpensive and compatible with the fabrication of the next generation of optical and magnetic recording media.

Keywords: Ferromagnetic Features, Micron-Scale Magnets, Organometallic CVD

236. **MICRO-HOLLOW CATHODE DISCHARGE ARRAYS: HIGH PRESSURE, NONTHERMAL PLASMA SOURCES**
$229,000
DOE Contact: Walter Polansky, (301) 903-5995
Old Dominion University Contact: Karl H. Schoenbach, (757) 683-4625

Hollow cathode discharges are known as nonthermal plasma sources: the electron energy distribution in the two stages of the discharge (Predischarge and main discharge) contains a large percentage of high energy (>10 eV) electrons. By reducing the size of the cathode holes from cm to ten's of μm we were able to extend their range of operation from subtorr range to almost atmospheric pressure. The presence of high-energy electrons and the measured characteristics of micro-hollow cathode discharges, such as: (1) positive current voltage characteristics, which allow the construction of discharge arrays without ballast, (2) stable operation for dc, ac, and pulsed voltages, (3) low applied voltage (several hundred volts), and (4) strong radiative emission in the UV, allow the utilization of micro-hollow cathode discharge arrays (MHCDAs) for flat panel displays, surface processing, gaseous emission treatment, and as broad area electron and ion sources. The MHCDAs consist either of sets of metal meshes, spaced a distance on the order of the hole diameter apart, or of metal-plated, perforated dielectric foils. The simplicity, low cost, and the low required voltage for hollow electrode arrays makes MHCDAs strong competitors to other electro-technologies which rely on nonthermal plasmas (such as barrier discharges, and pulsed corona discharges). This project will study the physics of micro-hollow cathode discharge operation in a positive differential conductivity mode. Particularly, the conditions for discharge array operation at atmospheric pressure will be explored, concentrating on the electron energy distribution and the spectral emission of micro-hollow cathode discharges. This project will focus on two applications: (1) UV light sources (excimer lamps) for food and water sterilization and for surface treatment; and (2) gas reactors for treatment of hazardous gases, such as perfluoro compounds, used in the semiconductor industry, and volatile organic compounds (VOC's).

Keywords: Plasma Sources, Hollow-Cathode Discharge

237. **RAPID MELT AND RESOLIDIFICATION OF SURFACE LAYERS USING INTENSE, PULSED ION BEAMS**
$300,000
DOE Contact: Walter Polansky, (301) 903-5995
Sandia National Laboratories Contact: Bob Turman, (505) 845-7119

In the past, the introduction of new material surface treatments like galvanizing, sputtering, and plasma spraying have enabled new products and opened new markets. The capability to rapidly melt and resolidify surface layers using intense, pulsed ion beams can enable another such advance. This project will develop a next generation surface processing technology based on new, repetitively pulsed ion bea Rapid solidification is known to greatly improve metal surface properties such as corrosion, wear, and fatigue resistance, but the lack of an economic and effective way to apply this technique to surfaces has prevented its use except in high value applications. Intense, pulsed, high energy ion beams treat surfaces based on surface melting followed by rapid thermal quenching by thermal diffusion into the underlying, untreated bulk material. This process produces non-equilibrium microstructures, nanocrystalline phases, and extended solid solutions leading to improved corrosion and friction properties of metals, as well as surface smoothing and defect healing, grain refinement, and modification of surface layer hardness. The low cost and in-depth deposition of high energy pulsed ion beams gives pulsed ion beam technology important advantages over laser treatment. The project will determine the capabilities and limitations of rapid melt and resolidification using pulsed ion beams. It will document the non-equilibrium micro-structures produced in treated layers and their effect on metal surface properties and will do the initial process development needed to show how this technique can be applied to commonly used metals. If successful, this will enable new ways to modify surfaces for enhanced properties and lifetimes with greatly improved energy efficiency and cost-effectiveness and will enable a significant reduction in the use of heavy metal and solvent-based surface treatment coating processes.

Keywords: Ion Beam Processing, Rapid Solidification, Surface Modification, Pulsed Ion Beams

238. **EXPERIMENTAL AND THEORETICAL INVESTIGATION OF DUAL-LASER ABLATION FOR STOICHIOMETRIC LARGE-AREA MULTICOMPONENT FILM GROWTH**
$147,000
DOE Contact: Walter Polansky, (301) 903-5995
University of South Florida Contact: Sarath Witanachchi, (813) 974-2789

We have recently discovered a novel dual-laser ablation process that dramatically alters the dynamics of the conventional single-laser ablation process. Initial experiments, using this process, allowed the production of high quality defect-free films of Y(2)O(3) that was not possible with single excimer laser ablation. This provides the motivation for our proposed research to investigate the physical mechanisms operative in this novel process. Two major problems associated with single laser ablation have hindered the development of this method as a manufacturing process. They are: (1) deposition of micron and submicron particulates; and (2) relatively narrow expansion profiles that limit the area of uniform film growth. Dual-laser ablation can potentially overcome both these major drawbacks while retaining the main advantages of the single laser ablation technique. We propose a systematic study to ascertain expansion characteristics of individual elements, with different volatility, in a multi-component material system, under the dual-laser ablation process that would determine the required conditions for large-area defect-free stoichiometric film growth. A species-sensitive hydrodynamic model is proposed. This will provide a clear understanding of the basic mechanisms operative in this process, and thus aid the process optimization for any material system. The dual-laser ablation system comprises a tandem combination of excimer and CO(2) laser pulses with an adjustable inter-pulse delay, that is spatially overlapped on the target. The primary objective of the research is to study experimentally the effect of the process parameters on the species velocity distribution and expansion profile for individual components, and to develop a species-sensitive theoretical model that is consistent with the experimental observations. The project will investigate a Cu target to establish the process characteristics for a single-element plume. It will also study the expansion characteristics of CuInSe(2) and Cu(In(1-x)Ga(x))Se(2) plumes to explore the behavior of individual elements in multi-component plumes. Investigation of spatial stoichiometric control of Ga in the Cu(In(1-x)Ga (x)) Se(2) will aid semiconductor doping studies. The new understanding of the dual-laser ablation process will facilitate the extension of this method to other material syste The method offers ease of control, simplicity and high-quality film growth, that could yield a method of choice for both epitaxial and highly oriented polycrystalline multi-component film growth.

Keywords: Laser Ablation, Stoichiometric Evaporation, Dual Laser Ablation

239. **'OFF-DIAGONAL' THERMOELECTRICITY FOR COOLING AND POWER GENERATION**
$166,000
DOE Contact: Walter Polansky, (301) 903-5995
TecOne Contact: Louis R. Testardi, (904) 562-9789

'Off-Diagonal' thermoelectricity, an uncommon effect which only occurs in low symmetry materials, allows unique and untried opportunities for thermal cooling, heat pumping and power generation. It utilizes the orthogonal coupling of heat and electric current flows in anisotropic media and opens new device as well as material development routes for the improvement of thermoelectric energy conversion. The advantages lie in a geometry naturally adapted to compact cooling, heat pumping and power generation with planar thermal boundaries, and also in electric impedances which allow a more compact, efficient and convenient device. The overall program goal is the development of a lightweight, flexible sheet material which will provide cooling, heat pumping and, with less application, power generation for objects or temperature baths of irregular geometry using 'off-diagonal' thermoelectricity. The principal materials thrust will be in conducting polymers because of their potential low cost and their ease of large scale processing to develop anisotropic properties. Applications include cooling of small volume consumer/industrial items, cooling and temperature control of the human body for medical treatment and comfort, and the utilization of waste heat from large area temperature baths.

Keywords: Off-Diagnonal Thermoelectricity, Thermal Cooling, Thermal Heating

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

240. EXPLOITATION OF ROOM TEMPERATURE MOLECULE/POLYMER MAGNETS FOR MAGNETIC AND ELECTROMAGNETIC INTERFERENCE SHIELDING AND ELECTROMAGNETIC INDUCTION APPLICATIONS

$322,000
DOE Contact: Walter Polansky, (301) 903-5995
Ohio State University Contact: Arthur J. Epstein, (614) 292-1133

There are increasing needs in today's society for lightweight, electromagnetic radiation shielding materials for operation at low frequencies (<Mhz range). This is partially driven by the growth of electric power distribution, telecommunications, and electromechanical power devices; concerns about electromagnetic interference; and an increasing need for lightweight inductive materials for efficient and portable motors and transformers. We reported the first polymer (tetracyanoethylene)-based magnet that remained strongly magnetic up to 350°K (170°F). We also demonstrated that more-than doubling of the room temperature magnetization can be achieved using a new route. Molecule/polymer-based magnetic materials are technologically attractive due to anticipated room temperature synthesis, processing, and device manufacture. Though these materials are relatively new, we already demonstrated that unoptimized versions of the materials shield magnetic fields independent of frequency between 10 and 10_4 Hz—a range difficult to shield using electrical conductors alone—with initial room-temperature real permeabilities, μ(i), of 13, which is close to iron. In late 1994, a preliminary report from a French group disclosed that a second class of molecule-based magnets (based on mixed-metal Prussian Blue type materials) has magnetic transitions near room temperature. The report suggests that additional molecule-based magnetic materials may be suitable for magnetic shielding. We have now synthesized similar (but not identical) Prussian Blue type materials with vanadium replacing iron. Our preliminary results on these modified Prussian Blue type materials revealed an even higher saturation magnetization, though a lower transition temperature than reported by the French group, indicating opportunity for chemical tuning of the magnetic properties including initial permeabilities and transition temperatures. This project involves an integrated synthesis/processing/characterization/modeling component to ascertain the feasibility of using molecule-based magnetic materials with emphasis on the study of the high Tc Prussian Blue-type magnetic materials from dc/low frequency to communications frequencies for shielding and induction applications. The objective of the project is to establish the ultimately achievable intrinsic real and imaginary magnetic permeabilities and corresponding electric permittivities and their control through synthesis and processing.

Keywords: Polymer Magnets, Molecule-Based Magnets, Electromagnetic Shielding

241. MOLECULAR SURFACE MODIFICATION AS A MEANS OF CORROSION CONTROL

$388,000
DOE Contact: Walter Polansky, (301) 903-5995
Princeton University Contact: Andrew B. Bocarsly, (609) 258-3888

Corrosion is a major materials problem in many industries. In the petrochemical industry which provides a major market for iron based materials, corrosion challenges exist from the production of hydrocarbons to their refining and conversion to chemical products. Corrosion of concern to the petrochemical industry occurs in a variety of environments ranging from highly acidic to alkaline, and temperatures ranging from room temperature up to ~1100°C. The goal of this research is to investigate the chemistry of novel organic films (corrosion inhibitors) of 5 Å to 20 Å dimension that may provide a corrosion resistant barrier on the surface of metallic materials. Joint studies at Princeton University and Exxon Research and Engineering Company suggest that developments in the fields of surface science and materials chemistry are now at a point where an utilitarian molecular view of corrosion processes is possible. This capability is expected to allow for the "molecular design" of next generation inhibitors having the requisite properties to provide for corrosion protection under extreme chemical and thermal conditions. In the proposed research, which is a collaborative effort involving members of the Princeton Materials Institute and scientists from Exxon's Research and Engineering Laboratory, state-of-the-art surface characterization tools will be brought together to generate a molecular level understanding of model organic films appropriate for corrosion control. The mechanisms of film protection and film breakdown will be investigated thoroughly. The order and packing density of the films will be studied as a function of temperature, using Grazing Incidence X-ray Diffraction involving synchrotron X-radiation as a main characterization tool. The interface stability of the molecule, its bonding mechanism and dissociation pathways will be studied by using a combination of spectroscopies such as Temperature Programmed Desorption, High Resolution Electron Energy Loss Spectroscopy and Auger Electron Spectroscopy on model substrate surfaces. Additionally, low energy electron diffraction will be used to characterize the material surface after molecular debonding. The mechanistic understanding derived from these different techniques will be used to construct molecular frameworks that may provide corrosion resistance. The performance of these molecular architectures in real environments will be investigated using electrochemical reactors available at Exxon's Corporate Research Laboratories.

Keywords: Surface Modification, Corrosion Control, Corrosion Inhibitors

SMALL BUSINESS INNOVATION RESEARCH PROGRAM

The Small Business Innovation Research (SBIR) program is mandated by the Small Business Innovation Development Act of 1982 and the Small Business Research and Development Enhancement Act of 1992. The program is designed for implementation in a three-phase process, with Phase I determining, insofar as possible, the scientific or technical merit and feasibility of ideas proposed for investigation. The period of performance in this initial phase is about six months with awards up to $75,000. Phase II is the principal research or research and development effort and is performed in a period of up to two years with awards up to $750,000. Under Phase III, commercial applications of the research or research and development are to be pursued by small businesses with non-Federal capital or, alternatively, Phase III may involve follow-on non-SBIR Federal contracts for products or processes desired by the Government.

The materials-related projects, like all other projects in the DOE SBIR program, were selected using the specific evaluation criteria listed in the program solicitation. Award selection was based on detailed reports returned by reviewers drawn from DOE laboratories, universities, private industry, and government. In the Phase II technical evaluation process, an additional evaluation criterion addresses the commercial potential of the proposed scientific/technical work.

The work supported in this program represents high-risk research, but the potential benefits are also high if the objectives are met. Brief descriptions of all DOE SBIR projects (not just those of interest in materials research) are given in the following publications: Abstracts of Phase I Awards, 1996 (DOE/ER-0686), Abstracts of Phase II Awards, 1996 (DOE/ER-0688), and Abstracts of Phase II Awards, 1995 (DOE/ER-0655). Copies of these publications may be obtained by calling (301) 903-1414.

MATERIALS, PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

PHASE I PROJECTS

Control of Glycol Dehydrator Benzene, Toluene, Ethylbenzene, and Xylene Emissions - DOE Contact Harold Shoemaker, (304) 285-4715; Membrane Technology And Research, Inc. Contact E. G. Weiss, (415) 328-2228

Composite Ceria Eletrolytes for Solid Oxide Fuel Cells - DOE Contact William Cary Smith, (304) 285-4260; Nextech Materials, Ltd. Contact William J. Dawson, (614) 766-4895

Nitrogen Selective Adsorption for Natural Gas Upgrading - DOE Contact Harold Shoemaker, (304) 285-4715; Northwest Fuel Development, Inc. Contact Dr. Peet M. Soot, (503) 699-9836

Gas-Solid Reaction and Separation Process for Simultaneous Removal of Toxic Metals and Particulates in Coal-Based Power Systems - DOE Contact Otis Mills, (412) 892-5890; Ceramem Corporation Contact Dr. Robert L. Goldsmith, (617) 899-0467

An Attrition-Resistant Zinc Titante Sorbent for a Transport Reactor - DOE Contact Daniel C. Cicero, (304) 285-4826; Intercat Development, Inc. Contact Wendy L. Hansen, (908) 223-4644

Noncontact Viscosity Measurement of Molten Glass Using Laser-Generated Ultrasound for Process Control During Melting and Forming Operations - DOE Contact Rolf Butters, (202) 586-0984; Karta Technology, Inc. Contact Dr. Satish Nair, (210) 681-9102

A Light Scattering Based Sensor for On-Line Monitoring of Fiber Diameter Distribution During Fiberglass Manufacturing - DOE Contact Rolf Butters, (202) 586-0984; Mission Research Corporation Contact Scot R. Fries, (805) 963-8761

Advanced Materials for Higher Temperature Glass Forming - DOE Contact Rolf Butters, (202) 586-0984; Ultramet Contact Craig N. Ward, (818) 899-0236

Novel Use of Gas Jet Plasma to Prepare Amorphous Silicon Alloy - DOE Contact Alec Bulawka, (202) 586-5633; Energy Conversion Devices, Inc. Contact Ms. Nancy M. Bacon, (810) 280-1900

High Rate Deposition of Transparent Conducting Zinc Oxide Using Activated Oxygen for Photo-voltaic Manufacturing Cost Reduction - DOE Contact Alec Bulawka, (202) 586-5633; Energy Photovoltaics, Inc. Contact David A. Jackson, (609) 587-3000

Innovative Bonding and Spray-Forming Techniques for Cost-Effectively Producing High Performance Induction Motors - DOE Contact Jim Merritt, (202) 586-0903; Satcon Technology Corporation Contact Steven St. Germain, (617) 349-0914

Tungsten Trioxide Films for Detection of Nitrogen Oxide in Automotive Exhaust Streams - DOE Contact Jim Merritt, (202) 586-0903; Sensor Research And Development Corporation Contact Carl J. Freeman, (207) 581-2265

Development and Testing of Environmentally-Safe Extractive Scintillator Solutions for Alpha Spectrometry - DOE Contact Wanda Ferrell, (301) 903-0043; Ordela, Inc. Contact Manfred K. Kopp, (423) 483-8675

Binary-Chalcogenides as Evaporation Source Material For Cu(In, Ga) $(Se,S)_2$ Thin-Film Deposition - DOE Contact Yok Chen, (301) 903-3428; Energy Photovoltaics, Inc. Contact David A. Jackson, (609) 587-3000

Development of Optimal SnO_2 Contacts for CdTe Photovoltaic Applications - DOE Contact Yok Chen, (301) 903-3428; Green Development, LLC Contact Dr. Jianping Xi, (303) 278-4571

Large Area, Low Cost Processing for CIS Photovoltaics - DOE Contact Yok Chen, (301) 903-3428; International Solar Electric Technology, Inc. Contact Dr. Bulent Basol, (310) 216-4427

Improved Processes for Forming CIS Films - DOE Contact Yok Chen, (301) 903-3428; Unisun Contact Dr. Chris Eberspacher, (805) 499-7840

Ultrafast Polysilylene Scintillators - DOE Contact Tim Fitzsimmons, (301) 903-9830; Adherent Technologies, Inc. Contact Susan K. Switzer, (505) 822-9186

Highly Branched, Lightly Crosslinked, Solid Polymer Electrolytes - DOE Contact Al Landgrebe, (202) 586-1483; Tpl, Inc. Contact H. M. Stoller, (505) 344-6744

An Innovative Approach to Synthesis of Porous Intermetallic Matrix Composites for Regenerative Cooling Below 20K - DOE Contact Jerry Peters, (301) 903-5228; Materials And Electrochemical Research (mer) Contact Dr. J. C. Withers, (520) 574-1980

Development of Artificial Pinning Center NbTiTa Conductor for High Field Applications - DOE Contact Jerry Peters, (301) 903-5228; Supercon, Inc. Contact Elaine Drew, (508) 842-0174

NbTi Ternary and Quarternary Alloys for High Field (>8T) Applications - DOE Contact Jerry Peters, (301) 903-5228; Supercon, Inc. Contact Elaine Drew, (508) 842-0174

Development of a New High-Field NbTi Superconductor with Mechanically Introduced Ta Inclusions - DOE Contact Jerry Peters, (301) 903-5228; Supercon, Inc. Contact Ms. Elaine Drew, (508) 842-0174

Improved Ultrafast Scintillators for Nuclear Physics - DOE Contact Richard Rinkenberger, (301) 903-3613; Alem Associates Contact Dr. Alexander Lempicki, (617) 353-9581

MATERIALS, PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

PHASE II PROJECTS (FIRST YEAR)

Low Cost, Contamination-Tolerant Electrocatalysts for Low-Temperature Fuel Cells - DOE Contact David Koegel, (301) 903-5997; Aspen Systems, Inc. Contact Dr. Kang P. Lee, (508) 481-5058

A Low Cost, High Temperature Superconductor Wire Manufacturing Technology - DOE Contact James Daley, (202) 586-1165; American Superconductor Corporation Contact Ramesh Ratan, (508) 836-4200

A Low Cost Receiver Plate Manfacturing Process for High Concentration Photovoltaic Systems - DOE Contact Alec Bulawka, (202) 586-5633; Amonix, Inc. Contact Mr. Vahan Garboushian, (310) 325-8091

An Intumescent Mat Material for Joining of Ceramics to Metals at High Temperatures - DOE Contact William J. Gwilliam, (304) 285-4401; CeraMem Corporation Contact Dr. Robert L. Goldsmith, (617) 899-0467

Development of Modulator Quality Rubidium Titanyl Arsenate Crystals for Remote Sensing Laser Systems - DOE Contact Michael O'Connell, (202) 586-9311; Crystal Associates, Inc. Contact G. M. Loiacono, (201) 612-0060

A Novel Method to Recycle Thin Film Semiconductor Materials - DOE Contact Alec Bulawka, (202) 586-5633; Drinkard Metalox, Inc. Contact Fred Gallagher, (704) 332-8173

An Improved Material and Low-Cost Fabrication Options for Candle Filters - DOE Contact William J. Gwilliam, (304) 285-4401; FluiDyne Engineering Corporation Contact Dr. Gary J. Hanus, (612) 544-2721

An Integrated Catalyst/Collector Structure for Regenerative Proton-Exchange Membrane Fuel Cells - DOE Contact David Koegel, (301) 903-5997; Giner, Inc. Contact Dr. Anthony B. LaConti, (617) 899-7270

Nanostructured Insterstitial Alloys as Catalysts for Direct Energy Applications - DOE Contact David Koegel, (301) 903-5997; Nanomaterials Research Corporation Contact Dr. Angelo Yializis, (602) 575-1354

Environmentally Responsible Recycling of Thin-Film Cadmium Telluride Modules - DOE Contact Alec Bulawka, (202) 586-5633; Solar Cells, Inc. Contact Frederick L. Yocum, (419) 534-3377

Low-Cost, Large-Area, High-Resistivity Substrates for Gas Microstrip Detectors - DOE Contact Richard Rinkenberger, (301) 903-3613; Spire Corporation Contact Richard S. Gregorio, (617) 275-6000

An Economic Sorbent for the Removal of Mercury, Chlorine, and Hydrogen Chloride from Coal Combustion Flue Gases - DOE Contact Sean Plasynski, (412) 892-4867; TDA Research, Inc. Contact Michael E. Karpuk, (303) 940-2301

PHASE II PROJECTS (SECOND YEAR)

A Ceramic Material and Process for Use in Monolithic Ceramic Cross-Flow Filters - DOE Contact Theodore McMahon, (304) 291-4865; Blasch Precision Ceramics, Inc. Contact David W. Bobrek, (518) 372-9416

Jet Vapor Deposition of Multilayer and Nanocluster Thick Film Targets for Radioactive Nuclear Beams and Medical Applications - DOE Contact Richard Rinkenberger, (301) 903-3613; Jet Process Corporation Contact Jerome J. Schmitt, (203) 786-5130

Design and Applications of Close-Spaced Thermionic Converters with Novel Isothermal Electrodes - DOE Contact David Koegel, (301) 903-5995; Space Power, Inc. Contact Joseph A. Dodson, (408) 434-9500

A Multilayer Silicon Carbide Fiber Coating for Toughened, Neutron Radiation-Resistant Silicon Carbide/Silicon Carbide Composites - DOE Contact F. W. Wiffen, (301) 903-4963; Hyper-Therm, Inc. Contact Wayne S. Steffier, (714) 375-4085

Economical and Reliable Niobium-Tin Conductors via Innovations in Stabilizers - DOE Contact T.V. George, (301) 903-4957; IGC Advanced Superconductors, Inc. Contact B. A. Zeitlin, (203) 753-5215

Carbon-Carbon to Copper Joining for Fusion Reactor Applications - DOE Contact T.V. George, (301) 903-4957; Surmet Corporation Contact Dr. Suri A. Sastri, (617) 272-3250

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

PHASE I PROJECTS

Thermally Stable Nitrogen-Absorbents - DOE Contact Harold Shoemaker, (304) 285-4715; Bend Research, Inc. Contact Dr. Walter C. Babcock, (541) 382-4100

Improved Sealing Molten Carbonate Fuel Cell Electrolyte Matrix - DOE Contact Diane Hooie, (304) 285-4524; M-C Power Corporation Contact Patrick R. McSweeney, (708) 986-8040

Intermediate Temperature (~650 Degrees Celsius), High Power Density Solid Oxide - DOE Contact Richard A. Johnson, (304) 285-4564; Materials and Systems Research, Inc. Contact Dr. Dinesh K. Shetty, (801) 466-1262

Carbon Monoxide Tolerant Anodes for Proton Exchange Membrane (PEM) Fuel Cells - DOE Contact Ronald J. Fiskum, (202) 586-9154; EIC Laboratories, Inc. Contact Dr. A. C. Makrides, (617) 769-9450

Novel Proton Exchange Membrane (PEM) for Fuel Cell Application - DOE Contact Ronald J. Fiskum, (202) 586-9154; Lynntech, Inc. Contact Dr. Oliver J. Murphy, (409) 693-0017

Low Cost Advanced Bipolar Plates for Proton Exchange Membrane Fuel Cells - DOE Contact Ronald J. Fiskum, (202) 586-9154; Materials and Electrochemical Research (mer) Contact Dr. J. C. Withers, (520) 574-1980

Natural Gas Reformer Cleanup System for Proton Exchange Membrane Fuel Cells - DOE Contact Ronald J. Fiskum, (202) 586-9154; Mechanical Technology, Inc. Contact Douglas McCauley, (518) 785-2424

Improved Bi-2223 Flux Pinning Through Chemical Doping - DOE Contact James Daley, (202) 586-1165; American Superconductor Corporation Contact Ramesh Ratan, (508) 836-4200

Low Cost Multifilament Composite Process - DOE Contact James Daley, (202) 586-1165; American Superconductor Corporation Contact Ramesh Ratan, (508) 836-4200

High Temperature Superconducting Composites With Low Alternating Current Loss - DOE Contact James Daley, (202) 586-1165; American Superconductor Corporation Contact Ramesh Ratan, (508) 836-4200

Template-Mediated Synthesis of Periodic Membranes for Improved Liquid-Phase Separations - DOE Contact Kristine Bilenki, (301) 903-1687; American Research Corporation Of Virginia Contact Anne Churchill, (540) 731-0655

Novel Fiber-Based Adsorbent Technology - DOE Contact Kristine Bilenki, (301) 903-1687; Chemica Technologies, Inc. Contact Daniel J. Brose, (541) 385-0355

Recyclable Bio-Reagent for Rapid and Selective Extraction of Contaminants from Soil - DOE Contact Kristine Bilenki, (301) 903-1687; Isotron Corporation Contact Henry L. Lomasney, (504) 254-4624

Innovative Method to Stabilize Liquid Membranes for Removal of Radionuclides from Groundwater - DOE Contact Kristine Bilenki, (301) 903-1687; Membrane Technology And Research, Inc. Contact E. G. Weiss, (415) 328-2228

Metal-Binding Silica Materials for Wastewater Cleanup - DOE Contact Kristine Bilenki, (301) 903-1687; Tpl, Inc. Contact Jacqueline Taylor, (505) 343-8890

A Low Cost Process for the Concentration and Stabilization of Mixed Low Level Waste - DOE Contact Michael Torbert, (301) 903-7109; TDA Research, Inc. Contact Michael Karpuk, (303) 940-2301

A Reusable, Non-Toxic, Non-Lethal Activated Barrier to Delay Unauthorized Intruders by Vision Obscuration - DOE Contact Michael O'Connell, (202) 586-9311; Advanced Safeguards, Inc. Contact Anthony D. Valente, (708) 833-1211

Coating Capillary Optics to Improve X-ray and Neutron Transmission - DOE Contact Tim Fitzsimmons, (301) 903-9830; X-ray Optical Systems, Inc. Contact David M. Gibson, (518) 442-2661

Monolithic Polycapillary Optic for Bending and Microfocusing Neutron Beams - DOE Contact Tim Fitzsimmons, (301) 903-9830; X-ray Optical Systems, Inc. Contact David M. Gibson, (518) 442-5250

Superhard Nanophase Cutter Materials for Rock Drilling Applications - DOE Contact Paul Grabowski, (202) 586-0478; Diamond Materials, Inc. Contact Dr. Bernard H. Kear, (908) 445-2245

Evaluation and Constitutive Modeling of Unidirectional SiC/SiC Composites with Engineered SiC Fiber Coatings Subjected to Neutron Irradiation - DOE Contact F. W. Wiffen, (301) 903-4963; Hyper-therm High-temperature Composites, Inc. Contact Wayne S. Steffier, (714) 375-4085

Innovative Fabrication of SiC/SiC Composites with High Through-the-Thickness Thermal Conductivity - DOE Contact F. W. Wiffen, (301) 903-4963; Materials And Electrochemical Research (MER) Contact Dr. R. O. Loutfy, (520) 574-1980

High Numerical Aperture Scintillating Fibers - DOE Contact Robert Woods, (301) 903-3367; Biogeneral, Inc. Contact Andrea Gray, (619) 453-4451

Low Loss Silicon Nitride Technology for High Power Rf Transmission Windows - DOE Contact Richard Rinkenberger, (301) 903-3613; Composite Technology Development, Inc. Contact Dr. Naseem A. Munshi, (303) 447-2226

PHASE II PROJECTS (FIRST YEAR)

Rotating, In-Plane Magnetization and Magneto-Optic Imaging of Cracks under Coatings on Ferromagnetic Metals - DOE Contact Dennis Harrison, (301) 903-2884; Physical Research, Inc. Contact Dr. William C. L. Shih, (310) 378-0056

Development of Laser Materials and Rugged Coatings as Components for Tunable Ultraviolet Laser Systems - DOE Contact Michael O'Connell, (202) 586-9311; Lightning Optical Corporation Contact Wayne Ignatuk, (813) 0938-0092

Application of Raman Spectroscopy to Identification and Sorting of Post-Consumer Plastics for Recycling - DOE Contact Simon Friedrich, (202) 586-6759; National Recovery Technologies, Inc. Contact Dr. Charles E. Roos, (615) 734-6400

A Sensor for Automated Plastics Sorting - DOE Contact Simon Friedrich, (202) 586-6759; Radiation Monitoring Devices, Inc. Contact Dr. Gerald Entine, (617) 926-1167

PHASE II PROJECTS (SECOND YEAR)

An Apparatus for Structural Analysis of High Temperature Materials Using Synchrotron Radiation - DOE Contact Manfred Leiser, (301) 903-3426; Containerless Research, Inc. Contact Dr. Paul C. Nordine, (708) 467-2678

A Novel High Strength Ceria-Zirconia Toughened Alumina Ceramic with Superior High Temperature Corrosion and Erosion Resistance - DOE Contact David Koegel, (301) 903-5995; Selee Corporation Contact Kenneth R. Butcher, (704) 697-2411

Improvement in the Characteristics of Ternary Niobium Titanium Tantalum Alloys - DOE Contact Jerry Peters, (301) 903-5228; IGC Advanced Superconductors, Inc. Contact B. A. Zeitlin, (203) 753-5215

X-Ray Absorption Spectroscopy for Trace Analysis of Chemical Phase and Composition - DOE Contact Manfred Leiser, (301) 903-3426; Advanced Fuel Research, Inc. Contact Dr. David G. Hamblen, (203) 528-9806

High Temperature Thermally Stable Multi-Layer Quantum Well Films - DOE Contact Bill Barnett, (301) 903-3097; Hi-Z Technology, Inc. Contact Norbert B. Elsner, (619) 535-9343

A Long Life Zinc Oxide-Titanium Oxide Sorbent - DOE Contact Ronald Staubly, (304) 291-4991; TDA Research, Inc. Contact Michael E. Karpuk, (303) 940-2301

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

PHASE I PROJECTS

Catalytic Membrane for High Temperature Hydrogen Separations - DOE Contact Otis Mills, (412) 892-5890; Ceramem Corporation Contact Dr. Robert L. Goldsmith, (617) 899-0467

Low Cost, Environmental Friendly Carbonate Fuel Cell Matrix Fabrication - DOE Contact Tom J. George, (304) 291-4825; Energy Research Corporation Contact Dr. Bernard S. Baker, (203) 825-6001

High Speed Manufacturing for Molten Carbonate Fuel Cell Components - DOE Contact Diane Hooie, (304) 285-4524; M-C Power Corporation Contact Patrick F. McSweeney, (708) 986-8040

High Performance Membranes for Removal of Carbon Dioxide from Natural Gas - DOE Contact Harold Shoemaker, (304) 285-4715; Membrane Technology And Research, Inc. Contact E. G. Weiss, (415) 328-2228

Advanced Coal Based Power System Components Using Reaction Bonded Silicon Carbide - DOE Contact Otis Mills, (412) 892-5890; Busek Company, Inc. Contact J. Budny, (508) 655-5565

A Real Time Hydrocarbon Emissions Sensor for Hybrid Electric Vehicles - DOE Contact Jim Merritt, (202) 586-0903; Southwest Sciences, Inc. Contact Dr. Alan C. Stanton, (505) 984-1322

A Sensor for In-Situ Detection, Identification, and Quantification of TCE for Cone Penetrometers - DOE Contact Eric Lightner, (904) 644-5517; Detection Limit, Inc. Contact Eugene L. Watson, (307) 742-0555

Cone Pentrometer Deployable Solid Phase Optical Chemical Sensor for Subsurface Detection of Halohydrocarbons - DOE Contact Eric Lightner, (904) 644-5517; Physical Optics Corporation Contact Patty Shaw, (310) 320-3088

Real Time Monitor for the Laser-Based Coatings Removal System - DOE Contact Eric Lightner, (904) 644-5517; Physical Sciences, Inc. Contact George E. Caledonia, (508) 689-0003

A New Separation and Treatment Method for Soil and Groundwater Restoration - DOE Contact Kristine Bilenki, (301) 903-1687; Lynntech, Inc. Contact Dr. Olive J. Murphy, (409) 693-0017

Continuous Analyzer for Monitoring Hydrogen Chloride and Chlorine During Site Cleanup Activity - DOE Contact Michael Torbert, (301) 903-7109; Ada Technologies, Inc. Contact Dr. Judith Armstrong, (303) 792-5615

A Practical Laser Induced Breakdown Spectrometer for Real Time On-Line Monitoring of Aqueous Process Streams - DOE Contact Michael Torbert, (301) 903-7109; J. and D. Scientific, Inc. Contact Dr. Larry D. McCormick, (352) 336-2599

A Low Level Tritium Monitor Based on a Multi-Phase Scintillator Material - DOE Contact Michael O'Connell, (202) 586-9311; Aerodyne Research, Inc. Contact Dr. Charles E. Kolb, (508) 663-9500

A Miniaturized Flow-Injection System for Unattended Monitoring of Uranium by Electrochemical Detection - DOE Contact Michael O'Connell, (202) 586-9311; Eltron Research, Inc. Contact Eileen E. Sammells, (303) 440-8008

Long-Life Electrical Neutron Generator - DOE Contact Michael O'Connell, (202) 586-9311; First Point Scientific, Inc. Contact Dr. John R. Bayless, (818) 707-1131

Tracktag-A GPS/RFID Tag for Location and Status Monitoring - DOE Contact Michael O'Connell, (202) 586-9311; Navsys Corporation Contact Steven G. Miller, (719) 481-4877

Development of an RF Tagging Method for Use in Monitoring International Nonproliferation Treaty Compliance - DOE Contact Michael O'Connell, (202) 586-9311; Randtec, Inc. Contact Donald K. Salmon, (703) 352-0833

A Compact Neutron Generator - DOE Contact Michael O'Connell, (202) 586-9311; Science Research Laboratory, Inc. Contact Dr. Jonah Jacob, (617) 547-1122

Intelligent Sensing and Control System for Ethylene Production Using Laser Ultrasonic Coke Detention - DOE Contact Ted Vojnovich, (301) 903-7484; Harvest Energy Technology, Inc. Contact Dr. David Warren, (818) 767-3157

Thin-Film, Micron-Scale Transformers - DOE Contact David Koegel, (301) 903-3159; Integrated Microtransducer Electronics Corporation Contact Dr. Richard Spitzer, (510) 841-3585

Passive Electronic Components from Nanostructured Materials - DOE Contact David Koegel, (301) 903-3159; Nanomaterials Research Corporation Contact Thomas Venable, (520) 294-7115

A Novel On-Line Ammonia Sensor for Energy Conversion Applications - DOE Contact Wanda Ferrell, (301) 903-0043; Giner, Inc. Contact Dr. Anthony B. LaConti, (617) 899-7270

A Multicore Optical Fiber Sensor for Mass Transport and Particulates - DOE Contact Wanda Ferrell, (301) 903-0043; Owen Research, Inc. Contact Brian L. Sperry, (303) 427-1312

Infrared Hollow Waveguide Organic Solvent Analyzer - DOE Contact Wanda Ferrell, (301) 903-0043; Polestar Technologies, Inc. Contact Karen K. Carpenter, (617) 449-2284

Stratospheric Water Vapor Microsensor - DOE Contact Wanda Ferrell, (301) 903-0043; Deacon Research Contact Dr. Olive Lee, (415) 493-6100

A Simple, Inexpensive Approach to Real-Time Calibration of Radiometric Instrumentation - DOE Contact Wanda Ferrell, (301) 903-0043; Ion Optics, Inc. Contact Dr. Edward A. Johnson, (617) 275-4004

High Altitude Water Vapor Concentration Measurement Using Diode Laser Interferometry - DOE Contact Wanda Ferrell, (301) 903-0043; Optra, Inc. Contact James R. Engel, (508) 887-6600

Miniature Spectrometer Based on a Novel Optical Filter with Spectral Selectivity Distributed Along the Aperture - DOE Contact Wanda Ferrell, (301) 903-0043; Physical Optics Corporation Contact Patty Shaw, (310) 320-3088

A High Resolution Bug Eye Orientation Sensor Based on Fuzzy Optical Metrology - DOE Contact Wanda Ferrell, (301) 903-0043; Physical Optics Corporation Contact Patty Shaw, (310) 320-3088

Compact, Airborne Laser Multigas Sensor - DOE Contact Wanda Ferrell, (301) 903-0043; Physical Sciences, Inc. Contact George E. Caledonia, (508) 689-0003

Microwave Radiometer for Passively and Remotely Measuring Atmospheric Water Vapor - DOE Contact Wanda Ferrell, (301) 903-0043; Radiometrics Corporation Contact Dr. Randolph Ware, (303) 497-8005

Advanced Water Sensor for Unmanned Aerial Vehicles - DOE Contact Wanda Ferrell, (301) 903-0043; Southwest Sciences, Inc. Contact Dr. Alan C. Stanton, (505) 984-1322

High-Gain Monocapillary Optics - DOE Contact Tim Fitzsimmons, (301) 903-9830; Aracor Contact Ed LeBaker, (408) 733-7780

High Performance X-Ray and Neutron Micro-focusing Optics - DOE Contact Tim Fitzsimmons, (301) 903-9830; Hirsch Scientific Contact Mr. Gregory Hirsch, (415) 359-3920

Thermally Stable Polycrystalline Diamond Cutters for Hard Rock Drilling - DOE Contact Paul Grabowski, (202) 586-0478; Novatek Contact David R. Hall, (801) 374-6000

Very Low Friction Small Radius Domed Cutters for Percussion Drill Bits - DOE Contact Paul Grabowski, (202) 586-0478; Novatek Contact David R. Hall, (801) 374-6000

Development and Testing of a Jet Assisted Polycrystalline Diamond Drilling Bit - DOE Contact Paul Grabowski, (202) 586-0478; Novatek Contact David R. Hall, (801) 374-6000

Advanced Low-Stress Bonding of Thermally Stable Polycrystalline Diamond Cutters to Tungsten Carbide Substrates - DOE Contact Paul Grabowski, (202) 586-0478; Science Research Laboratory, Inc. Contact Dr. Jonah Jacob, (617) 547-1122

Nanocrystalline Superhard, Ductile Ceramic Coatings for Roller Cone Bit Bearings - DOE Contact Paul Grabowski, (202) 586-0478; Spire Corporation Contact Richard S. Gregorio, (617) 275-6000

Solid-State Ultracapacitors for Electric Vehicles and Consumer Electronics - DOE Contact Al Landgrebe, (202) 586-1483; Cape Cod Research, Inc. Contact Katherine D. Finnegan, (508) 540-4400

A Four Volt per Cell Ultracapacitor with High Energy Density- DOE Contact Al Landgrebe, (202) 586-1483; Covalent Associates, Inc. Contact Dr. Margaret E. Langmuir, (617) 938-1140

A High Power Battery Based on Insertion Electrodes - DOE Contact Al Landgrebe, (202) 586-1483; EIC Laboratories, Inc. Contact Dr. A. C. Makrides, (617) 769-9450

A High Power Bipolar Ni-MH Battery for a Hybrid Vehicle - DOE Contact JoAnn Milliken, (202) 586-2480; Electro Energy, Inc. Contact Martin Klein, (203) 797-2699

Synergetic Ultracapacitor - DOE Contact Al Landgrebe, (202) 586-1483; Federal Fabrics-fibers Contact Bracha Horovitz, (508) 470-1859

High Surface Area Non-Oxide Ceramic Electrodes for Ultracapacitors - DOE Contact Al Landgrebe, (202) 586-1483; T/J Technologies, Inc. Contact Leslie Alexander, (313) 213-1637

Novel Ultracapacitor Electrodes for High Power Applications - DOE Contact Al Landgrebe, (202) 586-1483; Technical Research Associates Contact Charles D. Baker, (801) 485-4994

Wrappable Inorganic Electrical Insulators for Superconducting Magnets - DOE Contact T. V. George, (301) 903-4957; Composite Technology Development, Inc. Contact Dr. Naseem A. Munshi, (303) 447-2226

Novel Composite Insulators for Radio-Frequency Antenna Limiters - DOE Contact T. V. George, (301) 903-4957; Composite Technology Development, Inc. Contact Dr. Naseem A. Munshi, (303) 447-2226

Pulsed Induction Joining of Sapphire to Metal for Gyrotron Windows - DOE Contact T. V. George, (301) 903-4957; FM Technologies, Inc. Contact Dr. Frederick M. Mako, (703) 425-5111

Joining of Tungsten Armor Using Functional Gradients - DOE Contact T. V. George, (301) 903-4957; Plasma Processes, Inc. Contact Cheri McKechnie, (205) 851-7653

A Cost-Effective Technical Approach to Fabricating High Jc Bronze-Route $(Nb,Ti)_3Sn$ Superconducting Wire for Fusion Applications - DOE Contact T. V. George, (301) 903-4957; Supercon, Inc. Contact Elaine Drew, (508) 842-0174

Fabrication of a Copper-Backed Beryllium PFC Armor with a Built-In Diffusion Barrier Structure - DOE Contact T. V. George, (301) 903-4957; Surmet Corporation Contact Dr. Suri A. Sastri, (617) 272-3250

Development and Evaluation of Mineral Insulated Diagnostic Probes Subjected to High Dose Neutron Irradiation - DOE Contact F. W. Wiffen, (301) 903-4963; Delta M Corporation Contact A. D. White, (423) 483-1569

Silicon Detectors with 40Å Entrance Window for Low Energy Ions and Neutral Particles - DOE Contact Charles Finfgeld, (301) 903-3423; International Radiation Detectors Contact Dr. Raj Korde, (310) 534-3661

Carbon Thermostructure for Silicon-Based Particle Detectors - DOE Contact Richard Plano, (301) 903-4801; Energy Science Laboratories, Inc. Contact Dr. Timothy R. Knowles, (619) 552-2034

Light Amplifier - DOE Contact Richard Plano, (301) 903-4801; Nanosystems Inc. Contact Robert W. Boerstler, (203) 881-2827

High Performance Optical Detectors for Calorimetry - DOE Contact Robert Woods, (301) 903-3367; Radiation Monitoring Devices, Inc. Contact Dr. Gerald Entine, (617) 926-1167

Design, Development, and Fabrication of Hybrid High Temperature Superconducting Current Leads - DOE Contact Jerry Peters, (301) 903-5228; American Magnetics, Inc. Contact Roger M. Efferson, (423) 482-1056

Design of Novel Induction Accelerator Gaps - DOE Contact Jerry Peters, (301) 903-5228; Fusion and Accelerator Research Contact Dr Jin-Soo Kim, (619) 455-6607

A LaF_3:Nd + Photosensitive Wire Chamber for Gamma-Ray Imaging - DOE Contact Richard Rinkenberger, (301) 903-3613; Applied Physics Technologies Contact Dr. Argyrios Doumas, (516) 444-8802

Large Area Pixelated and Tiled X-Ray and Gamma - Ray Detector - DOE Contact Richard Rinkenberger, (301) 903-3613; Innova Laboratories, Inc. Contact Dr. George W. Webb, (619) 452-8760

Improved Cost and Radiation Hardness for Silicon Detectors - DOE Contact Richard Rinkenberger, (301) 903-3613; Intraspec, Inc. Contact John Walter, (423) 483-1859

Coplanar CdZnTe p-i-n, Gamma-Ray Detectors for Nuclear Spectroscopy - DOE Contact Richard Rinkenberger, (301) 903-3613; Spire Corporation Contact Richard S. Gregorio, (617) 275-6000

Large Room Temperature $Cd_{1-x}Zn_xTe$ Detectors - DOE Contact Richard Rinkenberger, (301) 903-3613; W. Peter Trower, Inc. Contact Dr. W. Peter Trower, (540) 953-2249

High Power Target Design for a Next Generation Radioactive Beam ISOL-Type Facility - DOE Contact Richard Rinkenberger, (301) 903-3613; Amparo Corporation Contact Dr. James J. Walker, (505) 982-6742

In-Situ Nondestructive Measurements of Key Mechanical Properties of Reactor Pressure Vessels Using Innovative SSM Technology - DOE Contact John Warren, (301) 903-6491; Advanced Technology Corporation Contact Fahmy M. Haggag, (423) 483-5756

Oxidation Induction Time Technology for Electric Cable Condition Monitoring and Life-Assessment - DOE Contact Duli Agarwal, (301) 903-3919; Pacific-sierra Research Corporation Contact Norman L. Duncan, (703) 516-6372

PHASE II PROJECTS (FIRST YEAR)

Advanced High Power Silicon Carbide Internally Cooled X-Ray - DOE Contact Bill Oosterhuis, (301) 903-3426; SSG, Inc. Contact Dexter Wang, (617) 890-0204.

Chemical Microsensor Arrays as Integrated Chip Compatible Devices for Chemical Weapons Nonproliferation Inspection- DOE Contact Robert Marianelli, (301) 903-5808; Microsensor Systems, Inc. Contact Dr. Hank Wohltjen, (502) 745-0099

A High Resolution Multi-hit Time to Digital Converter Integrated Circuit - DOE Contact Robert Woods, (301) 903-3367; Lecroy Corporation Contact Joseph Migliozzi, (914) 578-6006

A Helium-Cooled Faraday Shield Using Porous Metal Cooling - DOE Contact T. V. George, (301) 903-4957; Thermacore, Inc. Contact Donald M. Ernst, (717) 569-6551

Low Cost Fabrication of Large Silicon Carbide/Silicon Carbide Composite Structures - DOE Contact F. W. Wiffen, (301) 903-4963; Lanxide Corporation Contact Dr. Christopher Kennedy, (302) 456-6320

Bandgap-Engineered Thermophotovoltaic Devices for High Efficiency Radioisotope Power - DOE Contact Bill Barnett, (301) 903-3097; Edtek, Inc. Contact W. E. Horne, (206) 395-8084

Rugged, Tunable Infrared Laser Sources - DOE Contact Michael O'Connell, (202) 586-9311; Deacon Research Contact Dr. Olive Lee, (415) 493-6100

An Innovative Membrane and Process for Removal and Recovery of Natural Gas Liquids - DOE Contact William J. Gwilliam, (304) 285-4401; Membrane Technology And Research, Inc. Contact E. G. Weiss, (415) 328-2228

A Lower Cost Molten Carbonate Matrix - DOE Contact William J. Gwilliam, (304) 285-4401; M-C Power Corporation Contact Patrick F. McSweeney, (708) 986-8040

PHASE II PROJECTS (SECOND YEAR)

Economical Photochromic Films Based on Metal Oxides - DOE Contact David Koegel, (301) 903-5997; EIC Laboratories, Inc. Contact Dr. A. C. Makrides, (617) 769-9450

A Continuous Cryopump/Pellet-Fabrication Apparatus for Fusion - DOE Contact T.V. George, (301) 903-4957; Cryogenic Applications F, Inc. Contact Dr. Christopher A. Foster, (615) 435-5433

Development of Expansive Cements Using Dry Flue Gas Desulfurization Solid Wastes - DOE Contact Mary Ashbaugh, (304) 291-4966; Praxis Engineers, Inc. Contact Suzanne C. Shea, (408) 945-4282

Highly Selective Membranes for the Separation of Organic Vapors Using Super-Glassy Polymers - DOE Contact Robert Marianelli, (301) 903-5804; Membrane Technology and Research, Inc. Contact E. G. Weiss, (415) 328-2228

A Long Life Perovskite Oxygen Electrode for Calcium and Lithium Oxide Processing in Nuclear Fuel Cycles - DOE Contact Eli Goodman, (301) 903-2966; Eltron Research, Inc. Contact Eileen E. Sammells, (303) 440-8008

Fullerene Based Catalysts for Heavy Oil Upgrading - DOE Contact Udaya Rao, (412) 892-4743; TDA Research, Inc. Contact Michael E. Karpuk, (303) 940-2301

A Low Emission Alkali Metal Thermal to Electric Converter Automotive Power System - DOE Contact Robert Astheimer, (301) 903-4410; Advanced Modular Power Systems, Inc. Contact Dr. Thomas K. Hunt, (313) 677-4260

An Acoustic Plate Mode Sensor for Aqueous Mercury - DOE Contact Paul Hart, (301) 903-7456; BIODE, Inc. Contact Dr. Douglas McAllister, (207) 883-1492

SMALL BUSINESS TECHNOLOGY TRANSFER PROGRAM

The Small Business Technology Transfer (STTR) program was established by the Small Business Research and Development Enhancement Act of 1992, Public Law 102-564. Grant applications are solicited from small science- and technology-based U.S. firms (with 500 employees or less) in collaboration with a non-profit research institution (e.g. National laboratories and universities). Awards are made competitively to the small business with the collaborating research institution serving as a subcontractor. STTR supports innovative R&D and encourages conversion of that R&D into commercial applications of economic benefit to the Nation. The STTR program is designed for implementation in three phases, with Phase I determining, insofar as possible, the scientific or technical merit and feasibility of ideas proposed for investigation. The period of performance in this initial phase is about nine months, and awards are limited to $100,000. Phase II is the principal research or R&D effort, and only Phase I awardees can compete for Phase II awards of up to $500,000 for work to be performed in a period of up to two years. In Phase III, commercial application of the research or R&D is pursued using non-Federal funding or, alternatively, it may involve follow-on non-STTR Federal contracts for products or services desired by the Government.

The materials-related projects, like all other projects in the STTR program and the SBIR program, were selected on the basis of scientific and technical merit, as judged against the specific criteria listed in the solicitation. Award selections were based on reviews performed by personnel in DOE laboratories, universities, private industry, and government.

As in the SBIR program, these projects represent high-risk research, but the potential benefits are also high if the objectives are met. Brief descriptions of all DOE STTR projects, not only those of interest in materials research, are given in the following publications: Abstracts for Phase I Awards, 1996 (DOE/ER-0690) and Abstracts for Phase II Awards, 1995. Copies of these publications may be obtained by calling (301) 903-1414.

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

PHASE I PROJECTS

Cabled Monofilament Subelements for Improved Multifilament Niobium Tin Performance and Reduced Cost - DOE Contact Jerry Peters, (301) 903-5228; Supercon, Inc. Contact Elaine Drew, (508) 842-0174

Two-Phase Homogeneous Catalysis in Ionic Liquid and Liquid Cathrate Solvents - DOE Contact Paul Maupin, (301) 903-5808; Covalent Associates, Inc. Contact Dr. Margaret E. Langmuir, (617) 938-1140;

PHASE II PROJECTS (FIRST YEAR)

Laser Processing of Thermal Sprayed Beryllium Plasma Facing Components - DOE Contact T. V. George, (301) 903-4957; Plasma Processes, Inc. Contact Tim McKechnie, (205) 851-7653

Amorphous Silicon/Crystalline Silicon Heterojunctions for Nuclear Radiation Detector Applications - DOE Contact Richard Rinkenberger, (301) 903-3613; Quantrad Sensor, Inc. Contact Dr. Nicholas J. Szluk, (408) 727-7827

Low Loss Sapphire Windows for High Power Microwave Transmission - DOE Contact T. V. George, (301) 903-4957; Thoughtventions Unlimited Contact Dr. Stephen C. Bates, (203) 657-9014

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

PHASE I PROJECTS

Fuzzy Carbon Electrode Structures for Electrochemical Double Layer Capacitors - DOE Contact Jim Merritt, (202) 586-0903; Evans Company Contact David A. Evans, (401) 434-5600

High Speed Motor Alternators for Hybrid Electric Vehicle Energy Storage - DOE Contact Jim Merritt, (202) 586-0903 Satcon Technology Corporation Contact Steven St. Germain, (617) 349-0914

A Flywheel Motor Alternator for Hybrid Electric Vehicles - DOE Contact Jim Merritt, (202) 586-0903; Visual Computing Systems Corporation Contact Robert J. Westerkamp, (812) 923-7474

Feasibility of Correlating Vanadium-Chromium-Titanium Alloy Weld Strength with Weld Chemistry - DOE Contact F. W. Wiffen, (301) 903-4963; Charles Evans and Associates Contact Robert C. Ewing, (415) 369-4567

Development of Focussing Crystal Spectrometers for Extended X-ray Sources - DOE Contact Michael Crisp, (301) 903-4883; Radiation Science, Inc. Contact Dr. Allen S. Krieger, (617) 621-7076

Ultra-High Vacuum Radio Frequency Load - DOE Contact Jerry Peters, (301) 903-5228; Ferrite Components, Inc. Contact Aldo P. Elicone, (603) 881-5234

Advanced Electron Cyclotron Resonance Ion Source with Large Resonant Plasma Volume - DOE Contact Richard Rinkenberger, (301) 903-3613; Lambda Technologies, Inc. Contact Richard S. Garard, (919) 420-0275

Two-Phase Homogeneous Catalysis in Ionic Liquid and Liquid Cathrate Solvents - DOE Contact Paul Maupin, (301) 903-5808; Covalent Associates, Inc. Contact Dr. Margaret E. Langmuir, (617) 938-1140

PHASE II PROJECTS (FIRST YEAR)

Environmentally Benign Manufacturing of Compact Disk Stampers - DOE Contact Helen Kerch, (301) 903-2346; Prism Company Contact Peter Ciriello, (508) 785-2511

OFFICE OF FUSION ENERGY SCIENCES

The mission of the Office of Fusion Energy Sciences (OFES) is to advance plasma science, fusion science and fusion technology—the knowledge base needed for an economically and environmentally attractive fusion energy source. The policy goals that support this mission are: (1) advance plasma science in pursuit of national science and technology goals; (2) develop fusion science, technology and plasma confinement innovations as the central theme of the domestic program; and (3) pursue fusion energy science and technology as a partner in the international effort.

A significant component of the fusion energy program is the development and validation of the materials required for the fusion systems. Materials must be developed that will meet the unique requirements of fusion, as well as the standard requirements of a high efficiency, high reliability power generating system. The unique requirements of fusion are the result of the intense neutron environment, dominated by the 14 MeV neutrons characteristic of the deuterium-tritium fusion reaction. For performance, the materials must have slow and predictable degradation of properties in this neutron environment. For safety and environmental considerations, materials must be selected with activation products that neither decay too rapidly (affecting such safety factors as system decay heat) nor too slowly (affecting the waste management concerns for end-of-life system components). Materials that meet these requirements are referred to as "Low Activation Materials." Programs to develop the materials for plasma-facing components, for diagnostic and control systems, for structures in the high neutron flux regions, for the production of tritium in the blanket, and for the superconducting magnets required for confinement are sponsored by OFES.

The fusion program in the United States is conducted with a high degree of international cooperation. Of particular importance is the International Thermonuclear Experimental Reactor (ITER) engineering design activity, conducted in partnership with the European Union, Japan, and the Russian Federation. More than one-half of the materials work sponsored by OFES is in support of the ITER collaboration.

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

242. **STRUCTURAL MATERIALS DEVELOPMENT**
$1,250,000
DOE Contact: F. W. Wiffen (301) 903-4963
ANL Contact: D. L. Smith (708) 252-4837

This program is directed at the development of advanced, low activation structural materials for application in fusion power system first wall and blankets. Emphasis at ANL is on the development of vanadium-base alloys and on chemical corrosion/ ompatibility of the structural materials with other system materials. The vanadium alloy development is focused on the V-Cr-Ti system, with the goals of identifying promising candidate compositions, determining the properties of candidate alloys, and evaluating the response to irradiation conditions that simulate anticipated fusion system operation. The compatibility studies include vanadium and other candidate structural materials, and focus on the effects of exposure to projected coolants, especially liquid lithium.

Keywords: Vanadium, Compatibility, Lithium, Irradiation Effects, Alloy Development

243. **INSULATING CERAMICS FOR FUSION**
$30,000
DOE Contact: F. W. Wiffen, (301) 903-4963
LANL Contact: E. H. Farnum, (505) 665-5223

The goals of this project are to determine the changes in electrical, optical and structural properties of ceramic insulators in predicted fusion service, especially the effects of neutron irradiation. An understanding of the effects of radiation and of the controlling mechanisms are used to select or develop materials capable of extended life for use in fusion systems.

Keywords: Ceramics, Electrical Properties, Irradiation Effects

244. **MODELING IRRADIATION EFFECTS IN SOLIDS**
$80,000
DOE Contact: F. W. Wiffen, (301) 903-4963
LLNL Contact: T. Diaz de la Rubia, (510) 422-6714

Large scale computer simulation and experimental data on irradiation effects are combined to extend the understanding of the primary damage processes in solids. Special attention is given to the energy range appropriate for the 14 MeV neutrons produced in D-T fusion, and to the materials of interest for fusion systems.

Keywords: Modeling, Irradiation Effects

245. **FUSION SYSTEMS MATERIALS**
$3,493,000
DOE Contact: F. W. Wiffen, (301) 903-4963
ORNL Contacts: E. E. Bloom, (423) 574-5053 and A. F. Rowcliffe, (423) 574-5057

This program is directed at the development and qualification of structural materials and insulating ceramics for use in components of fusion power systems exposed to the intense neutron flux. Candidate low activation structural material systems include ferritic/martensitic steels, vanadium alloys and SiC/SiC composites. Investigations focus on the most critical questions or limiting properties in each of these systems: ferritic/ martensitic steels—DBTT transition shifts and fracture toughness, vanadium alloys—welding processes, effects of irradiation on fracture toughness, and compatibility in proposed coolant systems, SiC/SiC composites—definition of the effects of irradiation on properties and structure and evaluation of advanced composite fibers and coatings. The insulating ceramic activity is initially developing an understanding of irradiation effects in alumina, spinel and other materials. The greatest concern is to establish the permanent and transient changes in electrical properties, requiring measurement while the specimen is under irradiation. Work on these material classes involves irradiation in fission reactors, including HFIR, HFBR, and other test reactors, as partial simulation of the fusion environment.

Keywords: Ceramics, Steels, Vanadium, Silicon Carbide, Composites, Irradiation Effects, Electrical Properties

246. **STRUCTURAL MATERIALS FOR FUSION SYSTEMS**
$1,100,000
DOE Contact: F. W. Wiffen, (301) 903-4963
PNNL Contact: R. H. Jones, (509) 376-4276

The goal of this program is to develop an understanding of radiation effects that provides a basis for development of irradiation-insensitive materials. The objective is low activation materials for use as structures in divertor, first wall, and blanket components of fusion systems. Irradiation in fission reactors is used to simulate fusion conditions, with measurement of physical and mechanical properties used to track irradiation effects. A modeling activity complements the experimental measurements. The ultimate goal is optimized ferritic steels, vanadium alloys, and SiC/SiC composite materials for fusion power plant use.

Keywords: Steels, Vanadium, Silicon Carbide, Composites, Irradiation Effects, Modeling

247. **DEVELOPMENT OF RADIATION-HARDENED CERAMIC COMPOSITES FOR FUSION APPLICATIONS**
$36,000
DOE Contact: F. W. Wiffen, (301) 903-4963
RPI Contact: D. Steiner, (518) 276-4016

This research is directed at furthering the understanding of the effects of irradiation on the SiC/SiC composite system, as the basis for developing superior composite materials for fusion structural applications. The focus of the work is on the evaluation of improved fibers and alternative interface layer materials.

Keywords: Silicon Carbide, Composites

248. **RADIATION EFFECTS AND MICRO-MECHANICS OF SiC/SiC COMPOSITES**
$40,000
DOE Contact: F. W. Wiffen, (301) 903-4963
UCLA Contact: N. M. Ghoniem, (310) 825-4866

The goal of this program is to develop an understanding of the basic processes of neutron damage production, microstructural evolution, chemical compatibility, and micromechanics of fracture in SiC/SiC composite materials. This basic knowledge of materials behavior is used to model the effects of irradiation and the service performance of SiC/SiC components in fusion power systems. The critical goal is helping to evaluate the feasibility of using SiC/SiC in this application.

Keywords: Silicon Carbide, Composites, Modeling, Irradiation Effects

249. **DAMAGE ANALYSIS AND FUNDAMENTAL STUDIES FOR FUSION REACTOR MATERIALS DEVELOPMENT**
$200,000
DOE Contact: F. W. Wiffen, (301) 903-4963
UCSB Contacts: G. R. Odette, (805) 893-3525 and G. E. Lucas, (805) 893-4069

This research is directed at developing a fundamental understanding of both the basic damage process and microstructural evolution that take place in a material during neutron irradiation. This understanding is used with empirical data to develop physically-based models of irradiation effects. The focus is on the fracture properties of vanadium alloys, austenitic and ferritic stainless steels, including helium effects, to: (a) develop an integrated approach to integrity assessment, (b) develop advanced methods of measuring fracture properties, and (c) analyze the degradation of the mechanical properties of steels. The program also contributes to the assessment of the feasibility of using these alloys in ITER and other fusion systems.

Keywords: Vanadium, Steels, Irradiation Effects Fracture

250. **DEVELOPMENT OF LITHIUM-BEARING CERAMIC MATERIALS FOR TRITIUM BREEDING IN FUSION REACTORS**
$40,000
DOE Contact: S. Berk, (301) 903-4171
ANL Contact: C. Johnson, (708) 252-7533

Research activities are focused on critical issues of ceramic breeder blankets for fusion reactors, including ceramic breeder material tritium retention and release, ceramic breeder and beryllium irradiation response, chemical compatibility of ceramic breeder materials and beryllium with blanket coolant and structural materials and heat transfer and temperature control in ceramic breeder materials. Computer models are tested against data on irradiation of lithium-oxide and lithium-zirconate materials in a fast-spectrum fission reactor. There is good agreement between model predictions and experimental data in the area of transient tritium release.

Keywords: Ceramics, Compatibility, Tritium Release, Modeling, Lithium Ceramics

251. **POST-IRRADIATION EXAMINATION OF LITHIUM-BEARING CERAMIC MATERIALS FOR TRITIUM BREEDING IN FUSION REACTORS**
$70,000
DOE Contact: S. Berk, (301) 903-4171
PNNL Contact: G. Hollenberg, (509) 376-5515

Research activities are for post-irradiation examinations (PIE) of the ceramic breeder materials irradiated in the Fast Flux Test Facility. The PIE was conducted as part of the BEATRIX-II program under an International Energy Agency agreement between the US, Japan and Canada. PIE involved capsule disassembly, neutron radiography, plenum gas analysis, photography, mensuration characterization, tritium inventory measurements, microstructural characterization and thermal conductivity measurements. PIE for specimens from the BEATRIX-II Phase 1 irradiation (lithium-oxide irradiated to 5 percent lithium atom burnup) and the Phase 2 irradition (lithium-oxide and lithium-zirconate irradiated to 5 percent lithium atom burnup) was completed in FY 1995.

Keywords: Ceramics, Lithium Ceramics, Tritium Release

252. **INTERNATIONAL THERMONUCLEAR EXPERIMENTAL REACTOR (ITER) MATERIALS DEVELOPMENT FOR PLASMA FACING COMPONENTS**
$5,500,000
DOE Contact: M. M. Cohen, (301) 903-4253
SNL Contact: M. Ulrickson, (505) 845-3020

Research activities include: improved techniques for joining beryllium to copper alloys, determination of the tritium retention of beryllium, improvement of the thermal conductivity of plasma sprayed beryllium, development of radiation damage resistant carbon-fiber composites, determination of erosion rates of beryllium, tungsten and carbon under normal and disruption conditions and thermal fatigue testing of beryllium and carbon-fiber composites. The joining techniques being investigated include diffusion bonding, induction brazing, electroplating and inertial welding. Tritium retention and permeation measurements have been conducted on the Tritium Plasma Experiment. The improvements in the plasma spray technique are centered on improving the beryllium powder and selection of the proper powder sizes. Highly oriented pitch based carbon fibers have been used to produce carbon-fiber composite for neutron irradiation. The erosion rates are measured on both plasma simulators and tokamaks. The thermal fatigue testing is carried out on electron beam test systems.

Keywords: Plasma-Facing Components, Beryllium, Carbon-Fiber Composite, Joining, Erosion, Thermal Fatigue

253. **ITER CERAMIC MATERIALS**
$190,000
DOE Contact: F. W. Wiffen, (301) 903-4963
LANL Contact: E. H. Farnum, (505) 665-5223

The ITER will require ceramic materials in a number of the heating, current drive, and diagnostic elements of the plant. Behavior of these systems can be limited by their electrical, optical and/or structural properties. A program of in situ and post irradiation measurements to determine the effects of irradiation on these properties is conducted at LANL and other sites, with the goals of developing the properties database on candidate materials that will allow system designers to effectively include these components in the ITER plant.

Keywords: Ceramics, Electrical Properties, Optical Properties, Irradiation Effects

254. **ITER MATERIALS EVALUATION**
$380,000
DOE Contact: F. W. Wiffen, (301) 903-4963
ORNL Contact: E. E. Bloom, (423) 574-5053 and A. F. Rowcliffe, (423) 574-5057

ITER requires structural materials and insulating ceramics for use in a range of system components exposed to the neutrons produced by the fusion reaction. ORNL's part of the ITER materials program is directed at the selection of promising compositions of copper alloys, evaluating bonded copper alloy-stainless steel structures and assisting in the development of the database needed for the use of these materials. Irradiation effects and mechanical properties of these materials are under study. The insulating ceramics work is focused on the electrical properties under irradiation, and the in situ measurement techniques to determine this response are being developed. The work at ORNL emphasizes the use of the HFIR and of fission test reactors in Russia to perform the irradiations in support of the ITER materials development and evaluation.

Keywords: Steels, Copper, Vanadium, Ceramics, Irradiation Effects, Electrical Properties

255. **ITER STRUCTURAL MATERIALS EVALUATION**
$200,000
DOE Contact: F. W. Wiffen, (301) 903-4963
PNNL Contact: R. H. Jones, (509) 376-4276

Materials systems of interest to ITER for use as structural materials in the divertor, first wall and blankets are under evaluation to select the most attractive candidates in each system, and to develop the property database on these. The PNNL program is evaluating copper alloys and stainless steels for the ITER program. The emphasis is on irradiation effects, especially on fracture properties, for the bonded structures.

Keywords: Steels, Copper, Irradiation Effects

256. **DEVELOPMENT OF Nb_3Sn SUPERCONDUCTING WIRE FOR THE ITER MAGNET PROGRAM**
$4,000,000
DOE Contact: H. S. Staten, (301) 903-4950
MIT Contact: J. Minervini, (617) 253-5503

Activities include development of Nb_3Sn superconducting wire primarily for use in the high field magnets of the ITER model coils. Aggressive target specifications for high critical current density in the 12-13 tesla magnetic field range have been set and an industrial development program has begun to produce large quantities of this wire. U.S. superconducting wire industries involved include Intermagnetics General Corp./Advanced Superconductors Inc., and Teledyne Wah Chang Albany. Characterization of critical superconducting properties and ac losses has been carried out with measurements in university and national laboratories, including establishment of standardized samples and test procedures.

Keywords: Superconductors, Magnet Materials, Nb_3Sn

257. **STRUCTURAL MATERIALS DEVELOPMENT FOR THE CONDUIT OF ITER CABLE-IN-CONDUIT-CONDUCTORS**
$600,000
DOE Contact: H. S. Staten, (301) 903-4950
MIT Contact: J. Minervini, (617) 253-5503

Activities include fabrication of conduit for the conductors of the central solenoid and toroidal field model coils for ITER. The conduit material, Incoloy alloy 908, was developed via collaboration of INCO Alloys International and MIT. Work is proceeding on development of the database for this material. Alloy 908 has a low coefficient of expansion and minimizes the compressive strain in the Nb_3Sn superconductor upon cool down from the heat treatment temperature of approximately 1000°K to the operation temperature of 4°K. Industrial processing by various methods to finished conduit shape has been a priority. A second generation, improved weld filler metal has been developed.

Keywords: Conduit, Incoloy, Magnet Materials

OFFICE OF ENVIRONMENTAL MANAGEMENT

	FY 1996
Office of Environmental Management - Grand Total	$40,091,517
Office of Waste Management	$ 2,579,000
High Level Waste Division	2,579,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 1,979,000
The West Valley Support Project	1,609,000
Ceramic Final Forms	370,000
Materials Properties, Behavior, Characterization or Testing	$ 600,000
Materials Characterization Center Testing of West Valley Formulation Glass	100,000
Argonne National Laboratory High-Level Waste Borosilicate Glass Testing Program	500,000
Office of Science and Technology	$37,512,517
Office of Technology Development	$37,512,517
Office of Science and Risk Policy	$14,449,517
Materials Preparation, Synthesis, Deposition, Growth or Forming	$4,758,653
Adsorption/Membrane Filtration as a Contaminant Concentration and Separation Process for Mixed Wastes and Tank Wastes	609,987
An Alternative Host Matrix Based on Iron Phosphate Glasses for the Vitrification of Specialized Nuclear Waste Forms	624,834
Architectural Design Criteria for F-Block Metal Ion Sequestering Agents	50,000
Biofiltration of Volatile Pollutants: Engineering Mechanisms for Improved Design, Long-term Operation, Prediction and Implementation	26,389
Chemical and Ceramic Methods Toward Safe Storage of Actinides Using Monazite	750,000
De Novo Design of Ligands for Metal Separation	380,000
Design and Synthesis of the Next Generation of Crown Ethers for Waste Separations: An Inter-Laboratory Comprehensive Proposal	53,333
Development of Inorganic Ion Exchangers for Nuclear Waste Remediation	449,999
Extraction and Recovery of Mercury and Lead from Aqueous Waste Streams Using Redox-active Layered Metal Chalcogenides	333,000
Managing Tight-binding Receptors for New Separations Technologies	350,000
New Anion-Exchange Resins for Improved Separations of Nuclear Materials	36,111
Novel Ceramic-Polymer Composite Membranes for the Separation of Hazardous Liquid Waste	360,000
Polyoxometalates for Radioactive Waste Treatment	330,000
Removal of Heavy Metals and Organic Contaminants from Aqueous Streams by Novel Filtration Methods	330,000
Sensors Using Molecular Recognition in Luminescent, Conductive Polymers	41,667
Synthesis of New Water-Soluble Metal-Binding Polymers: Combinatorial Chemistry Approach	33,333

OFFICE OF ENVIRONMENTAL MANAGEMENT (continued)

	FY 1996
Office of Science and Technology (continued)	
Office of Technology Development (continued)	
Office of Science and Risk Policy (continued)	
Materials Properties, Behavior, Characterization or Testing	$9,690,864
Acoustic Probe for Solid-Gas-Liquid Suspensions	750,841
Analysis of Surface Leaching Processes in Vitrified High-Level Nuclear Wastes Using In-Situ Raman Imaging and Atomistic Modeling	559,000
Atmospheric-Pressure Plasma Cleaning of Contaminated Surfaces	422,556
A Broad Spectrum Catalytic System for Removal of Toxic Organics from Water By Deep Oxidation	327,000
Chemical Decomposition of High-Level Nuclear Waste Storage/Disposal Glasses Under Irradiation	489,000
Construction of Bending Magnet Beamline at the APS for Environmental Studies	810,000
Design and Development of a New Hybrid Spectroelectrochemical Sensor	850,000
Determination of Transmutation Effects in Crystalline Waste Forms	25,417
Development of an In-Situ Microsensor for the Measurements of Chromium and Uranium in Groundwater at DOE Sites	690,000
f-Element Ion Chelation in Highly Basic Media	499,998
Fundamental Studies of the Removal of Contaminants from Ground and Waste Waters via Reduction by Zero-Valent Metals	380,000
Improved Analytical Characterization of Solid Waste-Forms by Fundamental Development of Laser Ablation Technology	184,028
In-Situ Spectro-Electrochemical Studies of Radionuclide Contaminated Surface Films on Metals and the Mechanism of Their Formation and Dissolution	27,917
An Investigation of Homogeneous and Heterogeneous Sonochemistry for Destruction of Hazardous Waste	290,000
Investigation of Microscopic Radiation Damage in Waste Forms Using ODNMR and AEM Techniques	19,389
Investigation of Novel Electrode Materials for Electrochemically-Based Remediation of High- and Low-Level Mixed Wastes in the DOE Complex	650,000
Microstructural Properties of High Level Waste Concentrates and Gels with Raman and Infrared Spectroscopies	45,917
Novel Analytical Techniques Based on an Enhanced Electron Attachment Process	300,000
On-Line Slurry Viscosity and Concentration Measurement as a Real-Time Waste Stream Characterization Tool	691,154
Partitioning Tracers for In Situ Detection and Quantification of Dense Nonaqueous Phase Liquids in Groundwater Systems	776,903
Photooxidation of Organic Wastes Using Semiconductor Nanoclusters	64,750
Quantifyinig Silica Reactivity in Subsurface Environments: Controls of Reaction Affinity and Solute Matrix on Quartz and SiO_2 Glass Dissolution Kinetics	348,994
Radiation Effects in Nuclear Waste Materials	80,000
Radiation Effects on Materials in the Near-Field of Nuclear Waste Repository	408,000

OFFICE OF ENVIRONMENTAL MANAGEMENT (continued)

	FY 1996
Office of Science and Technology (continued)	
Office of Technology Systems	$23,063,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$11,015,000
Fixed Hearth Plasma Treatment Process	4,076,000
High Temperature Demonstrations on Actual Mixed Waste	716,000
Fixed Hearth Plasma Radioactive Waste Test	3,864,000
Phosphate-Bonded Ceramic Waste Forms	450,000
Kinetic Mixer Demonstration	150,000
Stainless Steel Beneficial Reuse	600,000
Recycle of Depleted Uranium Studies	430,000
Reuse of Concrete from Contaminated Structure	231,000
Surface Acoustic Wave Array Detectors	248,000
Versatile, Robust, Miniature Sized and Real-Time Radiation Detector	250,000
Materials Properties, Behavior, Characterization or Testing	$12,048,000
Fixed Hearth Plasma Radioactive Waste Test	3,864,000
Phosphate-Bonded Ceramic Waste Forms	450,000
Kinetic Mixer Demonstration	150,000
Cesium Removal Demonstration	1,500,000
Grout and Glass Waste Forms	900,000
T_c Qualification Studies	225,000
Vitreous Ceramic Compositional Envelope Study	100,000
Graphite DC Plasma Arc Melter	2,109,000
Crystalline Silicotitanate for Cs/Sr Removal	400,000
TUCS/Phosphate Immobilization of Actinides	300,000
Test Sorbents: Industrial Contracts	2,050,000

OFFICE OF ENVIRONMENTAL MANAGEMENT

The Office of Environmental Management (EM) was established to effectively coordinate and manage the Department's activities to remediate the DOE Defense Complex and to properly manage waste generated by current operations. EM conducts materials research within two offices:

Office of Waste Management - The Office of Waste Management uses current technologies to minimize production of DOE-generated waste, alter current processes to reduce waste generation, and work with the Office of Science and Technology to develop innovative technologies for the treatment and disposal of present and future waste streams. The mission of the Office is to minimize, treat, store, and dispose of DOE waste to protect human health, safety, and the environment.

Office of Science and Technology - The Office of Science and Technology (OST) is responsible for managing and directing targeted basic research and focused, solution-oriented technology development programs to support the DOE Office of Environmental Management (EM). Programs involve research, development, demonstration, and deployment activities that are designed to produce innovative technologies and technology systems to meet national needs for regulatory compliance, lower life-cycle costs, and reduced risks to both people and the environment. Certain areas of the OST program focus on materials research in order to provide better, safer and less expensive approaches to identify, characterize and remediate DOE's waste problem.

Four Focus Areas have been formed to focus the EM-wide technology development activities on DOE's most pressing environmental management problems and are co-led by all EM offices:

Subsurface Contaminants. Hazardous and radioactive contaminants in soil and groundwater exist throughout the DOE complex, including radionuclides, heavy metals, and dense, nonaqueous phase liquids. Groundwater plumes have contaminated over 600 billion gallons of water and 50 million cubic meters of soil. In addition, the Subsurface Contaminants Focus Area is responsible for supplying technologies for the remediation of numerous landfills at DOE facilities. Technology developed within this speciality area provides effective methods to contain contaminant plumes and new or alternative technologies for remediating contaminated soils and groundwater.

Radioactive Tank Waste Remediation. Across the DOE Complex, hundreds of large storage tanks contain hundreds of thousands of cubic meters of high-level mixed waste. Primary areas of concern are deteriorating tank structures and consequent leakage of their contents. Research and technology development activities must focus on the development of safe, reliable, cost-effective methods of characterization, retrieval, treatment, and final disposal of the wastes.

Mixed Waste Characterization, Treatment, and Disposal. DOE faces major technical challenges in the management of low-level radioactive mixed waste. Several conflicting regulations together with a lack of definitive mixed waste treatment standards hamper mixed waste treatment and disposal. Disposal capacity for mixed waste is also expensive and severely limited. DOE now spends millions of dollars annually to store mixed waste because of the lack of accepted treatment technology and disposal capacity. In addition, currently available waste management practices require extensive, and hence costly waste characterization before disposal. Therefore, DOE must pursue technology that leads to better and less expensive characterization, retrieval, handling, treatment, and disposal of mixed waste.

Decontamination and Decommissioning. The aging of DOE's weapons facilities, along with the reduction in nuclear weapons production, has resulted in a need to transition, decommission, deactivate, and dispose of numerous facilities contaminated with radionuclides and hazardous materials. While building and scrap materials at the sites are a potential resource, with a significant economic value, current regulations lack clear release standards. This indirectly discourages the recovery, recycling, and/or reuse of these resources. The development of enhanced technologies for the decontamination of these materials, and effective communication of the low relative risks involved, will facilitate the recovery, recycle, and/or reuse of these resources. Improved materials removal, handling, and processing technologies will enhance worker safety and reduce cost.

When materials development work is performed in any of these Focus Areas, the Focus Area is identified. Projects not so identified crosscut more than one Focus Area. Funding levels are reported for the total project, which includes materials development and demonstration. For most projects, materials development accounts for less than 25 percent of the funds.

Some of the projects listed in this report are managed under the Environmental Management Research Program (EMSP), a joint program of EM and the Office of Energy Research (ER). Basic research under the EMSP contributes to environmental management activities that decrease risk to the public and workers, provide opportunities for major cost reductions, reduce time required to achieve EM's mission goals, and, in general, address problems that are considered intractable without new knowledge. This program is designed to inspire "breakthroughs" in areas critical to the EM mission through basic research and is managed in partnership with ER. ER's well-established procedures are used for merit review of applications to the EMSP. Subsequent to the formal scientific merit review, applications that are judged scientifically meritorious are evaluated by DOE for relevance to the objectives of the EMSP. The initial EMSP portfolio consisted of 139 awards amounting to a total of $112 million in three-year funding, $47.2 million of which was expended in FY96. Forty of those awards were in scientific disciplines related to materials issues that have potential to solve Environmental Management challenges. The entire EMSP portfolio can be viewed on the World Wide Web at *http://www.em.doe.gov/science*.

OFFICE OF WASTE MANAGEMENT

HIGH LEVEL WASTE DIVISION

The objective of the High Level Waste Division is to conduct waste management activities for ending interim storage of high-level waste and achieving permanent disposal of high-level waste at the Savannah River Site in South Carolina. Additionally, Congress directed the Department in 1980 to demonstrate the solidification of liquid high-level waste at West Valley (New York) which originated at the nation's only commercial plant to reprocess spent nuclear fuel. At both of these sites a program is in place to immobilize the high-level waste in preparation for geologic disposal.

At Savannah River and West Valley, high-level waste will be immobilized in a borosilicate glass prepared in a liquid-fed ceramic joule-heated melter. The Defense Waste Processing Facility at Savannah River is beginning nonradioactive operations in preparation for radioactive operation. West Valley is constructing the vitrification cell. For these two projects, materials research focuses on verifying the product consistency of the waste form based on a reference formulation chosen some time ago.

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

258. **THE WEST VALLEY SUPPORT PROJECT**
$1,609,000
DOE Contact: J. J. May, (716) 942-2161
PNNL Contact: M. Elliot, (509) 376-9858

The West Valley Support Project (WVSP) conducted by the Pacific Northwest National Laboratory (PNNL) is designed to meet the technology needs for the West Valley Demonstration Project (WVDP) and provide support to the subsequent site stabilization activities. The current objectives of the WVDP, as understood by PNNL, are: (1) to complete nonradioactive process testing, operational readiness reviews, and radioactive start-up of the vitrification facility; (2) to maintain safe storage of liquid high-level waste at the West Valley site; (3) to maintain a knowledgeable core of process support personnel to resolve current and future technical issues; (4) to resolve issues related to the site Environmental Impact Statement and other documents; and (5) to proceed with development of site stabilization activities particularly in the area of tank heel removal.

Keywords: Process Control, Storage, Technology

259. **CERAMIC FINAL FORMS**
$370,000
DOE Contact: Martyn Adamson, (510) 423-2024
LLNL Contact: Robert Hoppert, (510) 423-2420

Operations of the Mixed Waste Management Facility (MWMF) will yield ash-like residues (oxides, nitrates, etc. containing RCRA metals and radioactive elements) from the organic components of low-level mixed waste. These residues will be stabilized as a durable and leach-resistant ceramic waste form produced by traditional high-temperature powder technologies. Formulations for various input waste streams are being optimized.

Keywords: Ceramic, Final Waste Form, Ash

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

260. **MATERIALS CHARACTERIZATION CENTER TESTING OF WEST VALLEY FORMULATION GLASS**
$100,000
DOE Contact: J. J. May, (716) 942-2161
PNNL Contact: G. L. Smith, (509) 372-1957

Materials Characterization Center (MCC) is evaluating the chemical durability of glasses whose compositions are within the expected range of composition of the West Valley Demonstration Project borosilicate glass waste form. These include nonradioactive glass containing surrogate elements for radionuclides and radioactive glass doped with appropriate radionuclides. The MCC also is testing of a small sample of glass containing actual West Valley high-level waste.

Keywords: Radioactive Waste Host

261. **ARGONNE NATIONAL LABORATORY HIGH-LEVEL WASTE BOROSILICATE GLASS TESTING PROGRAM**
$500,000
DOE Contact K. Picha, (301) 903-7199

Argonne National Laboratory (ANL) is continuing a series of tests of high-level waste borosilicate glass. These tests, which have been supported by the Office of Environmental Management since FY 1989, will provide a better understanding of the long-term borosilicate glass corrosion mechanisms and durability concerns. Included in these tests are: Defense Waste Processing (DWPF)-based glass drip tests, DWPF sludge-based glass performance tests, long term drip testing on actinide-doped ATM-10 glass, and continued performance testing of West Valley Demonstration Project reference 6 glass.

Keywords: Waste, Waste Form, Borosilicate Glass, Waste Acceptance Specifications

OFFICE OF SCIENCE AND TECHNOLOGY

OFFICE OF TECHNOLOGY DEVELOPMENT

OFFICE OF SCIENCE AND RISK POLICY

Within the Office of Science and Technology, the Office of Science and Risk Policy manages EM's Science Program (EMSP), which draws on information from its DOE customers in identify necessary basic research. The EMSP concentrates its efforts on the characterization of DOE's wastes and contaminants, interactions of radioactive elements with biosystems in various natural media and waste forms, extraction and separation of radioactive and hazardous chemical contaminants, prediction and measurement of contaminant movement within DOE facilities' environments.

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

262. **ADSORPTION/MEMBRANE FILTRATION AS A CONTAMINANT CONCENTRATION AND SEPARATION PROCESS FOR MIXED WASTES AND TANK WASTES**
$609,987
DOE Contact: Ramoncita Massey, (202) 586-3837
University of Washington Contact: Dr. Mark M. Benjamin, (206) 543-7645

This project researches novel approaches for separating colloidal matter, U, Sr, and Cs from the remaining constituents of the liquid radionuclide-bearing wastes with which they are associated, and from one another. Inorganic materials are generally much cheaper and less prone to deterioration in radioactive environments than organic materials, their long-term behavior is easier to predict, and they can be used in vitrification processes. However, significant improvements are needed in mechanical properties, adsorption and/or exchange capacity, and level of characterization. This project examines new processes that employ relatively inexpensive and easy-to-use inorganic materials specifically designed to satisfy the needs of mixed nuclear waste treatment. Another phase of this project is the combination of inorganic media with electrochemical methods to enhance, accelerate or create an additional useful control parameter in the treatment process.

Keywords: Adsorption, Membrane, Filtration, Inorganic, Radionuclide-bearing Waste, Treatment Process

263. **AN ALTERNATIVE HOST MATRIX BASED ON IRON PHOSPHATE GLASSES FOR THE VITRIFICATION OF SPECIALIZED NUCLEAR WASTE FORMS**
$624,834
DOE Contact: Dr. Gordon Roesler, (202) 586-3231
University of Missouri-Rolla Contact: Dr. Delbert E. Day, (573) 341-4354

The overall objective of this project is to gain an understanding of the structure-property relationships for iron phosphate glasses that could be used for cost-effective nuclear waste disposal. This research consists of a combination of structural modeling and analysis along with property measurements yielding the informational data base of those property values and processing conditions directly applicable to nuclear waste disposal technology. The research focuses on four areas: (1) investigating the glass composition and processing conditions that yield optimum properties for vitrifying radioactive waste, (2) determining the atomic structure of these glasses and how it influences selected properties, (3) determining how the physical and structural properties are affected by the addition of simulated radioactive waste components, and (4) investigating the process and products of devitrification of the waste forms.

Keywords: Vitrification, Radioactive Waste, Iron Phosphate Glasses, Structure, Composition

264. **ARCHITECTURAL DESIGN CRITERIA FOR F-BLOCK METAL ION SEQUESTERING AGENTS**
$50,000
DOE Contact: Ramoncita Massey, (202) 586-3837
PNNL Contact: Dr. Benjamin P. Hay, (509) 372-6239

The objective of this project is to provide the means to optimize ligand architecture for f-block metal recognition. The hypothesis underlying this work is that differences in metal ion binding with multidentate ligands bearing the same number and type of donor groups are primarily attributable to intramolecular steric factors. The project will quantify these steric factors through the application of molecular mechanics models. The research involves close integration of theoretical and experimental chemistry. The goal will be to obtain an accurate set of criteria for ligand design, enabling researchers to reduce the time and cost associated with metal-specific ligand development.

Keywords: F-block Metal, Ligand Design, Separations, Recognition, Steric

265. **BIOFILTRATION OF VOLATILE POLLUTANTS: ENGINEERING MECHANISMS FOR IMPROVED DESIGN, LONG-TERM OPERATION, PREDICTION AND IMPLEMENTATION**
$26,389
DOE Contact: Steve Domotor, (301) 903-5053
ORNL Contact: Brian H. Davison, (423) 576-8522

Biofiltration is a rapidly developing concept with a variety of treatment applications. This project seeks to produce information for successful biofiltration operation through: (1) innovative application of nutrient limitation and filter regeneration; (2) development of a nonsteady state mathematical model; (3) incorporating cosolvents into the recirculating media and embedding high viscosity organics into the packing material. The result could be the emission-free destruction of organic wastes through off-gas treatment that eliminates emissions to the environment that exceed EPA limits.

Keywords: Biofiltration, Regeneration, Off-gas Treatment, Packing Material, Organic Waste

266. **CHEMICAL AND CERAMIC METHODS TOWARD SAFE STORAGE OF ACTINIDES USING MONAZITE**
$750,000
DOE Contact: Dr. Gordon Roesler, (202) 586-3231
Rockwell International Corporation Contact: Dr. P.E.D. Morgan, (805) 373-4273

Monazite is a naturally occurring mineral of which billion-year-old samples containing radioactive materials are available to study. This project investigates the concept of using monazite ceramic as a safe, secure, very long term containment for actinide wastes. Information to be obtained will include: sintering mechanisms involved in forming high density monazite ceramics; physical and chemical properties of grain boundaries in these ceramics; interactions with impurities and additives used to promote densification; physical properties of polycrystalline monazite ceramics; and the precipitation of monazite phases in an efficient, simple and economical manner. This project will provide a knowledge base for using monazite as a nuclear waste form.

Keywords: Actinide Wastes, Storage Methods, Monazite, Ceramics, Preparation, Properties

267. **DE NOVO DESIGN OF LIGANDS FOR METAL SEPARATION**
$380,000
DOE Contact: Ramoncita Massey, (202) 586-3837
Washington University Contact: Dr. Garland R. Marshall, (314) 361-1567

This research focuses on the development of appropriate computational tools and parameters for the de novo design of selective metal ligands. The researchers have developed a successful suite of tools for computer-aided design of ligands for receptors of known three-dimensional structure (structure-based design), including the prediction of affinity. Appropriate geometrical parameters for metals can derived from crystal structures and force constants adapted from recent advances in theories in metal-ligand interactions. The practical goal is computer-aided design of ligands which would be selective for one metal over another with a predicted selectivity ratio and affinity.

Keywords: Ligands, Metal Separation, De Novo Designs, Algorithms

268. **DESIGN AND SYNTHESIS OF THE NEXT GENERATION OF CROWN ETHERS FOR WASTE SEPARATIONS: AN INTER-LABORATORY COMPREHENSIVE PROPOSAL**
$53,333
DOE Contact: Ramoncita Massey, (202) 586-3837
ORNL Contact: Dr. Bruce A. Moyer, (423) 574-6718

Crown ethers are organic molecules which can selectively remove metal atoms from complex mixtures. The goal of this project is to design, synthesize, and characterize the next generation of crown ethers for metal-ion separations applicable to U.S. DOE's environmental needs. The work combines three thrusts: (1) molecular mechanics and ligand design, (2) solvent-extraction properties, and (3) resin-immobilized crowns. Exploiting advances in molecular mechanics, this project seeks accelerated progress through ligand design and synthesis coupled with testing of predictions via structural, spectroscopic, and separation techniques. New crown compounds will be studied in solvent-extraction and polymer systems, emphasizing ion-exchange features. Selectivity principles governing the binding of such ions as Li^+, Cs^+, Sr^{2+}, and Ra^{2+}, all of which have been identified as contaminants at USDOE sites, will be investigated.

Keywords: Crown Ethers, Waste Separations, Ligand Design, Molecular Mechanics, Solvent-extraction Properties, Ion Exchange

269. **DEVELOPMENT OF INORGANIC ION EXCHANGERS FOR NUCLEAR WASTE REMEDIATION**
$449,999
DOE Contact: Ramoncita Massey, (202) 586-3837
Texas A&M University Contact: Dr. Abraham Clearfield, (409) 845-2936

This project is concerned with the development of highly selective inorganic ion exchangers for the removal of Cs^+ and Sr^{2+} from nuclear tank waste and from groundwater. It will study the origins of selectivity through detailed structural studies and the thermodynamics of the ion exchange processes. The compounds to be synthesized may have cavity or tunnel structures, layer structures, or be amorphous gels. Systematic substitutions of framework ions based on ionic radii and charge will be carried out, and their effect on selectivity determined. Crystallinity will be controlled by the time, temperature, and pressure of synthesis. These studies will be used to predict the thermodynamics of exchange and tested by carrying out measurements of their thermodynamic properties.

Keywords: Inorganic Ion Exchangers, Nuclear Waste Remediation, Crystallinity

270. **EXTRACTION AND RECOVERY OF MERCURY AND LEAD FROM AQUEOUS WASTE STREAMS USING REDOX-ACTIVE LAYERED METAL CHALCOGENIDES**
$333,000
DOE Contact: Dr. Gordon Roesler, (202) 586-3231
Colorado State University Contact: Dr. Peter K. Dorhout, (970) 491-0624

Contamination of surface water and groundwater has already occurred in many DOE locations, necessitating safe, efficient, and cost effective remediation. Heavy elements must be removed from the waste (along with certain other metals and radionuclides) before the bulk of the remaining waste can be disposed of in sub-surface repositories. Current technologies for the selective extraction of mercury and lead require improvements in: (1) selectivity for mercury and lead; (2) decontamination factors; (3) recoverability of mercury and lead from the extractants. This project will address these issues, and investigate the design, synthesis, and evaluation of new redox active materials. These materials should be capable of being selective for softer cations and express redox-active reversibility to enable recovery of the ions of interest. Although concerned with removing soft heavy metal ions from aqueous solutions, this work is relevant to the extraction of these metal ions from contaminated soils as well.

Keywords: Water Contamination, Mercury, Lead, Aqueous Water Streams, Redox-active Layered Metal Chalcogenides, Selectivity, Decontamination Factor, Regeneration

271. **MANAGING TIGHT-BINDING RECEPTORS FOR NEW SEPARATIONS TECHNOLOGIES**
$350,000
DOE Contact: Ramoncita Massey, (202) 586-3837
University of Kansas Contact: Dr. Daryle H. Busch, (913) 864-5172

Environmental pollution scenarios that are not susceptible to standard separation and purification methodologies are: (1) those involving extremely dilute streams of radioactive or RCRA elements and (2) those in which such substances are absorbed in soils. In both cases, tight-binding, adequately selective, receptors offer the possibility of effective new technologies. Using powerful ligands, metal ions can be taken away from other reasonably strong binding sites, metal ions can be sequestered from very dilute media, and along with high affinity comes the possibility of high selectivity. This project attacks the historically slow establishment of equilibria in such systems by looking at means of facilitating both the binding and release processes and considering a novel concept for a separations technology that is tolerant of slow equilibration. The project includes: (1) designing of tight-binding ligands that can photo-release a metal ion, (2) investigating means for facilitating rapid binding by ligands with very high affinities for selected metal ions, and (3) developing template polymeric receptors that are imprinted for metal complexes of tight-binding ligands, but not for the free ligands.

Keywords: Tight-binding Receptors, New Separations Technology

272. **NEW ANION-EXCHANGE RESINS FOR IMPROVED SEPARATIONS OF NUCLEAR MATERIALS**
$36,111
DOE Contact: Ramoncita Massey, (202) 586-3837
LANL Contact: Dr. Mary E. Barr, (505) 667-7991

Improved methods for the extraction and recovery of radioactive metal ions from process, waste, and environmental waters have been identified as critical needs. The goal of this project is to develop multifunctional anion-exchange resins that facilitate anion uptake by carefully controlling the structure of the anion receptor site. These new ion-exchange resins combine ion-specific chelating ligands with robust, commercial ion-exchange technology to provide materials which exhibit superior selectivity and kinetics of sorption and desorption. Synthesis and testing of multifunctionalized extractants and ion-exchange materials that implement key features of the optimized binding site will provide feedback to the modeling and design activities. Resin materials which actively facilitate the uptake of actinide complexes from solution should display both improved selectivity and kinetic properties. This new methodology of 'facilitated uptake' could improve ion-exchange technology, allowing this robust, inexpensive procedure to attain higher levels of ion affinity and selectivity.

Keywords: Anion-exchange Resins, Nuclear Materials Separations, Selectivity, Extractants, Facilitated Uptake, Sorption

273. **NOVEL CERAMIC-POLYMER COMPOSITE MEMBRANES FOR THE SEPARATION OF HAZARDOUS LIQUID WASTE**
$360,000
DOE Contact: Ramoncita Massey, (202) 586-3837
University of California, Los Angeles Contact: Dr. Yoram Cohen, (310) 825-8766

There is a need for processes capable of selectively separating and concentrating a target species, often present in dilute solution. Although membrane systems have been considered the most probable means to achieve difficult liquid-phase separations, having reduced energy consumption level relative to conventional technologies (e.g., distillation, extraction), selective membranes with adequate structural integrity and longevity are lacking. This project focuses on the development and demonstration of novel robust ceramic-supported polymer membranes for organic-aqueous and organic-organic separations. The membranes are fabricated by modifying the pore surface of a ceramic support membrane via a graft polymerization process, imparting specific separation properties to the membrane. Fouling can be significantly reduced by terminally anchored chains that minimize surface solute adsorption. This approach may allow for the rapid deployment of task-specific membranes for remediation applications, recovery and recycle, effluent treatment, and selective replacement of energy intensive separation processes.

Keywords: Ceramic Polymer Composite Membranes, Hazardous Liquid Waste Separation, Ceramic-supported Polymer Membranes, Fouling, Selectivity

274. **POLYOXOMETALATES FOR RADIOACTIVE WASTE TREATMENT**
$330,000
DOE Contact: Ramoncita Massey, (202) 586-3837
Georgetown University Contact: Dr. Michael T. Pope (202) 687-6073

This project addresses the questions of separating and concentrating radioactive components of tank wastes, especially lanthanide and actinide species and technetium. It is known that such radioactive isotopes constitute only a small fraction of the mass present in most tanks, so that if efficient separations can be devised, the total volume of high level wastes to be stored is reduced to more manageable quantities. Three areas will be pursued concurrently: (1) development of known robust polyoxometalate cryptands; (2) incorporation of technetium into stable, non-volatile polyoxometalate complexes for subsequent separation and immobilization; (3) conversion of polyoxometalates under relatively mild conditions to inert tungsten bronze-like materials that incorporate the radioactive waste cations and which could be used as alternative waste forms.

Keywords: Separation of Tank Wastes, Polyoxometalates, Radioactive Waste Treatment, Waste Treatment

275. **REMOVAL OF HEAVY METALS AND ORGANIC CONTAMINANTS FROM AQUEOUS STREAMS BY NOVEL FILTRATION METHODS**
$330,000
DOE Contact: Ramoncita Massey, (202) 586-3837
Northeastern University Contact: Dr. Nelly M. Rodriguez, (617) 373-2822

Catalytically grown carbon nanofibers are a novel material that is produced by the decomposition of selected hydrocarbons over metal particles. The material consists of graphite platelets perfectly aligned and stacked in various directions with respect to the fiber axis. Such an arrangement imparts the carbon nanofibers with a unique combination of physical and chemical properties, including a high electrical conductivity. They exhibit high surface areas, and it is possible to generate structures with different spacing between the platelets, thereby generating new types of sieves. This project exploits a process by which it is possible to produce large amounts of nanofibers at the laboratory level, and it is estimated that on a large scale this material could be produced very inexpensively. As one part of the project the nanofibers will be employed as the electrode material in unique types of electrochemical filtration collection devices for the removal of heavy metals, radionuclides and transuranic elements from liquid phase effluent streams. Another part of the project is to take advantage of the unique blend of properties of carbon nanofibers for the separation of organic residues including methylene chloride, tetrahydrofuran, chlorobenzene, toluene, and methylethylketone, from aqueous waste streams. This could result in an inexpensive and regenerative removal medium for contaminants.

Keywords: Heavy Metals Removal, Organic Contaminants, Aqueous Streams Filtration, Carbon Nanofibers

276. **SENSORS USING MOLECULAR RECOGNITION IN LUMINESCENT, CONDUCTIVE POLYMERS**
$41,667
DOE Contact: Steve Domotor, (301) 903-5053
ANL Contact: Dr. Michael R. Wasielewski, (630) 252-3570

This project integrates three individual, highly interactive projects that will use molecular recognition strategies to develop sensor technology based on luminescent, conductive polymers that contain sites for binding specific molecules or ions in the presence of related molecules or ions. Selective binding of a particular molecule or ion of interest to these polymers will result in a large change in their luminescence and/or conductivity, which can be used to quantitatively sense the presence of the bound molecules or ions. Research problems that will be addressed include: (1) designing molecular recognition sites that are highly selective for the ions and/or molecules of interest to DOE in the presence of a large background of other chemical species, (2) finding ways to incorporate many different selective groups into a single polymer, (3) fabricating polymer films, strips, sheets, and coatings that can be applied to other materials, such as fiber optics and surfaces, (4) developing interfaces between the polymers and substrates that can be used to produce prototype arrays of many sensor elements for rapid multi-contaminant detection and quantitation, and (5) developing multiplexed data collection techniques to rapidly process the data obtained from many polymer sensors into a chemical profile of a waste stream or waste site in real time.

Keywords: Molecular Recognition, Polymer, Sensor Technology, Luminescent Conductive Polymer

277. **SYNTHESIS OF NEW WATER-SOLUBLE METAL-BINDING POLYMERS: COMBINATORIAL CHEMISTRY APPROACH**
$33,333
DOE Contact: Ramoncita Massey, (202) 586-3837
LANL Contact: Dr. Barbara F. Smith, (505) 667-2391

A variety of metals that require removal and concentration exist in DOE waste, ground, or process waters. A robust process, Polymer Filtration®, that can address the various conditions that these dilute waste streams present, is under development for aqueous stream polishing. Polymer Filtration® combines specially prepared water-soluble metal-binding polymers with commercially available ultrafiltration membranes to effect a selective separation of metal ions. To further the development of this technology the discovery and optimization of new, selective, strong, and reversible chelating polymers is necessary. This project explores the combinatorial approach for the discovery of metal-binding chelators attached to water-soluble polymers. The new materials are screened and prepared in larger quantity for further evaluation of their physical properties of stability, solubility, capacity, etc. and probed spectroscopically to identify the specific nature of their binding sites.

Keywords: Water-soluble Synthesis, Metal-binding Polymers, Combinatorial Chemistry

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

278. **ACOUSTIC PROBE FOR SOLID-GAS-LIQUID SUSPENSIONS**
$750,841
DOE Contact: Ramoncita Massey, (202) 586-3837
Syracuse University Contact: Dr. Lawrence L. Tavlarides, (315) 443-1883

Treatment of the radioactive waste stored in tanks across the DOE complex will require real-time characterization and monitoring of the size and volume fraction of solids in slurries during retrieval, immobilization, and closure stages of waste processing. Acoustic probes have been shown to be quite effective in determining the solid content in solid-liquid suspensions. The goal of this project is to develop an acoustic probe for monitoring particle size and volume fraction in slurries both in the absence and the presence of gas bubbles. The initial theoretical and experimental studies will be devoted to relatively well characterized three-phase systems. The latter studies will be devoted to more complex suspensions whose properties are similar to those encountered in various waste processes at the Hanford Site.

Keywords: Acoustic Probe, Suspension, Slurry, Solid-liquid Fraction, Bubble Size

279. **ANALYSIS OF SURFACE LEACHING PROCESSES IN VITRIFIED HIGH-LEVEL NUCLEAR WASTES USING IN-SITU RAMAN IMAGING AND ATOMISTIC MODELING**
$559,000
DOE Contact: Dr. Gordon Roesler, (202) 586-3231
University of Florida Contact: Dr. Joseph H. Simmons, (352) 392-6679

In the development of criteria for the safe disposal of vitrified nuclear wastes, it is necessary to have an accurate understanding of the chemical corrosion, leaching, and deposition processes that may take place during storage. New methods of Raman surface imaging being developed in this project have the potential for *in-situ* measurements without removal of samples from the ambient liquid, and for scanning the surface of macroscopic samples to reveal spatial differences in chemical behavior and surface composition.

Keywords: Vitrified Nuclear Waste, Disposal, Raman, Surface Imaging, Corrosion, Leaching

280. **ATMOSPHERIC-PRESSURE PLASMA CLEANING OF CONTAMINATED SURFACES**
$422,556
DOE Contact: Ramoncita Massey, (202) 586-3837
University of California, Los Angeles Contact: Dr. Robert F. Hicks, (310) 206-6865

Converting transuranic waste (TRU) into low-level radioactive waste (LLW) represents a large cleanup cost associated with the nuclear weapons complex cleanup. The goal of this project is to develop a low-cost technology for converting TRU into LLW based on selective plasma etchinig of plutonium and other actinides from contaminated structures. Plasma etching has already been used to remove Pu films from materials. A major breakthrough in this field has been demonstrated by the operation of an atmospheric-pressure plasma jet (APPJ). This research will study elementary surface reactions and characterize the etched surfaces in order to discover the elementary chemical processes that control the rate and selectivity for etching Ta, W and Pu thin films with atmospheric-pressure plasmas. This work will enable the development of new technology for low-cost, environmentally-benign decommissioning of nuclear waste.

Keywords: Plasma Etching, Atmospheric-pressure Plasma Jet (APPJ), Etching, Plutonium, Actinide, Contaminated, Decommissioning

281. **A BROAD SPECTRUM CATALYTIC SYSTEM FOR REMOVAL OF TOXIC ORGANICS FROM WATER BY DEEP OXIDATION**
$327,000
DOE Contact: Steve Domotor, (301) 903-5053
Pennsylvania State University Contact: Dr. Ayusman Sen, (814) 863-2460

Toxic organics in water constitute a very serious and persistent environmental hazard. Many are difficult to remove efficiently either through bioremediation or by presently known catalytic systems. It has been found that metallic palladium affects the removal of toxic organics and polymers by catalyzing their deep oxidation. This project involves a comprehensive study of the metallic palladium-water system. The research will examine the detailed mechanism of oxidation, and the classes of organics that can be efficiently oxidized and thereby removed from water. In addition, the possibility of designing more efficient hybrid catalytic oxidation systems will be examined.

Keywords: Deep Oxidation, Toxic Organics, Catalytic, Palladium

282. **CHEMICAL DECOMPOSITION OF HIGH-LEVEL NUCLEAR WASTE STORAGE/DISPOSAL GLASSES UNDER IRRADIATION**
$489,000
DOE Contact: Dr. Gordon Roesler, (202) 586-3231
Naval Research Laboratory Contact: Dr. David L. Griscom, (202) 404-7087

DOE is developing and producing vitrified glass storage/immobilization media for high-level nuclear wastes and excess weapons plutonium. This project will: (1) investigate the nature of any radiation-induced gas phases which may be dissolved in high-level-nuclear-waste-glass forms and lead to bubble formation; (2) provide fundamental knowledge necessary to assess the vulnerability of these forms to high-energy chemical reactions, particularly if dissolved oxygen is verified; and (3) develop an efficient method of surveying wide ranges of potential waste glass compositions to determine the dependence of radiolytic oxygen evolution on glass composition and hence determine compositions with superior resistance to decomposition.

Keywords: High-level Nuclear Wastes, Glass Waste Forms, Irradiation, Chemical Decomposition, Bubble Formation

283. **CONSTRUCTION OF BENDING MAGNET BEAMLINE AT THE APS FOR ENVIRONMENTAL STUDIES**
$810,000
DOE Contact: Dr. Gordon Roesler, (202) 586-3231
University of Washington Contact: Dr. Edward A. Stern, (206) 543-2023

Synchrotron radiation studies of materials at the molecular scale can make important contributions to the understanding of the basic science issues underlying environmental cleanup efforts. To help satisfy the growing need for synchrotron radiation based environmental research, this project involves the design and construction of a bending magnet (BM) beamline at the Advanced Photon Source (APS). Environmental and cleanup issues are a major focus of the fundamental research being performed on the BM beamline. The beamline will utilize the experimental techniques of X-ray absorption spectroscopy for both bulk and surface studies, with spatial and time resolution and elemental imaging, on toxic and radioactive samples.

Keywords: Beamline Construction, Advanced Photon Source (APS), Environmental Studies, X-ray Absorption Spectroscopy

284. **DESIGN AND DEVELOPMENT OF A NEW HYBRID SPECTRO-ELECTROCHEMICAL SENSOR**
$850,000
DOE Contact: Ramoncita Massey, (202) 586-3837
University of Cincinnati Contact: Dr. William R. Heineman, (513) 556-9210

The characterization of the contents of over 300 underground nuclear waste storage tanks at U.S. DOE sites presents a major scientific challenge. The general aim of this project is to design and implement a new sensor technology which offers unprecedented levels of specificity needed for analysis of the complex chemical mixtures found at U.S. DOE sites nationwide. The new sensor concept proposed combines the elements of electrochemistry, spectroscopy and selective partitioning into a single device that provides three levels of selectivity.

Keywords: Spectroelectrochemical Sensors, Hybrid Sensors, Underground Nuclear Waste Storage, Remediation

285. **DETERMINATION OF TRANSMUTATION EFFECTS IN CRYSTALLINE WASTE FORMS**
$25,417
DOE Contact: Dr. Gordon Roesler, (202) 586-3231
ANL Contact: Dr. Denis M. Strachan, (630) 252-4479

The objective of this study is to characterize the effects of transmutation in a candidate waste form for ^{137}Cs, the highest-activity constituent of many DOE wastes. Aged samples of a cesium aluminosilicate mineral, pollucite, that have undergone "natural" decay of the Cs, will be carefully characterized. under ambient temperature while isolated from interfering chemical effects. There currently is no information on beta-decay transmutation effects in waste forms in which transmutation has occurred over the natural decay time of the decaying isotope. This causes large uncertainty as to the effect of the transmutation on the physical and chemical properties of the waste form. Information on the effects of irradiation will give support to the selection of alternate waste forms for separated ^{137}Cs and give information on the long-term behavior of candidate waste forms.

Keywords: Transmutation Effects, Crystalline Waste Forms, Cesium, Pollucite

286. **DEVELOPMENT OF AN IN-SITU MICROSENSOR FOR THE MEASUREMENTS OF CHROMIUM AND URANIUM IN GROUNDWATER AT DOE SITES**
$690,000
DOE Contact: Steve Domotor, (301) 903-5053
New Mexico State University Contact: Dr. Joseph Wang, (505) 646-2140

The goal of this project is to develop, optimize and deploy a silicon-based micromachined stripping analyzer for field monitoring of trace levels of chromium and uranium. The system will integrate the sample-handling steps and necessary chemical reactions (using a flow-injection operation) with already proven adsorptive-stripping voltammetric operation on a small planar chip. Besides the drastic reduction in the size of the analytical system, such miniaturization should lead to increased speed, minimal reagent consumption and disposal, higher sensitivity and improved precision in the monitoring of toxic metals.

Keywords: In-situ Microsensors, Chromium and Uranium Traces in Groundwater, Groundwater Contamination, Stripping Analyzer, Flow-injection Operations

287. **f-ELEMENT ION CHELATION IN HIGHLY BASIC MEDIA**
$499,998
DOE Contact: Ramoncita Massey, (202) 586-3837
University of New Mexico Contact: Dr. Robert T. Paine, (505) 277-1661

The dominant radioactive species in DOE high-level wastes are cesium-137 and strontium-90; however, technetium and actinide species (Np, Pu, Am, Cm) are also significant contributors. The wastes are often in highly alkaline environments. In addition, treatment efforts have introduced a number of complex inorganic and organic ions, chelating agents, and solvents. As a result, the radioactive elements in many storage tanks (e.g., at the Hanford facility) exist in complex and variable solid and liquid matrices. More information will be required in order to develop the necessary chemical separations. This project will: conduct a study of the speciation of several fission product elements that are present in the waste; gather data on the interactions of various ligands with the metal species present; and begin developing new ligand systems that may serve to selectively bind and separate individual ions from the various alkaline waste fractions. The information gained will contribute to the future development of improved extractants and solid waste washing agents.

Keywords: Chelation, F-element Ion, Speciation, Radioactive Waste, Ligand Systems

288. **FUNDAMENTAL STUDIES OF THE REMOVAL OF CONTAMINANTS FROM GROUND AND WASTE WATERS VIA REDUCTION BY ZERO-VALENT METALS**
$380,000
DOE Contact: Dr. Gordon Roesler, (202) 586-3231
University of California, Riverside Contact: J. A. Yarmoff, (909) 787-5336

To remove trace contaminants from wastewaters and groundwaters, elemental iron can be used for the reductive dechlorination of solvents and the removal of toxic trace elements, such as Se, Cr, and U. The design and operation of in situ reactive barriers and above-ground reactors, as treatment systems, requires a detailed process-level understanding of iron/ contaminant interactions. This research project investigates the interactions of the relevant chlorinated solvents, trace elements, and trace element-containing compounds with single- and poly-crystalline Fe surfaces. This work will providing a fundamental physical and chemical understanding of these interactions, which can impact the development of cleanup techniques and procedures.

Keywords: Removal of Contaminants, Ground and Waste Water Treatment, Zero-valent Metals, Reductive Dechlorination, Reactive Barrier

289. **IMPROVED ANALYTICAL CHARACTERIZATION OF SOLID WASTE-FORMS BY FUNDAMENTAL DEVELOPMENT OF LASER ABLATION TECHNOLOGY**
$184,028
DOE Contact: Ramoncita Massey, (202) 586-3837
LBNL Contact: Dr. Richard E. Russo, (510) 486-4258

Laser ablation must be understood on a fundamental level to ensure confidence in the characterization for DOE environmental applications. This research project addresses several fundamental issues, including energy coupling, mass removal, gas dynamics, and transport. Mechanisms responsible for particle generation are also addressed. Samples to be emphasized initially in this fundamental research include prototypic vitrified waste glass and metal/ metal-oxide systems. This fundamental work supports the efforts at all the National Laboratories investigating laser ablation technology for the management of DOE radioactive, hazardous chemical, and mixed waste.

Keywords: Analytical Characterization, Solid Waste Forms, Laser Ablation, Waste Management

290. **IN-SITU SPECTRO-ELECTROCHEMICAL STUDIES OF RADIONUCLIDE CONTAMINATED SURFACE FILMS ON METALS AND THE MECHANISM OF THEIR FORMATION AND DISSOLUTION**
$27,917
DOE Contact: Ramoncita Massey, (202) 586-3837
ANL Contact: Dr. C.A. Melendres, (630) 252-4346

The aim of this research is to gain a fundamental understanding of the structure, composition, and mechanism of formation of radionuclide-containing surface films on metals that are relevant to the problem of decontamination of piping systems and waste storage tanks at DOE nuclear facilities. Electrochemical studies include the corrosion and passivation behavior of iron, nickel, chromium, and stainless steel. The energetics and dynamics of film formation and dissolution and the effect of incorporation of heavy metal ions and radioactive elements will be examined. Synchrotron X-ray absorption and vibrational (infrared and Raman) spectroscopic techniques will be used define "in-situ" the structure and composition of the various oxide phases that are formed as a function of temperature.

Keywords: In-situ Spectro Electrochemical Studies, Radionuclide Contamination, Contamination of Metals, Corrosion, Passivation, Film

291. **AN INVESTIGATION OF HOMOGENEOUS AND HETEROGENEOUS SONOCHEMISTRY FOR DESTRUCTION OF HAZARDOUS WASTE**
$290,000
DOE Contact: Ramoncita Massey, (202) 586-3837
Purdue University Contact: Dr. Inez Hua, (317) 494-2409

This research explores the application and optimization of ultrasonic waves as a novel method by which aqueous contaminants are degraded. The primary objective is to acquire a deeper fundamental knowledge of acoustic cavitation and cavitation chemistry, and in doing so, to ascertain how ultrasonic irradiation can be more effectively applied to environmental problems. Special consideration is given to the types of problems and hazardous chemical substrates found specifically at Department of Energy (DOE) sites. The experimental work is to include: exploring the significance of physical variables during sonolysis, such as ultrasonic frequency; examining sonochemical degradation kinetics and by-products, and reactive intermediates; investigation of activated carbon regeneration; and studying the physics and hydrodynamics of cavitation bubbles and bubble clouds and correlating with sonochemical effects.

Keywords: Sonochemistry, Hazardous Waste Destruction, Activated Carbon, Physical Variables, By-products

292. **INVESTIGATION OF MICROSCOPIC RADIATION DAMAGE IN WASTE FORMS USING ODNMR AND AEM TECHNIQUES**
$19,389
DOE Contact: Dr. Gordon Roesler, (202) 586-3231
ANL Contact: Dr. Guokui Liu, (630) 252-4630

This project will investigate the microscopic effects of radiation damage in crystalline and glass forms. Information about the nature of electronic interaction and the chemical bonding properties of radionuclides in damaged phases will be provided. Connections between the consequences of alpha and beta-decay processes and radionuclide release and chemical decomposition in waste forms will be studied. Electronic and chemical binding properties and local structural changes of parent radionuclide species and their decay daughters in the radiation damaged regions of the waste forms will be probed. Theoretical models based on electronic and nuclear interactions of the actinides and their surrounding ligands will be developed to interpret the experimental results and correlate the microscopic effects of radiation damage to the macroscopic mechanical and chemical properties of the HLW materials.

Keywords: Microscopic Radiation Damage, Optically Detected Nuclear Magnetic Resonance (ODNMR), Analytical Electron Microscopy (AEM)

293. **INVESTIGATION OF NOVEL ELECTRODE MATERIALS FOR ELECTROCHEMICALLY-BASED REMEDIATION OF HIGH- AND LOW-LEVEL MIXED WASTES IN THE DOE COMPLEX**
$650,000
DOE Contact: Ramoncita Massey, (202) 586-3837
California Institute of Technology Contact: Dr. Nathan S. Lewis, (818) 395-6335

The focus of this project is on electrochemical oxidation, one promising method of waste stream remediation. The aim would be to demonstrate a successful remediation technique for the high level liquid wastes through the removal of the significant quantities of nitrate and nitrite in many high-level radioactive liquid waste streams. Electrochemical oxidation is well-documented to have some significant advantages relative to high and low temperature steam oxidation processes, including the fact that electrochemical treatment is an in-situ remediation process whereas the water oxidation processes and most other proposed methods are pump-and-treat technologies. The main uncertainty in using such processes for high-level waste concerns the scale-up of the effort and the harsh conditions present in the radioactive wastes at the DOE sites.

Keywords: Electrochemical Oxidation, Oxidation, Electrode Materials, Electrochemical Remediation, High and Low Level Radioactive Wastes

294. **MICROSTRUCTURAL PROPERTIES OF HIGH LEVEL WASTE CONCENTRATES AND GELS WITH RAMAN AND INFRARED SPECTROSCOPIES**
$45,917
DOE Contact: Ramoncita Massey, (202) 586-3837
LANL Contact: Dr. Stephen F. Agnew, (505) 665-1764

The aim of this project is to use FTIR, Raman, and NMR spectroscopies along with thermophysical heats of gelation to relate the microstructural physical and chemical properties of DOE waste concentrates to their macroscopic characteristics. Better understanding in this area of macroscopic characteristics will enhance waste retrieval, pretreatment, and final disposal. This project will relate microscopic properties to macroscopic characteristics by using water vapor pressure measurements for concentrates to unambiguously determine water activity as a function of composition and temperature; FTIR, Raman, and aluminum NMR spectroscopies to determine the form and solubility of aluminate in caustic slurries; micro-Raman spectroscopy to identify and quantify phases of each species for a variety of concentrates; measurements of the heat of gelation and its dependence on water activity, presence of organic, and other properties; and spectroscopic tools to assess the influence of organic salts on microstructural properties of slurries.

Keywords: Microstructural Properties, High Level Waste Concentrates, High Level Waste Gels with Raman, Infrared Spectroscopies

295. **NOVEL ANALYTICAL TECHNIQUES BASED ON AN ENHANCED ELECTRON ATTACHMENT PROCESS**
$300,000
DOE Contact: Steve Domotor, (301) 903-5053
University of Tennessee Contact: Dr. Lal A. Pinnaduwage, (423) 574-6540

The purpose of this technique is to improve analytical instrumentation for the detection of complex molecules, such as may exist in contaminated DOE sites or waste streams. Previous research has shown that highly-excited electronic states of molecules have electron attachment cross sections orders of magnitude larger than for ground-state molecules. Furthermore, this enhanced electron attachment process appears to occur in a wide variety of molecules. Three novel analytical techniques based on this enhanced negative-ion formation process will be examined. In one technique, the excited states of the (analyte) molecules are populated via laser excitation; the resulting negative ions are mass analyzed for identification. The other two techniques utilize a specialized gas discharge for the formation of excited species (and low-energy electrons for attachment), and may provide a cost-effective method if successful.

Keywords: Electron Capture Detector, Enhanced Electron Attachment Process, Electron Attachment

296. **ON-LINE SLURRY VISCOSITY AND CONCENTRATION MEASUREMENT AS A REAL-TIME WASTE STREAM CHARACTERIZATION TOOL**
$691,154
DOE Contact: Ramoncita Massey, (202) 586-3837
University of California, Davis Contact: Dr. Robert L. Powell, (916) 752-8779

The radioactive and mixed wastes currently stored in the 177 underground storage tanks at the Hanford Site are complex mixtures of insoluble sludge, soluble salts, and supernatant liquids. Cross-site transfer pipelines will be used to transport the waste to various processing plants and separation facilities. This process will investigate an online, real-time means is required to monitor the waste stream physical and chemical properties to prevent line plugging. Elemental analysis of tank sludges reveal that the major insoluble components expected to be present are oxides and hydroxides of Al, Fe, Zr, and Cr, insoluble salts such as calcium phosphates, and aluminosilicate minerals. There is a strong dependence of the rheological properties on the environment. The principal thrust is to address the issue of on-line viscosity measurement by examining two potential technologies, nuclear magnetic resonance imaging and acoustic velocimetry. The project will focus on the fundamental scientific issues that must be overcome in order to implement these techniques.

Keywords: On-line Slurry Viscocity, Real-time, Characterization Tool, Nuclear Magnetic Resonance Imaging, Acoustic Velocimetry

297. **PARTITIONING TRACERS FOR IN SITU DETECTION AND QUANTIFICATION OF DENSE NONAQUEOUS PHASE LIQUIDS IN GROUNDWATER SYSTEMS**
$776,903
DOE Contact: Gordon Roesler, (202) 586-3231
University of Arizona Contact:
Dr. Mark L. Brusseau, (520) 621-1646

At some DOE sites and across the nation, some underground aquifers are threatened with contamination by dense nonaqueous phase liquids (DNAPLs) spilled into the soils. Bulk-phase partitioning tracers will be investigated to detect and determine DNAPL saturation, while interface partitioning tracers will be investigated to measure the area of the DNAPL-water interface. The specific objectives of the project are to: (1) investigate the use of partitioning tracers to detect and determine both the saturation and interfacial area of DNAPLs in saturated porous media; (2) investigate the effect of rate-limited mass transfer on the transport behavior of partitioning tracers; (3) investigate the effect of porous-media heterogeneity on the transport behavior of partitioning tracers; and (4) develop and evaluate mathematical models capable of simulating the transport of partitioning tracers in complex systems. This project combines one-dimensional laboratory experiments, 3-dimensional intermediate-scale flow cell experiments, physical methods for DNAPL description (including dual-energy gamma radiation), and advanced modeling techniques. The use of the partitioning tracer method in the future may reduce the uncertainty associated with risk assessments and remediation planning.

Keywords: Tracers, In Situ Detection, Dense Nonaqueous Phase Liquids (DNAPLS), Groundwater System

298. **PHOTOOXIDATION OF ORGANIC WASTES USING SEMICONDUCTOR NANOCLUSTERS**
$64,750
DOE Contact: Ramoncita Massey, (202) 586-3837
Sandia National Laboratory Contact:
Dr. J.P. Wilcoxon, (505) 844-3939

Solar detoxification is a process wherein sunlight is captured by a semiconductor particle in suspension to create electrons and holes that then diffuse to the particulate surface to effect the oxidation and reduction of toxic pollutants. Using solar energy to oxidize organic chemicals to carbon dioxide and dilute mineral acids is very energy efficient compared to other methods such as incineration. Recent research has made possible the synthesis of photostable semiconductor nanoclusters with band gaps that can be tuned by adjusting the cluster size. The rate of electron-hole recombination is small in nanoclusters, so they have the potential to act as highly efficient solar detoxification agents. In effect, they act more like molecular organic photoredox catalysts, but with significant advantages in chemical stability because they are inorganic. The goal of this project is to investigate the use of these materials in practical detoxification applications.

Keywords: Photooxidation, Organic Wastes Photooxidation, Semiconductor Nanoclusters, Solar Detoxification, Solar Energy Detoxification

299. **QUANTIFYING SILICA REACTIVITY IN SUBSURFACE ENVIRONMENTS: CONTROLS OF REACTION AFFINITY AND SOLUTE MATRIX ON QUARTZ AND SiO_2 GLASS DISSOLUTION KINETICS**
$348,994
DOE Contact: Dr. Gordon Roesler, (202) 586-3231
Georgia Institute of Technology Contact:
Dr. Patricia M. Dove, (404) 894-6043

Disposal of radioactive wastes can only be performed safely with a knowledge of the chemical kinetics of the surrounding environment. The goal of this research is to address this gap in our current understanding by quantifying the reactivity of crystalline and amorphous SiO_2 phases in the complex fluids of natural systems. Using an experimental approach which integrates techniques from surface science and geochemical kinetics, this study will measure the dissolution rate of quartz and silica glass in a series of single and mixed solute solutions over a range of variable pH and temperature. These data should result in a comprehensive quantitative model of solute controls on the reactivity of crystalline and glassy SiO_2. The kinetic portion of the study will be conducted in parallel with in situ and ex situ surface sensitive analyses of selected samples/ conditions. Findings will establish quantitative relationships between silica reactivity and a number of solution chemistries. The hypothesis that the solvation properties of dissolved species govern silica reactivity will be tested in a systematic and predictable way. This may result in a powerful predictive tool for accurately estimating the influence of complex subsurface chemistries on silica reactivity and durability.

Keywords: Reactivity of Amorphous Sio_2 Phases, Solute Matrix, Quartz Kinetics, Sio_2 Glass, Kinetics, Reactivity of Crystalline Phases, Dissolution Kinetics

300. **RADIATION EFFECTS IN NUCLEAR WASTE MATERIALS**
$80,000
DOE Contact: Dr. Gordon Roesler, (202) 586-3231
PNNL Contact: Dr. William J. Weber, (509) 375-2299

This project is intended to develop a fundamental understanding of the atomic, microscopic, and macroscopic levels of radiation effects in glass and ceramics that will improve performance assessments of glass and ceramic waste forms for the immobilization and disposal of various radioactive wastes. Studies focus on the effects of ionization and elastic-collision interactions on defect production, defect interactions, structural rearrangements, diffusion, solid-state phase transformations, and gas accumulation using actinide containing materials, gamma irradiation, ion-beam irradiation and electron-beam irradiation to simulate the effects of alpha decay and beta decay on nuclear waste glasses and ceramics. A number of irradiation facilities and capabilities will be used, including user facilities at several national laboratories, to study in situ the effects of irradiation under different conditions.

Keywords: Nuclear Waste Materials, Ionization, Elastic Collision, Irradiation

301. **RADIATION EFFECTS ON MATERIALS IN THE NEAR-FIELD OF NUCLEAR WASTE REPOSITORY**
$408,000
DOE Contact: Dr. Gordon Roesler, (202) 586-3231
University of New Mexico Contact: Dr. Lu-Min Wang, (505) 277-7536

Many DOE wastes are ultimately slated for disposal in a geologic repository. Demonstrated containment of radionuclides in the near-field can greatly reduce the complexity of the performance assessment analysis of such a repository. Near-field containment of radionuclides depends critically on the behavior of these materials in a radiation field. This project involves a systematic study of elastic and inelastic damage effects in materials in the near-field. These include: (1) waste forms (glass and crystalline ceramics); (2) alteration products of waste forms; (3) back-fill materials (clays and zeolites). Materials selected are those whose durability or chemical behavior can potentially have a major effect on the retention of radionuclides (e.g., monazite as a waste form; smectite clays in back-fill), but for which there is very little previous systematic study.

Keywords: Radiation Effects, Nuclear Waste Repository, Waste Forms, Alteration Products, Backfill

OFFICE OF TECHNOLOGY SYSTEMS

The Office of Technology Systems is investigating various types of cement and polymer technology for stabilization and containment of wastes. The applicability of these substances is being demonstrated, tested and evaluated for implementation at specific sites. Technology development and demonstrations into glasses and ceramics are being pursued to better understand high-temperature technologies, useful for containment of contaminated soils. Vitrification and plasma technologies are being developed for treating specific mixed waste streams. OST will continue to fund these materials research projects, as well as others, to provide the basis for other applied research in the Technology Development Program.

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

302. **FIXED HEARTH PLASMA TREATMENT PROCESS**
$4,076,000
DOE Field Office Contact: Julie Conner, (208) 526-0648
DOE HQ Contact: Caroline Purdy, (301) 903-7672
Idaho Contact: Steve Bates, (208) 526-6790
EM Focus Area: Mixed Waste Characterization, Treatment and Disposal

This technology, the Plasma Hearth Process (PHP), converts entire drums of low-level mixed waste (LLMW) directly into an enhanced waste form without extensive pretreatment or characterization. Organics are destroyed while metals and inorganics are melted, creating a vitrified slag and molten metal. The process is characterized by high-efficiency destruction of organics, encapsulation of heavy metals and radionuclides in the vitrified final waste form, large volume reduction of waste to be disposed, possible recycling of metals, low off-gas flow rates, and the capability of processing many waste types in a single-step process. The non-radioactive proof-of-principle concept demonstration has been completed. The remaining work in this task focuses on design, fabrication, and demonstration of a near full-scale pilot system for non-radioactive operation.

Keywords: Plasma, Vitreous Slag, Final Form, Low-level Mixed Waste, Pilot-scale

303. **HIGH TEMPERATURE DEMONSTRATIONS ON ACTUAL MIXED WASTE**
$716,000
DOE Field Office Contact: Julie Conner, (208) 526-0648
DOE HQ Contact: Caroline Purdy, (301) 903-7672
Savannah River Contact: Ray Schumacher, (803) 725-5306
EM Focus Area: Mixed Waste Characterization, Treatment and Disposal

This project investigated innovative methods of vitrification that provide higher temperature processing capabilities. High temperature processing is desirable where there is insufficient fluxing agents available within the wastes. Higher temperatures however, can also increase volatilization which is undesirable. Methods of vitrification under consideration include induction, plasma, and high temperature joule heating.

Keywords: Vitrification, High Temperature, Plasma, Induction

304. **FIXED HEARTH PLASMA RADIOACTIVE WASTE TEST**
$3,864,000
DOE Field Office Contact: Julie Conner, (208) 526-0648
DOE HQ Contact: Caroline Purdy, (301) 903-7672
ANL-West Field Contact: Carla Dwight, (208) 533-7651
EM Focus Area: Mixed Waste Characterization, Treatment and Disposal

This project involves the design and construction of the facility modifications to house the bench-scale Plasma Hearth Process to be tested in the Plasma Hearth Process Radioactive Waste Test - Idaho. It also includes tasks to develop the mechanisms by which actual waste can be repackaged for testing in the bench-scale system, the radioactive waste forms produced by the process can be sampled and analyzed, and the pertinent analysis to be made to ensure safe operation of the plasma system in the ANL-West TREAT facility. Waste operations and sampling and analysis during the bench-scale demonstration are covered in the task.

Keywords: Plasma, Vitreous Slag, Final Form, Low-level Mixed Waste, Bench-scale

305. **PHOSPHATE-BONDED CERAMIC WASTE FORMS**
$450,000
DOE Field Office Contact: Julie Conner, (208) 526-0648
DOE HQ Contact: Caroline Purdy, (301) 903-7672
Argonne National Laboratory Contact: Arun Wagh, (708) 252-4295
EM Focus Area: Mixed Waste Characterization, Treatment and Disposal

Chemically-bonded ceramics (CBCs) are being investigated as an alternative final waste form for streams that cannot be handled by other established methods. Phosphate bonded ceramics are a subclass of CBCs and have several advantages over other systems for stabilization and encapsulation of LLMW. These include insolubility in water, high-temperature stability, and the ability to cure at room temperatures. Studies are underway to stabilize waste streams containing liquid mercury, mercury-contaminated aqueous liquids, toxic and heavy metal containing materials, salt cakes, beryllium wastes, and pyrophorics by encapsulating them in phosphate-bonded ceramics. A closely related study investigated the effectiveness of using harmonic compaction as a process modification for certain types of waste.

Keywords: Alternate Final Waste Form, Ceramics, Phosphate

306. **KINETIC MIXER DEMONSTRATION**
$150,000
DOE Field Office Contact: Julie Conner, (208) 526-0648
DOE HQ Contact: Caroline Purdy, (301) 903-7672
BNL Contact: Paul Kalb, (516) 282-7644
EM Focus Area: Mixed Waste Characterization, Treatment and Disposal

This project involves the testing of a commercially available mixer for the enhancement of microencapsulating mixed waste in polyethylene. This work expands on earlier work at BNL, and is expected to be used in conjunction with the macroencapsulation of mixed waste debris in a commercial facility in Utah. The process blends the waste to be microencapsulated with polyethylene while driving off water and volatile organics. Both surrogate and actual mixed waste streams were tested.

Keywords: Mixed Low-Level Waste, Kinetic Mixing, Final Form, Polyethylene, Microencapsulation, Macroencapsulation

307. **STAINLESS STEEL BENEFICIAL REUSE**
$600,000
DOE Field Office Contact: Paul Hart, (304) 285-4358
DOE HQ Contact: Jerry M. Hyde, (301) 903-7914
WSRC, SRS Principle Investigator: Bill Boettinger, (803) 725-4833
EM Focus Area: Decontamination & Decommissioning

The Stainless Steel Beneficial Reuse project involves participation of private industry to melt 304 stainless steel radioactive scrap metal (RMS), and then to fabricate the recycled metal into storage containers. The containers will include 100 cubic foot boxes, 55 gallon drums, 85 gallon overpacks, and other specialized items. The metal to be recycled primarily resides at the Savannah River Site (SRS), but the intent is to include other sites' RMS in the future. The SRS metals originate from process water heat exchanger components, primary piping, handling equipment, and duct work. All metals selected will meet the Department of Transportation requirement of low-specific activity (LSA) for transportation to the selected subcontractors. Two subcontractors, Manufacturing Sciences Corporation and Carolina Metals, Inc., participated in a full scale demonstration in FY 1995 and delivered the first complete products, 100 cubic foot boxes, in August. The SRS has already implemented the boxes for temporary storage of waste.

Keywords: Stainless Steel, Recycle, Storage, Containers

308. **RECYCLE OF DEPLETED URANIUM STUDIES**
$430,000
DOE Field Office Contact: Paul Hart, (304) 285-4358
DOE HQ Contact: Carl R. Cooley, (301) 903-7276
INEL Principle Investigator: W. J. Quapp, (208) 526-9443
EM Focus Area: Decontamination & Decommissioning

The primary objective of this project is to perform an initial assessment of the feasibility and economic incentives of alternative management options for storing, recycling, and/or disposing of the large depleted uranium (DU) reserves within the DOE Complex. As an alternative to disposal, a concept for converting depleted uranium into concrete shielding material has been developed. Laboratory work continues to improve pellet densities, and preparation for fabrication of depleted uranium DUROCK samples using UO3 from SRS was initiated, and leach testing of DUCRETE samples was also initiated.

Keywords: Depleted Uranium, DUROCK, DUCRETE, Shielding

309. **REUSE OF CONCRETE FROM CONTAMINATED STRUCTURE**
$231,000
DOE Field Office Contact: Paul Hart, (304) 285-4358
DOE HQ Contact: Carl R. Cooley, (301) 903-7276
Vanderbilt University Principle Investigator: Dr. Frank Parker, (615) 343-2371
EM Focus Area: Decontamination & Decommissioning

This study will examine the economic, risk, legal, and social implications of reusing/recycling radiologically contaminated concrete from the DOE complex. Current decontamination and decommissioning (D&D) practices within the DOE entail decontamination of concrete surfaces, disposing of the decontamination waste streams, demolishing the structure, and disposing of the concrete rubble and rebar at a construction and demolition landfill.

This practice is not only expensive but places a severe burden on ever diminishing land disposal capacity. Additionally, failure to utilize the decontaminated aggregate requires the production, and accompanying environmental degradation, of virgin materials. This study will examine potential for recycling concrete under various scenarios representing the possible paths.

Keywords: Radioactive Waste, Decontamination, Recycling

310. **SURFACE ACOUSTIC WAVE ARRAY DETECTORS**
$248,000
DOE Field Contact: Roger Christensen
(509) 372-4035
DOE HQ Contact: Caroline Purdy,
(301) 903-7672
PNNL Contact: Jay W. Grate,
(509) 375-4547

The purpose of this task is to design, develop and demonstrate array sensor systems for sensing volatile organic compounds (VOCs), including chlorinated hydrocarbons and other vapors of interest with regard to environmental cleanup and occupational safety. These sensor arrays will be based on polymer-coated surface acoustic wave (SAW) vapor sensors and data processing using pattern recognition and chemometric techniques. The advantages of the SAW vapor sensor technology include the rugged planar design of the devices; the suitability of polymer-coated devices for use in arrays with pattern recognition; the fast response times (seconds); rapidly reversible responses-the selective material is not altered by the vapor; the high vapor sensitivities (ppm to ppb detection limits depending on the particular vapor); and the flexibility of the array approach to be adapted to many detection problems. The analyte or analytes to be detected can be changed merely by the selection of the polymer coating and the pattern recognition algorithm used. The combination of the information from the sensor array with modern chemometric data processing techniques creates an intelligent sensor system. The sensor array approach provides greatly increased selectivity and reliability in field environments over a single sensor. Single sensors cannot determine if an interfering species is present that might invalidate the measurement. SAW sensors are more sensitive than other microsensors such as fiber optic devices.

Keywords: Array Sensor, Volatile Organic Compounds, Surface Acoustic Wave

311. **VERSATILE, ROBUST, MINIATURE SIZED AND REAL-TIME RADIATION DETECTOR**
$250,000
DOE Field Contact: Richard C. Baker
(708) 252-2647
DOE HQ Contact: Caroline Purdy,
(301) 903-7672
BNL Contact: Eng-Kie Souw,
(516) 282-5407

The objective for this project is to develop a miniature, real-time solid-state sensor capable of detecting alpha particles, beta particles and gamma rays. The project has applicability for rapidly scanning surface soils, waste processing streams and facility walls, floors and equipment for D&D. Although diamond is an ideal detector due to its physical hardness and chemical inertness, its low stopping power makes it suitable for detecting alphas, low energy betas and X-rays. For higher energy betas and gamma rays, stacked layers of cadmium telluride will be developed for the detector. For FY95 the objective is to design, develop and test carbon vapor deposited (CVD) diamond films for use on p-type intrinsic metal diamond nuclear detectors. The project is joint with Northrup-Grumman Corp. and the New Jersey Institute of Technology.

Keywords: Sensor, Alpha Particles, Beta Particles, Gamma Rays

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

312. **FIXED HEARTH PLASMA RADIOACTIVE WASTE TEST**
$3,864,000
DOE Field Office Contact: Julie Conner,
(208) 526-0648
DOE HQ Contact: Caroline Purdy,
(301) 903-7672
ANL-West Field Contact: Carla Dwight,
(208) 533-7651
EM Focus Area: Mixed Waste Characterization, Treatment and Disposal

This project involves the design and construction of the facility modifications to house the bench-scale Plasma Hearth Process to be tested in the Plasma Hearth Process Radioactive Waste Test - Idaho. It also includes tasks to develop the mechanisms by which actual waste can be repackaged for testing in the bench-scale system, the radioactive waste forms produced by the process can be sampled and analyzed, and the pertinent analysis to be made to ensure safe operation of the plasma system in the ANL-W TREAT facility. Waste operations and sampling and analysis during the bench-scale demonstration are covered in the task.

Keywords: Plasma, Vitreous Slag, Final Form, Low-Level Mixed Waste, Bench-Scale

313. **PHOSPHATE-BONDED CERAMIC WASTE FORMS**
$450,000
DOE Field Office Contact: Julie Conner, (208) 526-0648
DOE HQ Contact: Caroline Purdy, (301) 903-7672
Argonne National Laboratory Contact: Arun Wagh, (708) 252-4295
EM Focus Area: Mixed Waste Characterization, Treatment and Disposal

Chemically-bonded ceramics (CBCs) are being investigated as an alternative final waste form for streams that cannot be handled by other established methods. Phosphate bonded ceramics are a subclass of CBCs and have several advantages over other systems for stabilization and encapsulation of LLMW. These include insolubility in water, high-temperature stability, and the ability to cure at room temperatures. Studies are underway to stabilize waste streams containing liquid mercury, mercury-contaminated aqueous liquids, toxic and heavy metal containing materials, salt cakes, beryllium wastes, and pyrophorics by encapsulating them in phosphate-bonded ceramics. A closely related study investigated the effectiveness of using harmonic compaction as a process modification for certain types of waste.

Keywords: Alternate Final Waste Form, Ceramic, Phosphate

314. **KINETIC MIXER DEMONSTRATION**
$150,000
DOE Field Office Contact: Julie Conner, (208) 526-0648
DOE HQ Contact: Caroline Purdy, (301) 903-7672
BNL Contact: Paul Kalb, (516) 282-7644
EM Focus Area: Mixed Waste Characterization, Treatment and Disposal

This project involves the testing of a commercially available mixer for the enhancement of microencapsulating mixed waste in polyethylene. This work expands on earlier work at BNL, and is expected to be used in conjunction with the macroencapsulation of mixed waste debris in a commercial facility in Utah. The process blends the waste to be microencapsulated with polyethylene while driving off water and volatile organics. Both surrogate and actual mixed waste streams were tested.

Keywords: Mixed Low-Level Waste, Kinetic Mixing, Final Form, Polyethylene, Microencapsulation, Macroencapsulation

315. **CESIUM REMOVAL DEMONSTRATION**
$1,500,000
DOE Field Office Contact: J. O. Moore, (423) 576-3536
DOE HQ Contact: Dave Geiser, (301) 903-7688
ORNL Contact: Phil McGinnis, (423) 576-6845
EM Focus Area: Radioactive Tank Waste Remediation

All tank sites require Cs removal before processing the LLW immobilization to meet NRC acceptance criteria, cut radiation exposure to personnel and the environment, and reduce the volume of High Level Waste processed for glass formulation. Much work has been done on selecting technologies to do this, and the concept needs to be demonstrated on a full scale using real waste. ORNL has selected a crystalline silico-titanate (CST) as the material for cesium removal. The demonstration has been designed, fabricated, and will be operated during the first quarter of fiscal year 1997. The plan is to treat 25,000 gallons of Melton Valley Storage Tank Waste at ORNL. The system will then be transferred to Waste Operations at ORNL and the results reported to the Tank Focus Area. This project chooses sorbents studied in the ORNL hot cell tests to.

Keywords: Separations, Cesium, High Level Waste, CST

316. **GROUT AND GLASS WASTE FORMS**
$900,000
DOE Field Office Contact: W. LaVeille, (803) 725-7663
DOE HQ Contact: Dave Geiser, (301) 903-7688
ORNL Contact: John Harbor, (803) 725-8725
EM Focus Area: Radioactive Tank Waste Remediation

Disposal of low activity tank wastes is being approached very differently at individual DOE sites, and, in some cases, even within a single site. Application of a consistent approach would lead to reduced direct costs and technical uncertainties. In addition, a consistent approach across the DOE complex would also provide a straighter path through the regulatory maze, speeding the cleanup effort. Oak Ridge operations office is currently planning to perform a CERCLA treatability study to reduce the technical and cost uncertainties associated with tank remediation. The CERCLA study will focus on tank heel characterization and removal. Immobilization of the material will provide an ideal means to gain information which can be used across the DOE system to judge the suitability of glass and grout as the waste

Keywords: Immobilization, Grout, Glass

317. **T_c QUALIFICATION STUDIES**
$225,000
DOE Field Office Contact: J. A. Frey, (509) 372-4564
DOE HQ Contact: Dave Geiser, (301) 903-7688
PNNL Contact: D. Kurath, (509) 376-6752
EM Focus Area: Radioactive Tank Waste Remediation

In order to meet NRC Class A requirements for the low level waste form at Hanford, technetium must be removed from the liquid portion(supernate) of tank waste inventory prior to immobilization. During fiscal year 1997, this task will perform small scale batch tests with various ion exchange media (sorbents) which are designed to remove pertechnetate. This will give an estimate of pertechnetate concentration within the tank waste inventory. For supernates with a high technetium concentration and high percentage of pertechnetate, column tests with appropriate pertechnetate sorbents will be conducted.

Keywords: Separations, Technetium, Pertechnetate

318. **VITREOUS CERAMIC COMPOSITIONAL ENVELOPE STUDY**
$100,000
DOE Lead Office Contact: Jim Wright (803) 725-5608
DOE HQ Contact: Skip Chamberlain (301) 903-7248
ANL Contact: Dave Wronkiewicz, (630) 252-7362
EM Focus Area: Subsurface Contaminants

The objective of this program is to utilize tailored slag waste forms to expand the range of waste streams that can be treated using the Minimum Additive Waste Stabilization (MAWS) approach. Compositional ranges appropriate to the production of tailored slag waste forms will be identified for these waste streams. These studies will complement the composition envelopes being studied for glass waste forms.

Keywords: Composition, Characterization, MAWS

319. **GRAPHITE DC PLASMA ARC MELTER**
$2,109,000
DOE Lead Area Contact: Jim Wright, (803) 725-5608
DOE HQ Contact: Skip Chamberlain, (301) 903-7248
LIMIT Contact: Bill Bonner, (509) 372-6263
EM Focus Area: Subsurface Contaminants

The objective of this program is to demonstrate the applicability of the Graphite DC Plasma Arc Melter for treating mixed wastes and contaminated soils and for providing an extremely durable waste form for disposal. An engineering scale, radioactive capable furnace system has been installed and tested at Pacific Northwest Laboratory with radioactive waste. This furnace includes analytical instruments for making spatially resolved measurements of furnace and glass temperatures and for the on-line measurements of exhaust emissions, both in the furnace chamber and the offgas. The capacity of the system will be optimized through the use of process diagnostics. A larger pilot-scale melter has been constructed at Massachusetts Institute of Technology with a greater throughput capacity. It is undergoing testing with a microwave plasma analyzer to monitor plutonium in the offgas stream. Two series of tests have been completed on radioactive materials, providing fate data on transuranic species. An engineering scale system has been started and operated, and tests are underway on the fate of species contained in mixed waste.

Keywords: Graphite, DC, Plasma, Arc, Melter, Plasma Analyzer, Plutonium, Offgas, Mixed Waste

320. **CRYSTALLINE SILICOTITANATE FOR Cs/Sr REMOVAL**
$400,000
DOE Field Office Contact: Dennis Alona, (505) 845-4296
DOE HQ Contact: Kurt Gerdes, (301) 903-7289
SNL Contact: Maher Tadros, (505) 845-8930

The U.S. Department of Energy is faced with safely treating and disposing millions of gallons of Liquid Radioactive Waste stored in High Level Waste tanks across the United States. Only a small amount of radioactive material contributes to the millions of gallons of High Level waste. By removing the radioactive components from the waste, a large volume reduction of waste to be solidified is achieved. A separations program has been established to accomplish this task. A crystalline silicotitanate ion exchange material (IONSIV® IE-911) has been developed by SNL and Texas A&M University. The material is being manufactured by UOP for engineering scale processing. This material has been selected as the ion exchanger to process 25,000 gallons of tank waste at ORNL.

Keywords: Ion Exchange, Separations, High Level Waste

321. **TUCS/PHOSPHATE IMMOBILIZATION OF ACTINIDES**
$300,000
DOE Field Office Contact: Richard C. Baker, (708) 252-2647
DOE HQ Contact: Kurt Gerdes, (301) 903-7289
Argonne Contact: Ken Nash, (708) 252-3581

The U.S. Department of Energy facilities face the challenge of restoring facilities following years of radioactive materials processing. Various DOE sites have contaminated soil that needs remediation. The Thermally Unstable Complexants (TUCS) to sequester and immobilize actinides in soil by mineralization as phosphates technology is being developed and evaluated. This process will enhance DOE's ability to restore sites contaminated with radioactive constituents.

Keywords: Subsurface Contamination, Soil, Immobilization, Restoration

322. **TEST SORBENTS: INDUSTRIAL CONTRACTS**
$2,050,000
DOE Field Office Contact: Maria C. Vargas, (509) 372-4994
DOE HQ Contact: Kurt Gerdes, (301) 903-7289
PNNL Contact: Garret Brown, (509) 373-0165

The U.S. Department of Energy is faced with safely treating and disposing millions of gallons of Liquid Radioactive Waste found in various waste streams throughout the DOE Complex. Only a small amount of radioactive material contributes to the millions of gallons of waste. By removing the radioactive components from the waste, a large volume reduction of waste to be solidified is achieved. A separations program has been established to accomplish this task. PNNL, 3M, and IBC Advanced Technologies have teamed to provide a web technology that successfully removes these contaminants. Molecular recognition agents engineered into flow-through membranes have been developed for selective removal of cesium, strontium, and technetium from aqueous wastes. The agents provided by IBC Advanced Technologies are attached to 3M Empore™ membranes and have been demonstrated on a variety of DOE waste streams. A commercially available Process Absorber Development Unit (PADU) has been successfully used at INEL Test Area North, Hanford's N-Spring, and Hanford's N-Basin.

Keywords: PADU, 3M, IBC Advanced Technologies, Membrane

OFFICE OF NUCLEAR ENERGY, SCIENCE AND TECHNOLOGY

	FY 1996
Office of Nuclear Energy, Science and Technology - Grand Total	$51,830,000
Office of Engineering and Technology Development	$ 1,830,000
Space and National Security Programs	$ 1,830,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 1,250,000
Development of an Improved Process for the Manufacture of DOP-26 Iridium Alloy Blanks, Product Characterization and Exploratory Alloy Improvement Studies	910,000
Carbon-Bonded Carbon Fiber Insulation Production Maintenance, Manufacturing Process Development and Product Characterization	340,000
Materials Properties, Behavior, Characterization or Testing	$ 580,000
Development of Materials for Advanced Radioisotope Power Systems	340,000
T-111 Tantalum Alloy Characterization for Use as a Sealed Isotope Heat Source Capsule	240,000
Office of Naval Reactors	$50,000,000[1]

[1]This excludes $45 million for the cost of irradiation testing in the Advanced Test Reactor (ATR).

OFFICE OF NUCLEAR ENERGY, SCIENCE AND TECHNOLOGY

OFFICE OF ENGINEERING AND TECHNOLOGY DEVELOPMENT

SPACE AND NATIONAL SECURITY PROGRAMS

Space and National Security Programs include the development and production of radioisotope power systems for both space and terrestrial applications and the technical direction, planning, demonstration and delivery of nuclear reactor power and propulsion systems for military and civilian space missions and for special military terrestrial applications. All materials programs were designed to support the production of General Purpose Heat Source-Radioisotope Thermoelectric Generators for the NASA Cassini Mission and preliminary scoping studies for support of the future Pluto Express and other future NASA missions. Thus applied materials research programs are supported in the areas of thermoelectric materials and devices, advanced energy conversion systems, high temperature heat source materials, materials systems compatibility and safety related materials characterization and testing.

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

323. **DEVELOPMENT OF AN IMPROVED PROCESS FOR THE MANUFACTURE OF DOP-26 IRIDIUM ALLOY BLANKS, PRODUCT CHARACTERIZATION AND EXPLORATORY ALLOY IMPROVEMENT STUDIES**
$910,000
DOE Contact: W. Barnett, (301) 903-3097
ORNL Contacts: E. P. George, (615) 574-5085 and E. K. Ohriner, (615), 574-8519

An iridium alloy, DOP-26 (i.e., Ir-0.3 wt.% W with Th and Al dopant additions), serves as the fuel clad or capsule material for isotope heat sources employed in recent and contemporary space power systems for NASA deep space missions. This program is aimed at the optimization of the new improved process route previously selected for the production of DOP-26 iridium alloy sheet, namely a consumable vacuum arc cast/extrusion/"warm" rolling route. The effectiveness of this production process was further demonstrated in the FY1996 production of DOP-26 alloy blanks, foil and clad vent sets for the Cassini Mission. Production yields have continued to exceed our goals.

Continued progress was made in the preparation for introducing bare rolling into the sheet production process.

Studies of bare rolling of blank stock and bare forming of cups were continued with very promising results. It is anticipated that bare rolling elimination of molybdenum cover plates will be adopted as a production process in FY 1997.

Continued product characterization studies, particularly for simulated service conditions, continued to show behaviors equivalent or superior to the prior process product.

Studies of alternate iridium alloy doping agents were continued. The objective is to maintain or exceed the properties of the DOP-26 alloy at a significantly lower thorium dopant level. An iridium alloy containing 0.3 wt.%W with dopant additions of 40 appm cerium and 15 appm thorium was selected for scale-up. A 5KG ingot of this composition has been consumable arc melted, extruded and processing to sheet was initiated. This work will be continued in FY 1997.

Keywords: Consumable Arc Melt, Extrusion, Noble Metal

324. **CARBON-BONDED CARBON FIBER INSULATION PRODUCTION MAINTENANCE, MANUFACTURING PROCESS DEVELOPMENT AND PRODUCT CHARACTERIZATION**
$340,000
DOE Contact: W. Barnett, (301) 903-3097
ORNL Contacts: C. E. Weaver and R. Dunwiddie, (615) 574-9978

Carbon-bonded carbon fiber (CBCF) type thermal insulation material is employed in Isotopic General Purpose Heat Source (GPHS) Module assemblies for use in current GPHS-RTG (radioisotope thermoelectric generator). This material was originally employed in GPHS-R7Gs for the Galileo/NASA (1989 launch) and Ulysses/NASA-ESA (1990 launch) Missions. Material produced for the Cassini Mission (1997 launch) was made with a replacement carbon fiber (new vendor, former source not available) utilizing an optimized process and process controls. The FY 1996 program encompassed (1) maintenance of capability for both tube and plate billet production through the year, and (2) characterization of Cassini CBCF insulation thermal conductivity.

Particular attention was focused on evaluation of the effects of short-term very high temperature short-time exposures on thermal conductivity. Equations were developed which express thermal conductivity as a function of temperature and peak exposure temperature and time.

Keywords: Insulators/Thermal, High Temperature Service, Fibers

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

325. **DEVELOPMENT OF MATERIALS FOR ADVANCED RADIOISOTOPE POWER SYSTEMS**
$340,000
DOE Contact: W. Barnett, (301) 903-3097
Iowa State University, Ames Laboratory
Contact: B. Cook, (515) 294-9673

The objectives of this activity are: (1) evaluate the potential of new thermoelectric materials, (2) develop and characterize rare earth based selective emitters for potential thermophotovoltaic systems application, provide support in the areas of materials compatibility and transport.

Particular attention was focused on: (1) analytical studies of impurities transport during 238-Plutonia fuel processing to a pellet and during service, and (2) alumina carbon interactions in the electrical heat source employed in the processing of thermoelectric converters for the NASA Cassini mission.

Particular attention was continued to be focused on the evaluation of the effects of short-term (typically 1 to 20 seconds) very high temperature exposure (typically in the range of 2000°C to 3000°C). Equations which express thermal conductivity of CBCF insulation as a function of temperature and peak exposure temperatures and time were updated. Production maintenance capability was demonstrated by the production of flight quality plate and billet stock.

Evaluation of Ti-Ni-Sn and ZnO type thermoelectric materials were initiated. Equipment for high temperature optical emission characterization of candidate rare earth based selective emitters for potential use in thermophotovoltaic power systems was procured and following integration with a high temperature vacuum system will proceed through the start-up/calibration phase.

Keywords: Thermoelectrics, Thermophotovoltaics, Thermal Transport

326. **T-111 TANTALUM ALLOY CHARACTERIZATION FOR USE AS A SEALED ISOTOPE HEAT SOURCE CAPSULE**
$240,000
DOE Contact: W. Barnett, (301) 903-3097
Oak Ridge National Laboratory Contact:
D. DiStefano, (423) 574-4452

High temperature isothermal constant pressure test of two production T-111 welded capsules was completed. Creep rupture tests on base metal and welded samples of the T-111 material were conducted at temperature spanning the temperature range of 580° to 1100°C. Tests at 580°C, 680°C and 800°C are continuing using a more sensitive technique for strain measurement.

Keywords: Refractory Alloy, Creep Rupture, Tests

OFFICE OF NAVAL REACTORS

The materials program supports the development and operation of improved and longer life reactors and pressurized water reactor plants for naval nuclear propulsion.

The objective of the materials program is to develop and apply, in operating service, materials capable of use under the high power density and long life conditions required of naval ship propulsion systems. This work includes irradiation testing of reactor fuel, poison, and cladding materials in the Advanced Test Reactor at the Idaho National Engineering Laboratory. This testing and associated examination and design analysis demonstrates the performance characteristics of existing materials as well as defining the operating limits for new materials.

Corrosion, mechanical property, and wear testing is also conducted on reactor plant structural materials under both primary reactor and secondary steam plant conditions to confirm the acceptability of these materials for the ship life. This testing is conducted primarily at two Government laboratories—Bettis Atomic Power Laboratory in Pittsburgh and Knolls Atomic Power Laboratory in Schenectady, New York.

One result of the work on reactor plant structural material is the issuance of specifications defining the processing and final product requirements for materials used in naval propulsion plants. These specifications also cover the areas of welding and nondestructive testing.

Funding for this materials program is incorporated in naval projects jointly funded by the Department of Defense and the Department of Energy. This funding amounts to approximately $95 million in FY1996 including approximately $45 million as the cost for irradiation testing in the Advanced Test Reactor. The Naval Reactors contact is David I. Curtis, (703) 603-5565.

OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT

	FY 1996
Office of Civilian Radioactive Waste Management - Grand Total	$9,600,000
Materials Properties, Behavior, Characterization or Testing	$9,600,000
Waste Packages	$9,600,000

OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT

Materials research is ongoing in the Office of Civilian Radioactive Waste Management in the development of waste packages for eventual geologic disposal.

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OF TESTING

327. **WASTE PACKAGES**
$9,600,00
DOE Contact: David Haught (702) 794-5474
M&O Contacts: Hugh Benton,
(702) 295-4389 and David Stahl,
(702) 295-4383

The development of the nation's high-level waste repository has been delegated to DOE's Yucca Mountain Site Charactization Project Office. Framatome Cogema Fuels (formerly B&W Fuel Company), as part of the Civilian Radioactive Waste Management System Management & Operating (M&O) Contractor, is responsible for designing the waste package and related portions of the engineered barrier system. The advanced conceptual design was completed in 1996. Progress on the waste package and the supporting materials studies has been documented in various reports.

The waste package design effort includes the development of waste packages to accommodate uncanistered commercial spent nuclear fuel (SNF), canistered SNF, canistered defense high-level waste, Navy fuel, and other DOE owned spent nuclear fuel. The analytical process that is underway to support these designs included thermal, structural, and neutronic analyses. Also included are materials selection and engineering development. The waste package materials effort includes the testing and modeling of materials being considered for inclusion in the waste package and the engineered barrier system. The testing includes general aqueous and atmospheric testing, localized attack such as pitting and service corrosion, microbiologically-influenced corrosion, galvanic corrosion, and stress corrosion cracking. The corrosion test facility started the long-term (at least five-year) test program in FY 1996 with corrosion-allowance materials. Corrosion-resistant materials will be added in FY 1997. Waste form materials are also being evaluated for alteration and leaching under repository-relevant conditions. Chemical simulations have been performed to evaluate the performance of engineered barrier materials. These latter efforts support both design and performance assessment.

Keywords: Yucca Mountain Repository, Waste Package, Engineered Barrier System

OFFICE OF DEFENSE PROGRAMS

	FY 1996
Office of Defense Programs - Grand Total	$108,694,000
The Weapons Research, Development and Test Program	$108,694,000
Sandia National Laboratories	$ 64,697,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	
Fastcast	1,300,000
Ceramic Powder Process Modeling	130,000
New Optoelectronic and Photonic Materials	90,000
Diamond-Reinforced Composites	60,000
Phosphors for Flat-Panel Displays	280,000
New Materials and Processing Concepts for Tires	925,000
Thermal-Spray Deposited Coatings for Corrosion and Wear-Resistance	435,000
Laser Spraying	150,000
Engineered Monodisperse Porous Materials	331,200
Chemical Functional of Oligosilanes: Economically Attractive Routes to New Photoresponsive Materials	412,700
PbO-Free Composites for Low Temperature Packaging	299,000
Synthesis and Processing of High Strength SiC Foams: A Radically New Approach to Ceramic-Ceramic Composite Materials	385,000
Carbon Nanotube Composites	356,000
Nanocomposite Materials Based on Hydrocarbon-Bridged Siloxanes	440,000
New Adhesive Systems Based on Functionalized Block Copolymers	239,000
Synthesis and Modeling of Field-Structured Anistropic Composites	350,000
Nanocavity Effects on Misfit Accommodation in Semiconductors	293,000
Sol-gel Preservation of Mankind's Cultural Heritage in Objects Constructed of Stone	375,000
Tailorable, Visible, Room-Temperature Light Emission from Si, Ge and Si-Ge Nanoclusters	379,000
In Situ Optical Flux Monitoring for Precise Control of Thin Film Deposition	552,000
Molecular-Scale Lubricants for Micromachine Applications	400,000
Ultra-Hard Multilayer Coatings	449,000
Wide-Bandgap Compound Semiconductors to Enable Novel Semiconductor Devices	256,000
Photonic Band Gap Structures as a Gateway to Nano-Photonics	350,300
Power Sources	650,000
Casting Product Realization	450,000
Advanced Materials for High Performance Microelectronics	947,000
Ceramics Research Foundation	1,189,000
Polymeric Materials Research	2,050,000
Microelectronics and Photonics Materials	550,000
Gas and Solid Source MBE for High Performance Devices	250,000
DoD/DOE MOU	2,552,000
NIS Lab-to-Lab Interactions	1,000,000
Cooperative Measures Program	3,850,000
NIS Industrial Partnering Program	1,825,000
Development of Antimonide Based Semiconductors	600,000
High Temperature Underhood Electronics	341,000
Advanced Precursors and Chemistries for MOVPE	1,050,000

OFFICE OF DEFENSE PROGRAMS (continued)

	FY 1996
The Weapons Research, Development and Test Program (continued)	
Sandia National Laboratories (continued)	
Materials Structure and Composition	
Process Models for Aluminum Alloys	183,000
Adaptive Scanning Probe Microscopies	297,000
Extending the Applicability of Cluster-Based Pattern Recognition with Efficient Approximation Techniques	110,000
Smart Interface Bonding Alloys (SIBA): Tailoring Thin Film Mechanical Properties	432,900
Recognizing Atoms in Atomicallly-Engineered Nanostructures: An Interdisciplinary Approach	400,000
Artificial Atoms	336,000
Modeling and Characterization of Molecular Structures in Self Assembled and Langmuir-Blodgett Films	110,000
Semiconductor Physics	1,450,000
Nanostructures, Advanced Materials and Ion Beam Sciences	2,800,000
Materials Properties, Behavior, Characterization or Testing	
Lead-Free Solders	150,000
Welding Technology for Specialty Alloy AerMet 100	100,000
Welding Metallurgy for Austenitic Superalloys and Advanced Titanium-Base Alloys	232,000
Welding and Processing of an Advanced Titanium Alloy	160,000
Model Determination and Validation for Reactive Wetting Processes	351,000
In Situ Determination of Composition and Strain During MBE Using Electron Beams	295,000
Understanding and Control of Energy Transfer Mechanisms in Optical Ceramics	400,000
Physico-Chemical Stability of Solid Surfaces	397,000
AT-400 Surveillance	373,000
Metals	1,800,000
Materials Aging and Reliability	1,477,000
Materials Stability and Thin Coatings	2,400,000
Predictive Stewardship	2,600,000
Weapon Aging Characterization	2,500,000
NCMS High Temperature Solders - Alternatives to Lead-Based Solders	114,000
Device or Component Fabrication, Behavior or Testing	
Advanced Printed Wiring Board Technologies	450,000
Joining Silicon Nitride to Metals	491,000
Demonstration of Molecular-Based Transistors	330,500
Atomic-Scale Measurement of Liquid Metal Wetting and Flow	374,000
Modeling Electrodeposition for Metal Microdevice Fabrication	255,000
Surface-Micromachined Flexural Plate Wave Device Integrated on Silicon	500,000
Scanning Probe-Based Processes for Nanometer-Scale Device Fabrication	454,000
AT-400A Pit Container	3,470,000
MC4300	400,000
Smartprocesses	1,533,000
Materials and Process Design for Reliability	1,000,000
Applications-Driven Interdisciplinary Reserach	880,000

OFFICE OF DEFENSE PROGRAMS (continued)

	FY 1996
The Weapons Research, Development and Test Program (continued)	
Sandia National Laboratories (continued)	
Device or Component Fabrication, Behavior or Testing (continued)	
Repetitive PP-High Power Semiconductor Switch Research	499,000
Advanced Packaging	750,000
Advanced Lithography	1,000,000
IPP/SCT - Microwave Components	320,000
Phosphor Support Program for Field Emission Displays	343,000
Instrumentation and Facilities	
Intelligent Systems for Induction Hardening	350,000
Specialty Metals Processing Consortium	1,700,000
Catalytic Membrane Sensors	343,900
Integrated Thin Film Structures for IR Imaging	410,200
Molecular Imprinting in Aerogels for Remote Sensing of Chemical Weapons and Pesticides	366,300
Antipodal Focusing of Shock Energy from Large Asteriod Impacts on Earth	161,000
Biocavity Laser Microscopy/Spectroscopy of Cells	380,000
A New Paradigm for Near Real-Time Downhole Data Acquisition	
UV Spectroscopic Detection and Identification of Pathogens	100,000
Novel Laser-Based Diagnostics Capability for Chemical Science	150,000
Advanced Analytical Methods	1,058,000
Field Emission Source with Phosphor Screen	269,000
Lawrence Livermore National Laboratory	$16,970,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$4,675,000
Engineered Nanostructure Laminates	2,000,000
Sol Gel Coatings	335,000
KDP Growth Development	900,000
Vicarious Nucleophilic Substitution Chemistry	350,000[1]
CHEETAH Thermochemical Code	190,000[1]
Explosives Development	900,000[1]
Materials Properties, Behavior, Characterization or Testing	$1,260,000
Interfaces, Adhesion, and Bonding	460,000
Laser Damage: Modeling and Characterization	400,000
KDP Characterization	400,000

[1]This activity is jointly funded (50:50) by DOE DP and the DoD.

OFFICE OF DEFENSE PROGRAMS (continued)

	FY 1996
The Weapons Research, Development and Test Program (continued)	
Lawrence Livermore National Laboratory (continued)	
Instrumentation and Facilities	$11,035,000
Scanning Tunneling Microscopy (STM) and Atomic Force Microscopy (AFM)	250,000
Fatigue of Metal Matrix Composites	500,000
Materials Produced with Dynamic High Pressure	400,000
Properties of Hydrogen at High Shock Pressures and Temperatures	300,000
Atomic Level Explosive Calculations	400,000
Metastable Solid-Phase High Energy Density Materials	535,000
AFM Investigations of Crystal Growth	210,000
Superplastic Forming of Stainless Steel Automotive Components	150,000
Formability and Joining Analysis for Superplastic Panel Design	360,000
Microstructural Evolution in Welds	330,000
Uranium Casting Program	1,000,000
Uranium Spin Forming	1,500,000
Plutonium Near Net Shape Casting	2,500,000
Electron Beam Cold Hearth Melting of Uranium	900,000
NIF Capsule Mandrel R&D	600,000
Polyimide Coating Technology for ICF Targets	500,000
Berryllium Ablator Coatings for NIF Targets	600,000
Los Alamos National Laboratory	$27,027,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 5,055,000
Actinide Processing Development	1,350,000
Plutonium Oxide Reduction	150,000
Low Density Microcellular Plastic Foams	200,000
Physical Vapor Deposition and Surface Analysis	300,000
Chemical Vapor Deposition (CVD) Coatings	150,000
Polymers and Adhesives	430,000
Tritiated Materials	175,000
Salt Fabrication	800,000
Slip Casting of Ceramics	300,000
Plasma-Flame Spraying Technology	300,000
Rapid Solidification Technology	500,000
Bulk Ceramic Processing	250,000
Synthesis of Ceramic Coatings	150,000
Materials Structure or Composition	$ 1,237,000
Actinide Surface Properties	700,000
Neutron Diffraction of Pu and Pu Alloys and Other Actinides	237,000
Surface, Material and Analytical Studies	300,000
Materials Properties, Behavior, Characterization or Testing	$ 2,500,000
Mechanical Properties of Plutonium and Its Alloys	450,000
Phase Transformations in Pu and Pu Alloys	450,000
Plutonium Shock Deformation	350,000
Non-Destructive Evaluation	550,000
Powder Characterization	50,000
Shock Deformation in Actinide Materials	300,000
Dynamic Mechanical Properties of Weapons Materials	350,000

OFFICE OF DEFENSE PROGRAMS (continued)

	FY 1996
Los Alamos National Laboratory (continued)	
Device or Component Fabrication, Behavior or Testing	$ 3,900,000
Target Fabrication	1,500,000
Filament Winder	100,000
High Energy Density Welding in Hazardous Environments	800,000
Uranium Scrap Conversion and Recovery	1,500,000
Laboratory Directed Research and Development	$10,802,000
Electronically Correlated Materials at Ambient and Extreme Conditions	328,000
Organometallic Chemical Vapor Deposition	248,000
Polymer Sorbents for Hazardous Metal Uptake	164,000
Microscopic Materials Modeling: Textures and Dynamics	109,000
Surface Modification of Materials	315,000
Integration of Fundamental Knowledge in Plasticity and Textures to Provide Technical Tools for Microscopic Applications	290,000
High Resolution Electron Microscopy of Materials	350,000
Nano-Fabrication	255,000
Thin Film Micro-Electrochemical Sensor Development	210,000
Liquid Crystal Thermosets	200,000
Neutron and Resonant X-ray Scattering by Materials	350,000
Structural and Electronic Competitions in Low-Dimensional Materials	360,000
Fundamental Aspects of Photoelectron Spectroscopy in Highly Correlated Electronic Systems	300,000
Development of High Strength High Conductivity Materials for High Magnetic Field Devices	100,000
Low Temperature STM for Structural and Spectroscopic Studies of High Temperature Superconductors and Other Electronic Materials	50,000
Materials with Fine Microstructures	365,000
Ion Beam Materials Research	330,000
Texture Studies of Highly Deformed Composite Materials	192,000
Pressure Dependency of the Structure of High Explosives: Nitromethane	192,000
Neutron Reflection Studies of Thin Film and Multilayer Structures	300,000
Neutron Reflectivity Studies of In Situ Corrosion of Metal Surfaces	145,000
The Dynamics of Amorphous Materials	330,000
Advanced Material Science Algorithms for Supercomputer Architectures	75,000
Metal Vapor Synthesis in Organometallic Chemistry	235,000
Separation Chemistry of Toxic Metals	250,000
Polymers for Integrated Optical Interconnects	266,000
High Temperature Materials Synthesis Without Heat:Oxide Layer Growth on Electronic Materials Using High Kinetic Energy Atomic Species	164,000
Dynamic Deformation of Advanced Materials	855,000
Strain Measurements in Individual Phases of Multi-Phase Materials	130,000
Artificially Structured Nonlinear Optic and Electro-Optic Materials	465,000
Structural Phase Transitions in Non-Stoichiometric Oxides	275,000
Strongly Correlated Electronic Materials	495,000
Plasma Immersion Ion Implantation for Semiconductor Film Growth	261,000
Analysis of Structure and Orientation of Adsorbed Polymer in Solution Subject to Dynamic Shear Stress	172,000
Development of Pair Distribution Function Analysis of Mesostructural Details in Single Crystal Perovskites and Nanocrystalline Materials	170,000
Neutron Scattering as a Probe of the Structure of Liquid Crystal Polymer-Reinforced Composite Materials	180,000

OFFICE OF DEFENSE PROGRAMS (continued)

	FY 1996
Los Alamos National Laboratory (continued)	
Laboratory Directed Research and Development (continued)	
Strain Measurements in Individual Phases of Multi-Phased Materials During Thermomechanical Loading: LANSCE Neutron Scattering Experiment Support	318,000
A New Approach to Texture Measurements: ODF Determination by Rietveld Refinement	73,000
Applications of Fullerenes in Nuclear Technology	360,000
Ceramic Oxide Foams for Separation	400,000
Materials Modeling Project	125,000
Synthesis and Optical Characterization of Novel Fullerene-Based Composites	50,000
Technology Transfer Initiative	$ 3,533,000
A Pilot Program: Chemical Vapor Deposition of Diamond in a Fluidized-Bed for Cutting Tool and Tribological Applications	250,000
Advanced Beryllium Processing	632,000
Automated Pulsed Laser Deposition System	130,000
Plasma Source Ion Implantation for the Automotive Industry	1,326,000
Processing Modeling and Control for U.S. Steel Industry	1,195,000

OFFICE OF DEFENSE PROGRAMS

Summaries of materials activities which were selected to present the diversity of materials research, development and application projects conducted for the Office of the Assistant Secretary for Defense Programs are included in this section. Activities are organized in groupings that indicate the Defense Program Laboratory at which the specific project was performed. Funds for FY96 materials activities within Defense Programs were provided by the Weapons Research, Development and Test program including the Core Research and Development program and the Technology Transfer Initiative program and by the Inertial Confinement Fusion program, the Production and Surveillance program, and Laboratory Research and Development program. Projects with proprietary, patentable, or classified information were not reported.

THE WEAPONS RESEARCH, DEVELOPMENT AND TEST PROGRAM

SANDIA NATIONAL LABORATORIES

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

328. **FASTCAST**
$1,300,000
DOE Contact: Bob Dewitt, (301) 903-3311, (301) 903-3311
SNL Contact: Dave Larson, (505) 843-4165

Sandia National Laboratories and FASTCAST Consortium, Inc. will develop technologies of near-term application that improve the quality and reduce the cost of investment casting production. This agreement will serve as master terms and conditions for multiple cooperative research projects entered into between Sandia and FASTCAST through individual Project Task Statements as research projects are identified. The agreement provides a means for transferring Sandia's expertise and capabilities applicable to investment casting to consortium members, thereby offering them a commercial advantage in the international investment casting market.

Keywords: Investment Casting, FASTCAST

329. **CERAMIC POWDER PROCESS MODELING**
$130,000
DOE Contact: Bob Dewitt, (301) 903-3311
SNL Contact: Dave Larson, (505) 843-4165

Sandia National Laboratories and AACCMCI, Inc., a subdivision of the Association of American Ceramic Component Manufacturers (AACCM), are working together to develop and apply advanced computer modeling techniques for advanced materials processing to enhance capabilities in manufacturing ceramic components. The AACCM had identified forming, binder burnout, and sintering as three areas in ceramics manufacturing where improved understanding and process control will contribute to improved product quality can be improved significantly by identifying and exercising careful control over these critical manufacturing processes and process parameters. Computer process models can provide this insight. Los Alamos National Laboratory will also participate.

Keywords: Ceramics, Powder Processing

330. **NEW OPTOELECTRONIC AND PHOTONIC MATERIALS**
$90,000
DOE Contact: Bob Dewitt, (301) 903-3311
SNL Contact: Dave Larson, (505) 843-4165

Sandia and Amoco Chemical Company are developing new materials and processes for optoelectronic and photonic materials, resulting in a prototype, commercial-quality, optoelectronic materials process. The project joins Sandia's experience in developing nonlinear optical materials with Amoco's experience in developing and commercializing polyimide technology for the microelectronics industry and other industries, as well as expertise in passive wave-guide technology. The goal is to produce new materials and processes for marketable, competitive integrated optoelectronic and photonic devices for the microelectronics industry.

Keywords: Optoelectronics, Photonic

331. **DIAMOND-REINFORCED COMPOSITES**
$60,000
DOE Contact: Bob Dewitt, (301) 903-3311
SNL Contact: Dave Larson, (505) 843-4165

Sandia National Laboratories is working with Du Pont (E. I. Du Pont de Numours & Company) to develop technology and manufacturing capability for diamond-reinforced composites to produce materials with superior strength and improved thermal property. The three-way partnership of Du Pont, Sandia, and Los Alamos National Laboratory see improved plasma sources, gas recipes, and reactor designs for industrial production of diamond-film-reinforced polymers and composites.

Keywords: Diamond, Composites

332. **PHOSPHORS FOR FLAT-PANEL DISPLAYS**
$280,000
DOE Contact: Bob Dewitt, (301) 903-3311
SNL Contact: Dave Larson, (505) 843-4165

Sandia National Laboratories and Coloray Display Corporation are working together to identify and/or synthesize low voltage phosphors suitable for flat-panel displays. The cathode ray tubes (CRTs) used on most personal computers and televisions can use relatively high voltages to obtain the desired display luminance and color balance. The disadvantage of CRTs is their bulkiness. Field emission displays (FEDs) used for flat panel displays (such as laptop computers) have the advantages of thinner panels and greater portability but must use lower voltages, which affects the brightness, definition, and color of the display. This project aims to find or create improved phosphors for FED function. Applications for this project include any communication medium that needs visual display, including aircraft instrumentation. Other participants are FED Corporation, SI Diamond Technology, and Silicon Video Corporation.

Keywords: Phosphors, CRTs, FEDs

333. **NEW MATERIALS AND PROCESSING CONCEPTS FOR TIRES**
$925,000
DOE Contact: Bob Dewitt, (301) 903-3311
SNL Contact: Dave Larson, (505) 843-4165

Sandia National Laboratories and The Goodyear Rubber & Tire Company will develop new materials and processing concepts for tires that will improve tire performance, including economy, cost, traction, and safety. The partners are investigating foam technology to enable vehicles to run on punctured tires. Improved elastomers can decrease tire weight and rolling resistance, which translates into fuel savings and longer tire life. Extending a tire's lifetime reduce recycling and landfill needs. Using synthetic materials also decreases rubber consumption.

Keywords: Tires, Rubber

334. **THERMAL-SPRAY DEPOSITED COATINGS FOR CORROSION- AND WEAR-RESISTANCE**
$435,000
DOE Contact: Bob Dewitt, (301) 903-3311
SNL Contact: Dave Larson, (505) 843-4165

Sandia National Laboratories and General Motors Corporation are developing thermal spray-deposited bore coatings for corrosion- and wear-resistant cylinder walls in aluminum automotive engine blocks. Sandia has experience with a wire arc plasma coating device and with thermal spray process and materials development. In addition Sandia's Thermal Spray Research Lab and Engineering Sciences Center have special experimental capabilities and theoretical modeling expertise. General Motors has produced thermal spray coatings on aluminum engine cylinder bores, tested them, and identified technical issues that must be resolved to assure reliable high-volume production of sprayed cylinder bores. The new technology will include enhanced process quality and reliability achieved through improvements in the design of prototype spray equipment, especially the design of an air cap; and increased material deposition rate to enhance production throughput and decrease costs; and the development of a comprehensive theoretical model for gas dynamics, energy transfer, and particle dynamics in the high-velocity oxy-fuel fore coating process.

Keywords: Coatings, Thermal Spray, Corrosion

335. **LASER SPRAYING**
$150,000
DOE Contact: Bob Dewitt, (301) 903-3311
SNL Contact: Dave Larson, (505) 843-4165

Sandia National Laboratories and Pratt Whitney, a division of United Technologies, are developing a new laser coating and joining technology known as laser spraying to deposit metals and ceramics onto a variety of substrates and weld joints. The development of this technology will benefit U.S. industry by allowing expansion to new markets, reductions in operating costs, and wear-resistant coating that enables a broader use of lightweight components. The project combines the laser-process diagnostics, laser/material interaction and laser joining expertise of Sandia National Laboratories with United Technologies expertise in laser spraying process development. The intent of the project is to improve wear and corrosion resistance of components in critical locations in gas turbine and space engines.

Keywords: Laser, Coating, Joining

336. **ENGINEERED MONODISPERSE POROUS MATERIALS**
$331,200
DOE Contact: M. J. Katz, (202) 586-5799
SNL Contact: Chuck E. Meyers, (505) 844-3459

Porous materials are available with pore sizes ranging from 1s to 100s of microns and beyond. Beyond 15 it becomes difficult to obtain complete control over pore size, size distribution, ordering, and pore architecture. We are using the novel properties of block copolymers to create monodisperse, controllable, ordered porous materials spanning the mesoporous range (20-500). Block copolymers consist of homopolymers chemically attached at their ends. These polymers want to phase separate from each other by are limited by the chemical attachment. The result is well-ordered, monodisperse, meso-size domains of one polymer surrounded by the other. We are making block copolymers where one phase can be crosslinked and the other can be chemically or thermally removed. This would give the desired controllable mesoporous materials. Block copolymer phase separation also gives a variety of architectures, including spherical, cylindrical, tetrahedral, and lamellar. These will lead to unique mesoporous architectures. In conjunction with the synthesis of these materials, we are modeling our block copolymers systems using Density Functional Theory, which can predict architecture based on chemical and physical aspects of the block copolymer. The synthetic technique being used is called Ring-Opening Metathesis Polymerization, and gives us tremendous control over polymer chain length, block ratios, and chemical composition. This control leads directly to control of the pore size and architecture. We are characterizing our polymers with Gel Permeation Chromatography, SAXS, SANS, TEM, and Gas Adsorption, all of which have shown the presence of a block copolymer system that leads to phase separated morphologies, and ultimately to mesoporous materials.

Keywords: Porous Materials, Block Copolymers

337. **CHEMICAL FUNCTIONAL OF OLIGOSILANES: ECONOMICALLY ATTRACTIVE ROUTES TO NEW PHOTORESPONSIVE MATERIALS**
$412,700
DOE Contact: M. J. Katz, (202) 586-5799
SNL Contact: Chuck E. Meyers, (505) 844-3459

Polysilanes, [Si(R)(RŌ)]n, are saturated macro-molecules whose unusual electronic absorption behavior closely resembles those of conjugated polyenes. They are not commercially viable as photointeractive materials, as current production (restricted to Japan) involves a very hazardous and unreliable synthetic approach. Low molecular weight oligosilanes can be formed under mild conditions, with reactive silane (Si-H) residues. We propose to utilize these oligo(hydrido)silanes as versatile precursors to a wide variety of new photo-active materials. Computer aided molecular design (CAMD) will be employed to select rational synthetic targets for oligosilane elaboration. Chemical modification at the Si-H bond will access numerous new oligosilanes and permit development of a wide variety of hybrid polymeric systems with novel polymer architectures; applications may include photoactive elastomers, thermoplastics and sensor materials, graft/block copolymers, LED display devices and controlled porosity thin films, fibers and monolithic bodies.

Keywords: Polysilanes, Molecular Design

338. **PbO-FREE COMPOSITES FOR LOW TEMPERATURE PACKAGING**
$299,000
DOE Contact: M. J. Katz, (202) 586-5799
SNL Contact: Chuck E. Meyers, (505) 844-3459

We will develop new inorganic sealing materials that will have the requisite thermal and chemical properties to replace PbO-solder glasses currently used in a variety of low temperature packaging applications. These new materials include PbO-free glasses that we have successfully sealed at temperatures as low as 525°C and composites of low temperature, chemically stable glasses and low expansion, chemically compatible ceramics. Composites will be designed with thermal contraction coefficients between 70 and 100 x 10^{-7}/Degrees Celsius and seal temperatures below 450°C so that they can replace PbO-solder glasses used to seal flat panel displays, alumina sensor packages, and other hermetic packages.

Keywords: Composites, Scaling

339. **SYNTHESIS AND PROCESSING OF HIGH STRENGTH SiC FOAMS: A RADICALLY NEW APPROACH TO CERAMIC-CERAMIC COMPOSITE MATERIALS**
$385,000
DOE Contact: M. J. Katz, (202) 586-5799
SNL Contact: Chuck E. Meyers, (505) 844-3459

Prohibitively high processing costs due to restricted fiber preform connectivity have kept silicon carbide, SiC, composites from entering mass commercial markets despite their favorable strength to weight ratio and oxidative stability. Our novel approach will bypass expensive fiber processing steps by providing a 3D interconnected network of struts having open connectivity to all pores. We have developed several routes to synthesize and process the SiC foams. We will explore whether incorporation of nucleation sites in the foams during pyrolysis can induce crystallinity of the SiC resulting in increased strength. A variety of characterization techniques are performed on the resulting new and unique materials.

Keywords: SiC, Foams, Ceramics, Composite

340. **CARBON NANOTUBE COMPOSITES**
$356,000
DOE Contact: M. J. Katz, (202) 586-5799
SNL Contact: Chuck E. Meyers, (505) 844-3459

Carbon fiber composites are important advanced materials because of their exceptional mechanical properties (high strength to weight ratios) and electromagnetic properties (EM shielding). We propose to investigate carbon fiber composites in which the carbon fibers are 1000 times smaller than the currently used micron-sized PAN or pitch derived fibers. This revolutionary decrease in the size of the fibers is expected to lead to materials with unique mechanical, and especially unique electromagnetic properties. These properties derive from: (1) the size of the fiber, which increases the fiber surface area to volume (or weight) ratio and (2) the unusual, high curvature of the fiber surface that increases its reactivity.

We propose to use carbon "fibrils" ($35/pound—less expensive than PAN fiber!) and related new specialty carbon fibrils (obtained through nondisclosure agreements already in place), to modify the surfaces of these fibrils, and to prepare composites and test their mechanical and electromagnetic properties.

Keywords: Carbon Nanotube, Composite

341. **NANOCOMPOSITE MATERIALS BASED ON HYDROCARBON-BRIDGED SILOXANES**
$440,000
DOE Contact: M. J. Katz, (202) 586-5799
SNL Contact: Chuck E. Meyers, (505) 844-3459

Silicones are attractive for general elastomer applications because of their safety and their performance over a wide temperature range. However, polydimethylsiloxane (PDMS) is inherently weak due to its low glass transition temperature (Tg) and lack of stress crystallization. The major goal of this project is to create a family of reinforced elastomers based on silsesquioxane/PDMS networks. By achieving this goal we will not only produce materials which are suitable for a variety of applications, but also have the potential of establishing a new manufacturing technology for the U.S. silicone industry based on an in situ reinforcement method. This study will allow novel composite materials with applications in encapsulant, coating and moldmaking technologies for military and commercial use to be prepared and fully characterized.

Keywords: Nanocomposite, Siloxane

342. **NEW ADHESIVE SYSTEMS BASED ON FUNCTIONALIZED BLOCK COPOLYMERS**
$239,000
DOE Contact: M. J. Katz, (202) 586-5799
SNL Contact: Chuck E. Meyers, (505) 844-3459

The need to control and optimize the properties of polymer/solid interfaces is critical in a host of technologies. Often the adhesive strength of the interface, the resistance to moisture, and the ability to transfer stress through the interface are critical to the overall performance of the product. We propose to design and test new adhesive systems based on block copolymers, where one block (A) attaches to the surface while the second block (B) is compatible with and bonds to the polymeric matrix. An important advantage of block copolymers is that the B block can easily be made long enough to span the weak region of 10-100 nm and form a strong interlock with the matrix. We believe that these systems will lead to improved adhesion, more systematic design of the interphase region, and a decreased dependence on mechanical roughness and the environmentally unfriendly processes which are currently required.

Keywords: Adhesive, Block Copolymers

343. **SYNTHESIS AND MODELING OF FIELD-STRUCTURED ANISTROPIC COMPOSITES**
$350,000
DOE Contact: M. J. Katz, (202) 586-5799
SNL Contact: Chuck E. Meyers, (505) 844-3459

We propose to develop the 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 linear field will create one-dimensional particle chains. But we have recently discovered that rotating fields create two-dimensional particle sheets in the plane of the field. These unique structures will be captured by polymerizing the continuous phase during a field anneal. A key aspect of this program will be modeling and controlling the evolution of structure in these materials. For example, chains aggregate into columns because of attractive interactions generated by one-dimensional transverse and longitudinal fluctuations. Computer simulations indicate that in an electric field columns have a circular cross section, whereas in a magnetic field columns have a curtain-like structure, the difference being attributable to strong image dipoles in the electric field case. The sheet-like structures created in a rotating field are considerably more complex; very little is known about their detailed structure or interactions between sheets.

We are in a position to create novel anisotropic nanocomposite materials. The potential utility of these materials is great, with obvious applications as structural materials; anisotropic heat, current, and magnetic flux conductors; high dielectric constant materials for capacitors etc. Our approach can be applied to a variety of systems, so we feel that tailorable, field-structured nanocomposites could become an important new nanotechnology.

Keywords: Composite, Polymer, Metal

344. **NANOCAVITY EFFECTS ON MISFIT ACCOMMODATION IN SEMICONDUCTORS**
$293,000
DOE Contact: M. J. Katz, (202) 586-5799
SNL Contact: Chuck E. Meyers, (505) 844-3459

We are mechanistically exploring the use of nanometer-scale cavities to influence strain relaxation and associated dislocation behavior in heteroepitaxial semiconductor structures. This is a novel approach to the growth of strain-relaxed epitaxial layers with few threading defects on lattice-mismatched substrates, a long-standing and technologically important objective that has yet to be achieved in a generally satisfactory way. The central challenge is the control of dislocations, which beneficially accommodate lattice misfit between substrate and overlayer but are detrimental when they thread into the overlayer and remain there. Introducing nanocavities into the interfacial region is expected to alter lattice relaxation and dislocation behavior substantially through a variety of effects, including (1) enhanced dislocation nucleation, (2) strong attractive forces between dislocations and cavities, and (3) reduction of dislocation line energies. We have two broad objectives: first, to understand these effects at a mechanistic level, and, second, to manipulate them to maximize relaxation while minimizing dislocation threading into the epitaxial layer.

Keywords: Semiconductor, Nanoscale

345. **SOL-GEL PRESERVATION OF MANKIND'S CULTURAL HERITAGE IN OBJECTS CONSTRUCTED OF STONE**
$375,000
DOE Contact: M. J. Katz, (202) 586-5799
SNL Contact: Chuck E. Meyers, (505) 844-3459

Our cultural heritage, as reflected in artifacts and works of art, is being lost at an astonishing rate due to the ravages of nature and especially mankind. Since the industrial revolution, chemical by-products of man's technological advances have caused the deterioration of our most precious cultural treasures. Most vulnerable are stone objects that are subjected to outdoor environments in industrialized or urban settings. The combination of acid rain, salt crystallization, and freezing and thawing of ice have disfigured sculpture to unrecognizable states and have led to the widespread and costly problem of erosion of buildings and other architectural works. Although moderately effective conservation treatments exist for sandstones (silicates), no proven system has been developed for limestones (carbonates). Our approach to preserve these objects incorporates mineral-specific sol-gel methodologies designed to both passivate the rock against new chemical and physical degradation and to strengthen or consolidate the existing weathered state to arrest granular disintegration. Our research comprises three basic elements: (1) molecular modeling of the weathering mechanisms and resultant surface structure of model limestones, (2) mineral-specific passivation of the weathered surface to prevent further hydrolytic attack, and (3) *in situ* polymerization (within the weathered surface) to form a UV stable network that imparts strength and hydrophobicity. This research has been conducted in collaboration with The Metropolitan Museum of Art (MMA) and The Getty Conservation Institute (GCI), who have provided samples and ensured relevance to the conservation communities. In addition to solving the urgent need to preserve our cultural treasures, the methodology developed here can be applied to other mineral-corrosion problems such as the degradation of concrete infrastructure, environmental contamination by leached mine tailings, protection of ship hulls, and scale formation in petroleum wells.

Keywords: Sol Gel, Preservation

346. **TAILORABLE, VISIBLE, ROOM-TEMPERATURE LIGHT EMISSION FROM Si, Ge AND Si-Ge NANOCLUSTERS**
$379,000
DOE Contact: M. J. Katz, (202) 586-5799
SNL Contact: Chuck E. Meyers, (505) 844-3459

Although its outstanding properties are the key to modern microelectronics technology, silicon (Si) has a major drawback as a semiconductor: its indirect bandgap prevents it from emitting light efficiently. The goal of modifying Si to achieve intense, tailorable visible light emission at room temperature is one of the most important current challenges in materials science. Realization of this goal, which would have an enormous technological impact, requires a practical synthesis approach and understanding of the physics involved. Size-selected nanoclusters represent the best hope for the foreseeable future, but the tried cluster synthesis techniques are inadequate.

We have recently developed and patented a novel synthesis method based on using inverse micelles as reaction vessels to produce useful quantities of size selected clusters from different classes of materials. We propose to use this method to produce the first size-selected Si and germanium (Ge) nanoclusters, to study and understand the size dependence and mechanisms for their expected intense, tailorable room temperature photoluminescence and to assess their technological potential. A unique feature of our synthesis method is the ability to produce mixed or composite clusters. We shall capitalize on this feature to produce and study both Si/Ge alloy clusters and composite clusters consisting of a shell of Ge over Si or vice versa. These clusters will be truly novel and could have unusual and useful properties.

Keywords: Nanoclusters, Silicon, Germanium

347. **IN SITU OPTICAL FLUX MONITORING FOR PRECISE CONTROL OF THIN FILM DEPOSITION**
$552,000
DOE Contact: M. J. Katz, (202) 586-5799
SNL Contact: Chuck E. Meyers,
(505) 844-3459

We propose to lay the foundation for a Sandia led program in in situ sensors for materials processing science by developing a new, quantitative laser-based monitor of atomic and molecular reactants used in thin film vacuum deposition processes called optical flux monitoring (OFM). Our goal is to demonstrate precise real-time control of thickness and composition of multilayer materials fabricated by one such process: molecular beam epitaxy (MBE). The OFM will measure beam densities and velocities with chemical specificity near the substrate surface and discriminate incident from desorbing or background species using fluorescence or absorption detection methods. This program will develop robust coherent sources of tunable UV and visible radiation with the necessary amplitude and spectral characteristics to make quantitative in situ measurements of atomic beam densities in real time. We will optimize the OFM sensitivity for this deposition process to explore detection of atoms at dopant concentrations. We will also demonstrate proof of concept OFM for molecular species.

Keywords: Optical Flux Monitor, Thin Film, Deposition

348. **MOLECULAR-SCALE LUBRICANTS FOR MICROMACHINE APPLICATIONS**
$400,000
DOE Contact: M. J. Katz, (202) 586-5799
SNL Contact: Chuck E. Meyers,
(505) 844-3459

Friction- and wear-related failures have been identified as key issues for advanced micromachine devices such as micro-actuators. While unlubricated micromachines have demonstrated significant lifetimes, we must be able to improve the lifetimes against catastrophic friction and wear. Since the physical and chemical interactions that control friction are more significant and complex at micromachine dimensions than they are for large-scale machines, the purpose of this proposal is to develop the physics and chemistry base for designing molecular-scale lubricants for micromachine applications. We will acquire this new knowledge by combining capabilities for 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 on new micromachine test structures specifically designed for these studies. With Interfacial Force Microscopy (IFM), we will explore the role of molecular size, chemical end group, and chain structures on the lubricating properties of self-assembling monolayer (SAM) films in model and real-world lubrication studies. In addition to the SAM films, we will also explore the lubricating properties of extremely thin films that are assembled from nanoclusters of traditional sliding-plane lubricants, such as MoS_2. We will use these systems to explore the lubricating properties as a function of cluster size and film thickness. We will extend the application of IFM by incorporating near-field optical capabilities (SNOM). This unique combination will provide a completely new capability to correlate the mechanical response of the lubricating film with a direct optical signature of the lubricating film structure. We can either use fluorescence emission from the MoS_2 nanocrystals or emission from dilute concentrations of "guest" chromophores in SAMs to monitor local changes in the lubricating film structure as a function of mechanical contact conditions. This approach will provide the first ever simultaneous correlation between film structure and dynamic mechanical response. Our measurements will form a very important link for molecular dynamics calculations (simulations). The calculations will provide the key to interpreting the molecular level behavior of our experimental lubricant systems. Finally, we will apply these surface treatments to actual micromachined devices. In addition to evaluating the effect of these surface treatments on the operating lifetime of these devices, we will study the interaction of our SNOM/IFM probe tip with actual moving parts of micromachines. This information will provide a direct connection between our model lubrication studies, molecular dynamics calculations, and the operating performance of these extremely small devices. This research project will provide the physics- and chemistry-based rules that can be used to design and fabricate micromachine-based components that are reliable and have a long life span.

Keywords: Molecular, Lubricant, Micromachine

349. **ULTRA-HARD MULTILAYER COATINGS**
$449,000
DOE Contact: M. J. Katz, (202) 586-5799
SNL Contact: Chuck E. Meyers, (505) 844-3459

We propose to explore production of ceramic multilayer structures that are potentially harder than any natural or artificial material. Experiment indicates 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 mainly due 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.

This project seeks to identify and grow the most likely materials for ultra-hard multilayers. We will develop a fundamental experimental and theoretical understanding of the interfacial interactions between layers of these materials and the larger scale mechanical properties. The technological impact of this work is broad and exciting—unsurpassed performance for protective coatings, cutting tools, etc. We are poised to embark on the synthesis and understanding of the mechanical properties of a new class of ultrahard materials.

Keywords: Ultra-Hard, Ceramics, Multilayer

350. **WIDE-BANDGAP COMPOUND SEMICONDUCTORS TO ENABLE NOVEL SEMICONDUCTOR DEVICES**
$256,000
DOE Contact: M. J. Katz, (202) 586-5799
SNL Contact: Chuck E. Meyers, (505) 844-3459

We propose 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 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 two important areas in the development of these materials. A portion of the effort will concentrate on understanding the growth of III-N materials by gas-source molecular beam epitaxy (GSMBE). We will investigate the effects of substrate preparation, substrate temperature, V/III ratio, and growth rate on the nucleation and growth of AlGaInN on 6H-SiC (000(1) surfaces using in-situ reflection high-energy electron diffraction (RHEED), reflection mass spectroscopy (REMS), and scanning tunneling microscopy (STM). In combination with efforts to study crystal growth processes in these materials, we will also investigate 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 which will include an exact treatment of Coulomb effects. Steady state and time-resolved luminescence will be performed to evaluate the nature of defect states in these materials as well as to study the excitonic properties which are expected to be enhanced for wide-bandgap semiconductors. Magnetoluminescence experiments will be performed to determine energy dispersion and effective masses and these results will be directly compared with bandstructure calculations. A final aspect of our proposal is an evaluation of how various processing techniques which 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.

Keywords: Semiconductor, Wide Bandgap

351. **PHOTONIC BAND GAP STRUCTURES AS A GATEWAY TO NANO-PHOTONICS**
$350,300
DOE Contact: M. J. Katz, (202) 586-5799
SNL Contact: Chuck E. Meyers, (505) 844-3459

The goal of this LDRD proposal is to explore the fundamental physics of a new class of photonic materials, photonic band gap structures (PBG), and to exploit its unique properties for the design and implementation of photonic devices on a nano-meter 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, >105, for optoelectronic applications and for the exploration of novel photonic physics, such as photonic localization, tunneling and modification of spontaneous emission rate. Moreover, the photonic bandgap 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. The PBG materials offer many unique features: We propose in this project to: (1) build and test PBG devices in the mm-wave regime because sample fabrication is much easier in this frequency range while the underlying physics is essentially the same for all frequencies; (2) design and fabricate micro-cavities on semiconductor substrates in visible and infrared regime using the study in (1) as a foundation and (2) to design a new scheme for probing the nano-meter scale micro-cavities utilizing built-in LED light sources. Such an internal LED would overcome many difficulties associated with the microscopic light focusing and also greatly relax the process requirements for nano-fabrication.

Keywords: Photonics, Nanoscale

352. **POWER SOURCES**
$650,000
DOE Contact: Edwin E. Ives, (202) 586-4879
SNL Contact: Daniel Doughty, (505) 845-8105

Develop state-of-the-art carbon anode for lithium ion rechargeable batteries and demonstrate its performance by a prototype that demonstrates performance and manufacturability. Provide fundamental electrochemical understanding of voltage delay and self-discharge kinetics to permit precise lifetime projections for Li/Thionyl Chloride Batteries. Collaborate with domestic Li/Thionyl Chloride producers to transfer our fundamental understanding of this system, enabling them to enter the growing market of high reliability, long life Li/Thionyl Chloride Batteries.

Keywords: Carbon, Anode, Li Battery

353. **CASTING PRODUCT REALIZATION**
$450,000
DOE Contact: Bob Dewitt, (301) 903-3311
SNL Contact: Michael C. Maguire, (505) 845-3105

Incorporation of science-based modeling into casting simulation to speed product and process delivery times. Developing different pattern materials and fabrication methods in rapid prototyping and optimizing investment shell materials for use with rapid prototyping patterns. Developing improved materials for tooling production for medium lot size builds of castings (i.e. 10 to 100 parts). Demonstration of titanium investment casting capability in the new Investment Casting Addition.

Keywords: Casting, Fabrication, Rapid Manufacturing

354. **ADVANCED MATERIALS FOR HIGH PERFORMANCE MICROELECTRONICS**
$947,000
DOE Contact: Bob Dewitt, (301) 903-3311
SNL Contact: S. T. Picraux, (505) 844-7681

Develop advanced Si-based microelectronics employing strained alloys to enhance performance and delay scaling requirements. This aggressively collaborative effort brings together a range of elements including: (1) epitaxial growth science (CVD and MBE), (2) advanced thin film structural and electronic-properties characterization tools such as X-ray analysis, ion scattering, photoluminescence, C-V analysis, (3) low temperature gate oxide processes such as HIPOX, RPCVD, and ECR-plasma deposition, (4) extensive device modeling for transport and parameter sensitivity analysis, and (5) state of the art pilot-line short-channel device fabrication. Evaluate performance gains and manufacturability of strain-enhanced integrated structures.

Keywords: Silicon, Thin Films, Microelectronics

355. **CERAMICS RESEARCH FOUNDATION**
$1,189,000
DOE Contact: Bob Dewitt, (301) 903-3311
SNL Contact: Duane Dimos, (505) 844-6385

This project supports sub-projects on electronic ceramics and covalent ceramic films. The electronic ceramic sub-projects are to: (1) develop chemistries to fabricate new dielectric/ferroelectric films (7001.400), (2) understand the role of stress in ferroic thin films (7001.600), (3) understand the role of defects in electronic ceramics (7001.900), and (4) develop a new class of photosensitive thin films for optical devices (7001.800). The covalent ceramics sub-projects are (1) to enhance the understanding of covalent ceramics film fabrication (7001.100), (2) to achieve enhanced properties in covalent ceramic films by tailoring microstructure (7001.200), and (3) to develop covalent ceramic films for sensors and displays (7001.300).

Keywords: Ceramics, Electronics

356. **POLYMERIC MATERIALS RESEARCH**
$2,050,000
DOE Contact: Bob Dewitt, (301) 903-3311
SNL Contact: Jill Hruby, (510) 294-2596

The project consists of multiple sub-projects to address mid- and long-term needs for national security programs in the area of polymeric materials. Projects are grouped into topical areas which include: porous and microporous materials, adhesives and blends, encapsulant materials, and photoresists.

Keywords: Polymer, Adhesives, Photoresists, Porous

357. **MICROELECTRONICS AND PHOTONICS MATERIALS**
$550,000
DOE Contact: Bob Dewitt, (301) 903-3311
SNL Contact: Jeffrey Y. Tsao, (505) 844-7092

This project entails the development of semiconductor materials and heterostructures for discrete and integrated microelectronic and photonic devices and systems. These band-gap and refractive-index engineered materials and heterostructures are foundational to the microelectronic and photonic technologies that will replace present-day optical, electronic, electro-mechanical and mechanical components. They will enable a new generation of intelligent, reliable and affordable weapons and stockpile technologies.

Keywords: Photonics, Microelectronics, Heterostructures

358. **GAS AND SOLID SOURCE MBE FOR HIGH PERFORMANCE DEVICES**
$250,000
DOE Contact: Bob Dewitt, (301) 903-3311
SNL Contact: Jeffrey Y. Tsao, (505) 844-7092

This project will establish a unique and powerful gas and solid source molecular beam epitaxy (GSS-MBE) capability at Sandia and will apply it to a new generation of heterostructure-based communications and sensor systems.

Keywords: MBE, Heterostructures

359. **DoD/DOE MOU**
$2,552,000
DOE Contact: Edwin E. Ives, (202) 586-4879
SNL Contact: John T. Hitchcock, (505) 844-2340

The DoD and the DOE intend to fund jointly and support a stable level of effort at the DOE weapons laboratories on applied research and development of mutual interest. The work under this MOU is to be of a basic, general purpose, and long-term nature similar to that normally conducted in the DOE weapons technology base. The Five-Year Project Plan contains the detail descriptions of the individual projects under this MOU. Must focus on DP needs as well.

Keywords: DoD/DOE MOU

360. **NIS LAB-TO-LAB INTERACTIONS**
$1,000,000
DOE Contact: Edwin E. Ives, (202) 586-4879
SNL Contact: C. D. Croessmann, (505) 845-9517

Develop projects (including materials science and engineering) between Sandia and NIS (Russia, Ukraine, Belarus, Kazakhstan) weapon experts that bring mutual benefit by supporting stability at design institutes, assisting conversion to peaceful and commercial activities, encouraging surety best practices and developing long term relationships with scientists and experts in the FSU.

Keywords: NIS, FSU

361. **COOPERATIVE MEASURES PROGRAM**
$3,850,000
DOE Contact: Edwin E. Ives, (202) 586-4879
SNL Contact: K. D. Nokes, (505) 844-3744

Develop projects (including materials science and engineering) between Sandia and NIS (Russia, Ukraine, Belarus, Kazakhstan) weapon experts that bring mutual benefit by supporting stability at design institutes, assisting conversion to peaceful and commercial activities, encouraging surety best practices and developing long term relationships with scientists and experts in the FSU. Engage the nuclear weapon design complex of the PRC in mutually beneficial surety and nonproliferation activities.

Keywords: NIS, FSU

362. **NIS INDUSTRIAL PARTNERING PROGRAM**
$1,825,000
DOE Contact: Edwin E. Ives, (202) 586-4879
SNL Contact: Dennis Croessmann, (505) 845-9517

This project has established a portfolio of 68 SNL-NIS institute collaborations representing a mutually interesting cross section of technical and commercial applications (including materials science and engineering). The collaborations will be formalized with contracts and involve standard project management practices including periodic reviews, budget and technical reporting, and business plans for those demonstrating commercial potential. Sandia is also participating in efforts to develop metrics to measure the success of the IPP program, develop improved communication channels, and establish information resources for the collaborators.

Keywords: NIS, Industrial Partnering

363. **DEVELOPMENT OF ANTIMONIDE BASED SEMICONDUCTORS**
$600,000
DOE Contact: Edwin E. Ives, (202) 586-4879
SNL Contact: P. Esherick, (505) 844-5857

This program will develop the technology base required to manufacture magnetic field sensors and related devices based on a commercially viable use of MOCVD. This project will focus on the materials growth issues for antimonide based III-V compound semiconductors relevant to both magnetic sensors and infrared lasers and emitters relevant to DP sensor needs. Emphasis will on developing manufacturable materials growth processes using novel sources that will enable growth of critically needed Al containing materials for use as electrical isolation layers in magnetic sensors or for optical and carrier confinement in near-IR laser structures Applications for the latter include sensors for decomposition of explosives in weapons systems.

Keywords: Semiconductor, MOCVD

364. **HIGH TEMPERATURE UNDERHOOD ELECTRONICS**
$341,000
DOE Contact: Edwin E. Ives, (202) 586-4879
SNL Contact: T. J. Allard, (505) 844-5581

Microelectronic packaging techniques, which include die attach, wire bonding, hermetic glass sealing, and high temperature solders, are the focus of this CRADA. Numerical analysis, modeling, materials analysis, tests, and evaluations will be performed on the various materials to quantify reliability and manufacturability of each system. The ultimate goal is to identify those materials for use in the manufacture of microelectronic circuits for use in severe high temperature environments.

Keywords: Microelectronics, Packaging

365. **ADVANCED PRECURSORS AND CHEMISTRIES FOR MOVPE**
$1,050,000
DOE Contact: Edwin E. Ives, (202) 586-4879
SNL Contact: P. Esherick, (505) 844-5857

This project entails four task areas: precursor chemistry, equipment modeling, equipment design and manufacture, and materials growth and device evaluation. We will identify safer precursors, compatible with high-quality materials growth, to replace arsine and/or phosphine, develop kinetic mechanisms to models their chemistries and use these models in collaboration with Motorola to improve equipment design. We will develop manufacturing processes using these safer chemistries and demonstrate growth of device-quality material from which state-of-the-art microelectronic and photonic devices may be fabricated.

Keywords: Precursors, MOVPE

MATERIALS STRUCTURE AND COMPOSITION

366. **PROCESS MODELS FOR ALUMINUM ALLOYS**
$183,000
DOE Contact: Bob Dewitt, (301) 903-3311
SNL Contact: Dave Larson, (505) 843-4165

Sandia National Laboratories and ALCOA (Aluminum Company of America) are developing computational tools and codes for the analysis and design of the processing and manufacture of both existing and new aluminum alloys. These models will enable scientists to predict and follow (by computer simulation) the evolution of a precipitate microstructure as a function of the entire processing history from melt solidification to the final mill product. The partners will perform thermal and stress analyses of various processing steps.

Keywords: Aluminum, Alloys, Computational Methods

367. **ADAPTIVE SCANNING PROBE MICROSCOPIES**
$297,000
DOE Contact: M. J. Katz, (202) 586-5799
SNL Contact: Chuck E. Meyers, (505) 844-3459

Current data acquisition and analysis procedures used in scanning tunneling microscopy (STM) severely restrict our ability to extract quantitative information regarding, for example, atomic scale rate processes or local chemical compositions. In this program we combine innovative pattern recognition techniques with state-of-the-art STM to develop a new paradigm for operating STM whereby the microscope adapts its data acquisition to focus on the most important features of the structures that is under examination. Currently, the STM scans a region of material by devoting an equal amount of time to all areas of the image. However, for most materials problems, only the data that are associated with specific features, such as defects or possibly nucleation centers, are used to analyze the state of the material. An adaptive scanning approach can be used to locate, track and image features of interest without the overhead of acquiring data over the entire sample region. By using this novel approach, the time required to collect information will be decreased several orders of magnitude which will enable us to study the kinetic processes with unprecedented microscopic-real-space resolution. Pattern recognition techniques will be applied to these local data to distinguish and recognize features based on local electronic properties of the surface. The ability of the instrument to "recognize" specific features will greatly increase the operator's ability to examine and analyze complex materials structures. This new capability will place us in a strong position to apply STM to a wider range of technologically important problems such as catalysis, corrosion, lubrication, and biological processes.

Keywords: STM, Adaptive Scanning

368. **EXTENDING THE APPLICABILITY OF CLUSTER-BASED PATTERN RECOGNITION WITH EFFICIENT APPROXIMATION TECHNIQUES**
$110,000
DOE Contact: M. J. Katz, (202) 586-5799
SNL Contact: Chuck E. Meyers, (505) 844-3459

This project will develop, implement and evaluate a set of approximation techniques for Sandia's VERI pattern recognition technique. The approximations will make the technique applicable to problems with very large numbers of training points, test points, and measurement dimensions. The project will emphasize approximations which are especially suited to large problems of programmatic interest, e.g. chemical sensing of complex chemical mixtures, image analysis of Landsat and MTI nonproliferation satellite images, and personnel access control applications, which can have huge numbers of points representing many classes of interest. This project will provide the advantages of VERI pattern recognition while maintaining practical computation times in SPARC workstation and embedded PC environments. The approximation methods will include: (1) Faster approximate cluster computations (2) Replacing large training sets with sparse training sets which occupy the same phase space (3) Fast cluster neighbor search techniques.

Keywords: Pattern Recognition, Cluster Computation

369. **SMART INTERFACE BONDING ALLOYS (SIBA): TAILORING THIN FILM MECHANICAL PROPERTIES**
$432,900
DOE Contact: M. J. Katz, (202) 586-5799
SNL Contact: Chuck E. Meyers, (505) 844-3459

We will explore the use of the newly discovered strain-stabilized 2-D interfacial alloys as smart interface bonding alloys (SIBA). These materials will be used as templates for the heteroepitaxial growth of metallic thin films. SIBA are formed by two metallic components which 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, SIBA can be used to tailor the dislocation structure of thin films. Since dislocations directly affect mechanical properties, chemical resistance, electromigration and conductivity of thin films, control of their structure will allow enhanced performance and longevity of thin film materials. 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 interface force microscopy (IFM) and nanoindenter, and measurement of the electronic structure of the SIBA with synchrotron photoemission. Resistance of films to sulfidation and oxidation will also be examined. The Paragon parallel processing computer will be used to calculate the structure of the SIBA and thin films. 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.

Keywords: Strain Stabilized, Alloys, Bonding

370. **RECOGNIZING ATOMS IN ATOMICALLY-ENGINEERED NANOSTRUCTURES: AN INTERDISCIPLINARY APPROACH**
$400,000
DOE Contact: M. J. Katz, (202) 586-5799
SNL Contact: Chuck E. Meyers, (505) 844-3459

Scanning Tunneling Microscopy (STM) is a powerful tool for both characterizing and manipulating the atomic topographies of surfaces. For chemically-uniform model systems, e.g. clean Si surfaces, STM can provide considerable scientific insights. However, STM has typically been unable to provide unambiguous chemical recognition of atomic sites in many technologically relevant systems. This limitation is due to several problems: (1) There are no direct means for verifying proposed STM atomic identifications, and no theoretical guidance on what multivariate STM features would best characterize the atoms; (2) It is difficult to directly observe chemical information by inspecting individual STM images, and this chemical information is buried among the multiple-bias images; (3) STM tip structures have important yet poorly understood effects on STM data, and these tips often change due to tip-surface interactions during imaging. We will develop the theoretical and experimental underpinnings necessary to address the three issues above with the goal of enabling 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) We will seek to develop the first database of multivariate STM spectral features (i.e., the analogue of satellite ground truth spectra). This will be done by pseudopotential-based theoretical simulation of expected STM imagery and by carrying out a bootstrap pattern recognition procedure on experimental STM spectra from a series of samples with known and varying average atomic concentrations. (2) We will 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. This will also be done by cluster-based electronic structure calculations on STM tips under large electric fields and by correlating STM measured spectra with direct in-situ examination of the structure of the STM tip by field-ion microscopy. Mathematical approaches for minimizing the variability of the pattern recognition results with tip variability will be evaluated. (3) We will use pattern recognition of STM spectral imagery, based on the results of A and B tasks, 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 (spatial abruptness and chemical composition) of MOCVD-grown III-V structures of current programmatic interest for IR device applications.

Keywords: STM, Chemical Recognition

371. **ARTIFICIAL ATOMS**
$336,000
DOE Contact: M. J. Katz, (202) 586-5799
SNL Contact: Chuck E. Meyers, (505) 844-3459

Our goal is fundamental research in the new area of artificial atoms (AAs). Recent advances in semiconductor technology can now artificially tailor matter on a nanometer scale, and thus fabricate "working models" of atoms. AAs are defined by laterally patterning the 2D electron layer in a GaAs quantum well (QW) to sizes small enough (a few 100) that the electron wavefunctions are confined in all three dimensions. These quantized electron states are similar to those in actual atoms, except that they can be individually controlled and detected, offering unprecedented opportunities for new physics. Measurements of AA's single electron energy levels will produce breakthroughs in understanding of, e.g., magnetic field effects and electron-electron interactions, areas difficult to probe in bulk semiconductors. Further, the study of AAs may lead to such future applications as high efficiency LEDs, and cellular automata logic.

The difficulty in AA work has been detecting the tiny signals of single electrons. We propose to: (1) extend the study of AAs to geometries other than simple quantum dots, e.g., quantum rings; and (2) use a more sensitive technique to detect individual FQHE quasiparticles. We will use two approaches based on new techniques that offer significant advantages. The first measures changes in the capacitance of an artificial atom between two conducting planes, as individual carriers are added to it. Previously transistors were used to sense the voltage on the capacitor plates. We will instead use a new quantum device pioneered by one of the PIs, the Coulomb blockade electrometer (CBE), having a charge sensitivity of 3x10-4 electrons/ Hz1/2, and allowing ~2 orders of magnitude better sensitivity than previous techniques. The second approach measures individual electrons by resonant tunneling through their energy levels. Previous implementations did not allow the size of the dot to be directly controlled, introducing ambiguity. Our new method of gating isolated submicron area allows direct control of the size of the AA.

Keywords: Semiconductor, Nanoscale

372. **MODELING AND CHARACTERIZATION OF MOLECULAR STRUCTURES IN SELF ASSEMBLED AND LANGMUIR-BLODGETT FILMS**
$110,000
DOE Contact: M. J. Katz, (202) 586-5799
SNL Contact: Chuck E. Meyers, (505) 844-3459

Self Assembled (SA) thin films and Langmuir-Blodgett (LB) thin films are emerging technologies for the development of chemical and bio-chemical sensors, electrooptic films, second harmonic generators (frequency doublers), templates for biomimetic growth etc. However, the growth of these technologies is dependent on the development of our understanding and control of the molecular arrangement of these films. This is not trivial since SA and LB films are essentially two-dimensional monolayer structures. We intend to start a collaboration between Sandia National Laboratories (SNL) and Los Alamos National Laboratory (LANL) to extend characterization techniques and molecular modeling capabilities for these complex two-dimensional geometries with the objective of improving our control of the fabrication of these structures for specific applications. Achieving this requires understanding both the structure throughout the thickness of the films and the in-plane lattice of the amphiphilic molecules. To meet these objectives we intend to use molecular modeling and non-standard investigative procedures for transmission electron microscopy (TEM), atomic force microscopy (AFM), X-ray reflectivity, and neutron reflectivity. The neutron reflectivity studies will be completed in a non-monetary collaboration with Charles Majkrzak at NIST according to Sandia's pending Memorandum of Understanding.

Keywords: Modeling, Molecular Structures

373. **SEMICONDUCTOR PHYSICS**
$1,450,000
DOE Contact: Bob Dewitt, (301) 903-3311
SNL Contact: S. T. Picraux, (505) 844-7681

Characterize and understand through experiment and theory the synthesis and properties of new semiconductor materials and structures required for future microelectronic and photonic applications. We employ advanced growth (MBE, MOCVD), microscopic characterization of structural (TEM, X-ray, ion beam), optical (photoluminescence, magnetoluminesence, stimulated emission), transport (low temperature and high field), and extensive theoretical modeling (ab initio bandstructure, transport, laser gain, massively parallel tools, etc.) techniques. Surface emitting lasers, nanoelectronic and nanophotonic structures, laser arrays and other new structures are studied. New device concepts, theoretical models and processing approaches being developed.

Keywords: Semiconductors, Synthesis, Microelectronics

374. **NANOSTRUCTURES, ADVANCED MATERIALS, AND ION BEAM SCIENCES**
$2,800,000
DOE Contact: Bob Dewitt, (301) 903-3311
SNL Contact: G. A. Samara, (505) 844-6653

This project aims to keep Sandia at the forefront of materials science relevant to DP needs. It includes research on: nanoclusters and nanostructures for potential sensor, environmental, electronic and gettering applications; shock compression and high pressure phenomena for improved component designs and above ground diagnostics; dielectrics, borides, and amorphous diamond-like carbon materials for electronic, wear-resistant, thermoelectric and harsh environment applications; electrorheological fluids for novel control systems and vibration damping of interest in ADaPT; superconductors for novel sensors and high speed electronic devices; computational tools for improved structural and electronic properties simulations; development of new approaches, including ultra-high resolution accelerator microbeam methods, to understand/predict the performance of materials/components; invention/implementation of advanced atomic-level in-situ and ex-situ diagnostic capabilities.

Keywords: Nanostructures, Ion Beam

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

375. **LEAD-FREE SOLDERS**
$150,000
DOE Contact: Bob Dewitt, (301) 903-3311, (301) 903-3311
SNL Contact: Dave Larson, (505) 843-4165

Sandia National Laboratories and members of the National Center for Manufacturing Sciences (NCMS) will work together to develop and characterize alternatives to lead-based solders and to perform thermophysical and mechanical properties measurements. The health hazards associated with lead have prompted state and federal law makers to consider banning lead form manufactured products, including electronic solders. Electronic components, circuit board materials, and assembly processing have been optimized for tin-lead solders through the multi-billion dollar electronics industry. The selection of one or more alternative lead-free solders will require a complete evaluation of laminate materials, device leads and terminations, manufacturing processes, and solder joint performance on prototype assemblies.

Keywords: Solder, Thermophysical Properties, Mechanical Properties

376. **WELDING TECHNOLOGY FOR SPECIALTY ALLOY AerMet[a] 100**
$100,000
DOE Contact: Bob Dewitt, (301) 903-3311
SNL Contact: Dave Larson, (505) 843-4165

Sandia National Laboratories and Carpenter Technology Corporation will develop welding technology for the high-strength specialty alloy AerMet[a] 100, assess the effects of welding on the alloy's performance, and optimize the welding process. AerMet 100 is a high-strength, high-fracture toughness alloy developed by Carpenter Technology for use in structural components for aerospace applications. Potential commercial and military applications include armor plate, gas turbine main shafts and welded structural components for military and commercial aircraft, hand tools, bolts and fasteners, and bicycle frames. AerMet is registered trademark of CRS Holdings, Inc., a wholly-owned subsidiary of Carpenter Technology Corporation.

Keywords: Welding, Alloys

377. **WELDING METALLURGY FOR AUSTENITIC SUPERALLOYS AND ADVANCED TITANIUM-BASE ALLOYS**
$232,000
DOE Contact: Bob Dewitt, (301) 903-3311
SNL Contact: Dave Larson, (505) 843-4165

Sandia National Laboratories and General Electric Aircraft Engines will investigate and characterize the welding metallurgy, weldability, and mechanical properties for two classes of aerospace alloys: austenitic superalloys and advanced titanium-base alloys. The project goal is to accelerate commercial use of the alloys in gas turbine engines for improved aircraft performance. This project will help maintain the United States' superior performance in the aircraft industry through engine weight reduction, increased engine efficiency, reduced fuel consumption, and reduced aircraft fabrication costs. The partners will develop a database of the alloy's welding-related information.

Keywords: Austenitic, Titanium, Welding

378. **WELDING AND PROCESSING OF AN ADVANCED TITANIUM ALLOY**
$160,000
DOE Contact: Bob Dewitt, (301) 903-3311
SNL Contact: Dave Larson, (505) 843-4165

Titanium Alloy C (Ti-35V-15Cr) represents a major advance in properties over conventional titanium alloys, particularly in the areas of high temperature strength, cold-formability, and burn resistance. These properties make Alloy C an attractive alloy choice in areas where nickel alloys or high-performance stainless steels are used, and offers significant performance advantages due to its lower density and inherent corrosion resistance. At present, however, Alloy C is underutilized because of high material costs, limited availability of product forms, and difficulty in secondary fabrication. These problems arise from limited hot ductility in some instances, and are not well understood. This project will characterize the microstructural evolution and deformation mechanisms which occur in Alloy C during welding and thermomechanical processing, the apply both the fundamental knowledge and processing data base developed to optimize primary and secondary fabrication processes.

Keywords: Welding, Titanium, Alloys

379. **MODEL DETERMINATION AND VALIDATION FOR REACTIVE WETTING PROCESSES**
$351,000
DOE Contact: M. J. Katz, (202) 586-5799
SNL Contact: Chuck E. Meyers, (505) 844-3459

The wetting and spreading of a liquid over a surface has garnered much interest from numerous industries: printing, textiles, painting, and foliage insecticide to name a few. All of these processes are similar in that they are examples of nonreactive wetting. Under these conditions the liquid does not react chemically with the substrate to form new compounds. Because of this the information that has been collected on nonreactive systems fails to describe the behavior seen in reactive systems, specifically soldering. In soldering the liquid solder reacts with the substrate to form an intermetallic layer and the dynamic behavior of this type of system is seen to disagree with the nonreactive systems by many orders of magnitude. In order to better understand the reactive wetting process it is necessary to understand the driving forces that control the system. This project proposes to investigate the dominating physical forces in a reactive wetting system. Concurrent with these experiments is the numerical modeling of the system that incorporates the relevant discoveries of the experiments. The first year of the project will be dedicated to ranking the relative importance of what are believed to be the important driving forces and to perform experiments that investigate the effect of a local heat source at the triple-line. This will be accomplished by a careful study of the reaction of palladium plated copper with tin, as well as a an experiment to raster a laser in a line across the wetting front. Sn/Bi solder spreading on Bi experiments will also be done to test the effect of dissolution of the constituents as will an experiment to examine the electrochemical effects of the flux. The numerical analysis will be enhanced by the use of the SNL massively parallel Direct Simulation Monte Carlo (DSMC) code. This method directly simulates the Boltzmann Equation by transporting and interacting millions of computational particles. So far the DSMC has been used only in the realm of gas phase systems, but we intend to expand its applicability to include the liquid phase by adding attractive and repulsive potentials to the computational particles. This new simulation capability will be incorporated as a boundary condition model into the continuum transport codes to obtain parametric design results. Such numerical models could provide a platform for practical analysis of reactive processes.

Keywords: Wetting, Reaction

380. **IN SITU DETERMINATION OF COMPOSITION AND STRAIN DURING MBE USING ELECTRON BEAMS**
$295,000
DOE Contact: M. J. Katz, (202) 586-5799
SNL Contact: Chuck E. Meyers, (505) 844-3459

MBE growth of semiconductor heterostructures for advanced electronic and opto-electronic devices requires precise control of the surface composition and strain. Without in situ monitoring, the control of composition is limited to worse than 1 at. % by the instability of the growth sources. Since the misfit strain is determined both by the composition and the strain relaxation kinetics, it is even more difficult to control without direct monitoring. The development of advanced in situ diagnostics for real-time monitoring and process control of strain and composition would enhance the yield, reliability and process flexibility of material grown by MBE at Sandia and benefit leading-edge programs in microelectronics and photonics. We propose to develop real-time electron beam- and laser-based techniques to enhance composition and strain control. For strain relaxation, our goal is to use RHEED measurements of lattice spacing and laser measurements of wafer curvature as online process control tools with resolution of <0.1% in strain determination. In addition, we will develop a new technique using electron-induced X-ray fluorescence to determine surface composition with a resolution of better than 1 at. %. All these techniques will allow the monitoring to be performed in real-time without growth interruptions.

Keywords: MBE, Electron Beam, Diagnostic

381. **UNDERSTANDING AND CONTROL OF ENERGY TRANSFER MECHANISMS IN OPTICAL CERAMICS**
$400,000
DOE Contact: M. J. Katz, (202) 586-5799
SNL Contact: Chuck E. Meyers, (505) 844-3459

We propose a radically new material strategy for rare-earth (RE) hosts which will allow the development of new materials with emissive optical capabilities previously unattainable using conventional single-phase ceramics. This program will examine rare-earth ion optical behavior, and its theoretical basis, in multiphase, multicomponent host materials which exhibit nanoscale heterogeneities designed to influence ion-ion and ion-lattice energy transfer dynamics through atomic-level engineering of the ion local environment. Successful realization of this structural concept would dramatically impact the technological viability of these materials, resulting in higher efficiency, higher gain emissive optical components offering a broader range of operational wavelengths than that currently available, while preserving physical robustness. Blue light sources for high density optical data storage and optical amplifier elements compatible with 1.3 and 1.06 micron operating wavelengths for short haul data transmission and manipulation are just two application areas that will immediately profit from this enabling materials technology. The versatility of the strategy will also allow next generation optical components, with even more stringent operational requirements, to be readily attained. We will model the local atomic structure in the dopant vicinity using a computational approach based on local density functional theory, thus providing dopant site symmetry and vibrational structure information of critical importance to RE ion optical performance. This technique will be used in this work to model amorphous structures for the first time and will allow the investigation of a variety of dopant site types characteristic of these multiphase hosts (e.g., interfacial, mixed chemistry, cluster interior). These results will be interpreted in terms of direct optical evaluation of the RE excited state behavior in novel materials structures, based on Al_2O_3 and oxide glass compositions, incorporating both structural and compositional nanoscale inhomogeneties of varied size and stoichiometry. The study will result in a new, computer-based, predictive materials modeling capability which will enable RE optical behavior (e.g., RE 4f-4f transition characteristics and the relative dominance of different energy transfer mechanisms) to be estimated in both single and multiphase candidate hosts before fabrication.

Keywords: Energy Transfer, Optical, Ceramics

382. **PHYSICO-CHEMICAL STABILITY OF SOLID SURFACES**
$397,000
DOE Contact: M. J. Katz, (202) 586-5799
SNL Contact: Chuck E. Meyers, (505) 844-3459

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 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 understanding of the elementary events involved in surface damage and mobility. We are 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, (2) atomic-level imaging of surface and near-surface structure and defects using Field Ion Microscopy and Transmission Electron Microscopy, and (3) first-principles modeling of the effect 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 the developing true predictive models that are needed for wide application of these important new approaches to modifying the surface sensitive properties of materials.

Keywords: Surface, Stability

383. **AT-400 SURVEILLANCE**
$373,000
DOE Contact: Edwin E. Ives, (202) 586-4879
Sandia Contact: Ronald F. Hahn, (505) 844-7787

Conduct test and evaluation on approximately 22 AT-400 containers each cycle (tentatively 18 months) throughout the projected 50 year container life. Evaluate the Pit Storage container compliance with design requirements, detect deterioration that may affect container performance, and evaluate the container's ability to satisfy design requirements through the 50 year lifetime.

Keywords: AT-400, Container

384. **METALS**
$1,800,000
DOE Contact: Bob Dewitt, (301) 903-3311
SNL Contact: M. I. Baskes, (510) 294-3226

Failures and degradations in weapons components often can be traced to interfaces. Goals of the project are development of understanding of generic interface behavior, of how impurities affect the mechanical properties and structure of interfaces, relationships between processing, structure, and interface behavior, and microstructural evolution models of materials containing interfaces. Joining of metal hardware is ubiquitous in weapon systems. Our goals are to understand how process parameters affect joint behavior through microstructural change and to continue to develop an understanding of the process physics for weapon-relevant joining technologies.

Keywords: Metals, Characterization

385. **MATERIALS AGING AND RELIABILITY**
$1,477,000
DOE Contact: Bob Dewitt, (301) 903-3311
SNL Contact: Richard Salzbrenner, (505) 844-9408

The Materials Aging and Reliability Project will advance the understanding of the microstructural mechanisms which control the aging, reliability, and performance of materials. The selection of sub-projects is based on the risk (likelihood vs. consequence) of the failure of a specific material to weapon performance or surety. All sub-projects seek to develop fundamentally-based prediction capability to determine the effects of aging on the performance and reliability of non-nuclear materials in nuclear weapons. This project supports materials science work that is collaborative with other Research Foundations (9100, 9200, and 1100) to develop predictive capability that can be applied to the enduring stockpile.

Keywords: Aging, Reliability

386. **MATERIALS STABILITY AND THIN COATINGS**
$2,400,000
DOE Contact: Bob Dewitt, (301) 903-3311
SNL Contact: T. A. Michalske, (505) 844-5829

Develop and apply atomic- and molecular-level microscopies, spectroscopies, and theoretical models to examine fundamental materials processes that control phenomena, including: interfacial adhesion, lubrication, wear thermal stability, thin-film and surface kinetics, radiation effects, corrosion, hydrogen effects, curing, fracture, and chemical and physical vapor deposition processes. Develop scientific basis for design, manufacture and application of small smart products. Transfer degradation resistant/ stable materials technology to U.S. advanced materials industries and develop new models to predict useful lifetimes for currently used materials and structures.

Keywords: Coatings, Interfaces, Deposition, Stability

387. **PREDICTIVE STEWARDSHIP**
$2,600,000
DOE Contact: Edwin E. Ives, (202) 586-4879
SNL Contact: M. W. Perra, (510) 294-2093

This project is being conducted to develop predictive capability to quantify performance and *reliability* of stockpile materials throughout their specified service life. Specific materials used in the stockpile are identified based on their susceptibility to aging degradation. These have been prioritized in terms of their potential impact on the performance and reliability of weapons in the enduring stockpile. Sub-projects have been selected for funding based on this prioritization. Current sub-projects include: Stress Voiding, Degradation of Energetic Materials, Thermomechanical Fatigue of Solders, O-ring Embrittlement, and Slow Crack Growth in Glasses/ Ceramics. Starting in FY96, predictive models will be applied to selected weapon comps.

Keywords: Stockpile, Performance, Reliability

388. **WEAPON AGING CHARACTERIZATION**
$2,500,000
DOE Contact: Edwin E. Ives, (202) 586-4879
SNL Contact: M. W. Perra, (510) 294-2093

This project will be conducted to assure the availability of the people, equipment, and facilities that are required to support DP stockpile responsibilities. Capabilities will be applied, enhanced, or developed to meet DP needs in (1) production support, (2) solving production problems, (3) assessing stockpile materials, and (4) analyzing aging and failure of stockpile materials and components. For each sub-project, a single page Sub-project Description will be completed which includes: (1) title, (2) principal investigator, (3) brief description of the sub-project, (4) FY95 Goals/Objectives, (5) FY95 Deliverables (w/dates), (6) Goals/ Objectives for future FYs, (7) DP customers who directly benefit and (8) dual benefit.

Keywords: Stockpile, Aging

389. **NCMS HIGH TEMPERATURE SOLDERS - ALTERNATIVES TO LEAD-BASED SOLDERS**
$114,000
DOE Contact: Edwin E. Ives, (202) 586-4879
SNL Contact: Paul T. Vianco, (505) 844-3429

The three primary tasks of the Sandia participation in this project are: (1) the study of low Pb solders and the effects of Pb contamination on Pb-free solders; (2) intermetallic compound layer growth with Pb- solders; and (3) mechanical testing of Pb-free solders. In the first task, new low-Pb solders are being fabricated and their mechanical and physical properties measured for applicability in electronic system. The second task examine the intermetallic layer formation and substrate dissolution of the molten solder as well as at elevated temperatures in the solid state. The third task determines the creep and fracture properties of new Pb-free solders.

Keywords: Solder, Pb-Free, Low-Pb

DEVICE OR COMPONENT, FABRICATION, BEHAVIOR OR TESTING

390. **ADVANCED PRINTED WIRING BOARD TECHNOLOGIES**
$450,000
DOE Contact: Bob Dewitt, (301) 903-3311
SNL Contact: Dave Larson, (505) 843-4165

Sandia National Laboratories is working with three members of the National Center for Manufacturing Sciences—AT&T, Texas Instruments, and Hamilton Standard—to develop advanced printed wiring board technologies. These technologies must accommodate the ever increasing requirements of higher operating speeds and greater number of interconnections of electronic devices. The partners are researching printed wiring board materials, solderability, and chemical processes.

Keywords: Printed Wiring Boards, Solder

391. **JOINING SILICON NITRIDE TO METALS**
$491,000
DOE Contact: Bob Dewitt, (301) 903-3311
SNL Contact: Dave Larson, (505) 843-4165

Sandia National Laboratories and Allied Signal, Inc., will work together to develop reliable low-cost, commercially viable techniques for joining silicon nitride to metals for turbomachinery applications. Silicon nitride has superior rust resistance and superior performance at high temperatures. These physical properties make silicon nitride ideal use in stators, airfoils, rotors, and seal plates in turbomachinery. Worldwide commercial air travel is predicted to triple over the next twenty years. To accommodate this increase and to replace older aircraft, 6,000-7,000 wide-body aircraft are expected to enter service, development of advanced materials and process techniques to improve the performance aircraft engines will allow U.S. aircraft engine manufacturers to compete against heavily subsidized foreign companies. Allied Signal has expertise in silicon nitride fabrications, materials processing, and commercializations. Sandia has expertise in joining and welding technologies, as well as ceramic joining, braze metallurgy, and mechanical modeling.

Keywords: Silicon Nitride, Joining

392. **DEMONSTRATION OF MOLECULAR-BASED TRANSISTORS**
$330,500
DOE Contact: M. J. Katz, (202) 586-5799
SNL Contact: Chuck E. Meyers, (505) 844-3459

Increased research attention is being focused on molecular scale devices built from the bottom up, that is small, smart assemblies built using chemical techniques. In the past year, we have begun to explore the chemistry and physics of molecules that offer the promise of intermarriage of electronic and optical information in such a molecular scale device. We have dubbed devices that may be fabricated from such materials "molecular transistors." In analogy to a regular transistor, in which a base current regulates current flow, in molecular transistors, current flow is regulated photonically.

A photochromic compound is one that isomerizes from an initial form A to a different form B when irradiated with light of wavelength l1, and B in turn isomerizes to A when irradiated with light of wavelength l2. The materials we are developing feature photochromic side chains coupled to conducting polythiophenes, such that the photochromic reaction can attenuate the electronic properties of the thiophene backbone.

Keywords: Molecular Transistors, Photochromic

393. **ATOMIC-SCALE MEASUREMENT OF LIQUID METAL WETTING AND FLOW**
$374,000
DOE Contact: M. J. Katz, (202) 586-5799
SNL Contact: Chuck E. Meyers, (505) 844-3459

The wetting and flow of liquid metals plays an important role in materials synthesis and joining technologies. For example, soldering, brazing and welding require a liquid metal to wet the interface between two solids, and the fabrication of light-weight, metal-matrix structural composites involves the infiltration of a liquid metal into a porous ceramic preform. Despite the pervasive presence of liquid metal interfaces in materials problems, solutions are almost always the result of trial and error, rather than an atomic-scale scientific understanding. Just as microscopic flow processes determine the stability of atomically-thin grain boundary films, the wetting and flow of a macroscopic liquid are controlled by atomic motions at the leading edge of the spreading droplet. Current continuum models of spreading do not address atomic-scale flow mechanisms and fail to predict correctly wetting, flow, and stability of interfacial liquid metals. In this project we will (1) develop a new Acoustic Wave Damping experimental technique that can measure the atomic-scale flow behavior of liquid metals on solid substrates, and (2) use this technique to make the first viscoelastic measurements of well-characterized liquid metal layers.

Keywords: Liquid Metal, Wetting

394. **MODELING ELECTRODEPOSITION FOR METAL MICRODEVICE FABRICATION**
$255,000
DOE Contact: M. J. Katz, (202) 586-5799
SNL Contact: Chuck E. Meyers, (505) 844-3459

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. In LIGA, high-energy lithography is used to produce a deep non-conducting mold that is subsequently filled by means of electrodeposition to produce metal parts. This process offers a means to manufacture high resolution, high aspect-ratio devices including microscale valves, motors, solenoid actuators, and gear trains. Such devices cannot be fabricated either by silicon micromachining or by precision machine tool operations

.

Most research in LIGA has focused on lithography. Electrodeposition for LIGA has been relatively neglected, despite several serious problems. Device-scale voids in the deposited metal occur frequently and often without apparent cause. In addition, deposition surfaces are frequently rough or wavy, necessitating post-deposition polishing to produce parts having acceptable tolerances and surface finish. These problems are 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 electrodeposition for LIGA from all traditional electroplating and electroforming processes. To optimize the electroforming portion of the LIGA process, we will develop a model describing the electrodeposition of metal into high aspect-ratio molds having lateral dimensions on the micron scale. To validate this model we will also design and conduct a series of one and two-dimensional laboratory experiments

Keywords: Electrodeposition, Fabrication

395. **SURFACE-MICROMACHINED FLEXURAL PLATE WAVE DEVICE INTEGRATED ON SILICON**
$500,000
DOE Contact: M. J. Katz, (202) 586-5799
SNL Contact: Chuck E. Meyers, (505) 844-3459

Small, reliable chemical sensors are needed for a wide range of applications, such as weapon state-of-health monitoring, nonproliferation activities, and manufacturing emission monitoring. Surface acoustic wave (SAW) devices have been demonstrated as the basis for extremely sensitive (gravimetric) vapor phase chemical sensors. However, significant improvements in these acoustic sensors could be achieved by developing a flexural plate-wave (FPW) architecture, in which acoustic waves are excited in a thin sensor membrane. This architecture would improve sensitivity, reduce the operating frequency so that the devices would be compatible with standard digital microelectronics, and would permit sensing in liquid media.

Development of FPW devices requires integration of: (1) acoustic sensor technology, (2) silicon micromachining techniques to fabricate thin membranes, and (3) piezoelectric thin films. Consequently, the key materials innovation required to enable this approach is the development of piezoelectric thin films with large coupling coefficients and low losses that can be integrated with silicon. Pb(Zr,Ti)Of (PZT) ceramics offer exceptional piezoelectric properties for this application and have been successfully integrated at Sandia with silicon microelectronics. AlN and ZnO are alternative materials that have reasonable piezoelectric properties, can be integrated as thin films directly onto silicon, and eliminate the use of Pb.

Successful development and integration of these technologies would permit monolithic integration of vapor/ liquid-phase acoustic sensors with the drive electronics resulting in increased reliability, miniaturization, and reduced costs. Further miniaturization could be achieved by using micromachined structures and piezoelectric thin-film actuators to integrate flow control and chemical separation capabilities. Integration of this sampling technology would lead to a monolithic, microanalytical system. In addition, the piezoelectric thin film/ micromachined membrane structures could form the basis for pyroelectric detectors and micro-actuators for microelectromechanical systems and smart packages.

Keywords: Micromachine, Plate Wave Device, Silicon

396. **SCANNING PROBE-BASED PROCESSES FOR NANOMETER-SCALE DEVICE FABRICATION**
$454,000
DOE Contact: M. J. Katz, (202) 586-5799
SNL Contact: Chuck E. Meyers, (505) 844-3459

Nanometer-scale electronic device technology 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. Our object is to achieve an order of magnitude decrease in feature size compared to conventional fabrication technology. This order of magnitude jump in the ability to make small structures opens new areas of fundamental physics research on the properties of mesoscopic structures, and enables new types of electronic devices with enhanced functionality, speed, and reliability. We will explore approaches to nano-structure fabrication using scanning probe-based (STM, AFM) processes. We will emphasize limits to performance and fabrication and characterization of electronic effects in nanostructures. For prototype device structures critical nanoscale components will be integrated with conventional test structures to allow full electrical accessibility. Two approaches to nanostructure fabrication will be explored. First, we will investigate electron induced chemical vapor deposition of metals. Electrons from an STM tip locally decompose precursor molecules adsorbed on the sample surface or in the gas in the vicinity of the tip to produce polycrystalline Fe, Al, or Ni wires with dimension <10 nm. Second, we will develop a more general AFM-based nanolithographic capability, based on molecular scale resist processes. Mechanical modification of molecular scale resists can produce nanoscale images suitable for conventional pattern transfer by etching or deposition. We will also investigate molecular layer resists based on simple adsorbed atoms and molecules which can be patterned by electron induced desorption or reaction. In parallel with these fabrication approaches, low temperature electrical measurements will be performed, and selected nanoelectronic devices will be fabricated and characterized. The low-T magneto-transport of sub-10 nm metallic wires will be investigated. Field effects on extremely narrow metallic wires, a kind of metal-oxide-metal FET (MOM-FET), will be investigated for the first time. Finally we will attempt to demonstrate the single electron coulomb blockade (CB) effect at liquid nitrogen temperatures and above, by fabricating tunnel junctions with dimensions <100 nm2. Such single electron devices potentially have great metrology applications as current standards and quantum-noise-limited electrometers.

Keywords: Nanoscale, STM, AFM, Fabrication

397. **AT-400A PIT CONTAINER**
$3,470,000
DOE Contact: Edwin E. Ives, (202) 586-4879
SNL Contact: R. L. Alvis (505) 844-5400

The program requires the design, development, certification, and procurement of a container for the shipment and storage of nuclear weapon pits. Development will require extensive testing to verify that the container will meet the requirements of federal regulations. Procurement will include selection of contractors, production oversight and product acceptance. Certification will require the preparation of a Safety Analysis Report—Packaging (SARP) which is the major record on which the certification will be granted. Additional efforts will be required to support Pantex by providing procedural source data and participating in "Quality Evaluations." The welding system and associated processes will also be developed by SNL.

Keywords: AT-400, Container

398. **MC4300**
$400,000
DOE Contact: Edwin E. Ives, (202) 586-4879
SNL Contact: Carla Busick, (505) 844-2919

Design and develop in a timely and cost effective manner, a universal neutron tube satisfying the requirements of all stockpile weapons by the year 2002. Specifically, evolve a design which minimizes fabrication parts and processing through studies to advance technologies such as diffusion bonding, ion optics, and cermets.

Keywords: Neutron Tube

399. **SMARTPROCESSES**
$1,533,000
DOE Contact: Bob Dewitt, (301) 903-3311
SNL Contact: K. W. Mahin, (505) 844-2222

The SmartProcessing projects provide the science-base knowledge and models required for intelligent processing of materials and advanced product realization for DP. The products of this research are the process knowledge and understanding required to generate empirical (experimentally-supported) or predictive (mathematical/FEA-based) models for integration into Smart, computer-based product/process design systems, as prototyped by SmartWeld and FastCast. Research in this case is integrated with the more applied Advanced Manufacturing Processes projects under the Prouct Realization Backbone and covers several manufacturing processes.

Keywords: SmartWeld, FastCast

400. **MATERIALS AND PROCESS DESIGN FOR RELIABILITY**
$1,000,000
DOE Contact: Bob Dewitt, (301) 903-3311
SNL Contact: Michael Cieslak, (505) 845-9144

This project has the goals of developing: (1) materials whose weapon-functional properties are time- and environment-invariant or that have large tolerance to variations in composition and structure relative to performance requirements over their lifetime of use (i.e. in their own initial creation, during weapon manufacture, and throughout the STS), and (2) manufacturing processes that insure lower variability of fabricated weapons products through verified process control methodologies. We plan to initiate projects that support these concepts within the needs of the Block Change Diagram proposal as well as potential future weapon designs.

Keywords: Processing, Reliability

401. **APPLICATIONS-DRIVEN INTERDISCIPLINARY RESEARCH**
$880,000
DOE Contact: Bob Dewitt, (301) 903-3311
SNL Contact: S. T. Picraux, (505) 844-7681

Applications-driven interdisciplinary research with DP sector, including Micromechanical (IMEMS) reliability and high-reliability neutron tube fabrication and mid-IR based chemical sensors. Focus of research is to collaborate outside Center with specific DP focus and build on emerging technology core capabilities.

Keywords: Interdisciplinary Research, Micromachine

402. **REPETITIVE PP-HIGH POWER SEMICONDUCTOR SWITCH RESEARCH**
$499,000
DOE Contact: Bob Dewitt, (301) 903-3311
SNL Contact: Malcolm Buttram, (505) 845-7117

The primary issue with fast, high gain semiconductor switches is lifetime, a contact damage problem. We have demonstrated the ability to control this damage somewhat with ion implants at the contact edge. Based on those results we will fabricate and test contacts that appear to be much less susceptible to damage. We also need a better understanding of the carrier formation process than we have at present. We have developed a theory (with 1300) and begun to develop a Monte Carlo code to make quantitative predictions. We will continue research to improve thyristors for handling higher power and higher current.

Keywords: Semiconductor, Switch

403. **ADVANCED PACKAGING**
$750,000
DOE Contact: Bob Dewitt, (301) 903-3311
SNL Contact: Gilbert V. Herrera, (505) 845-8465

This project facilitates the transition of our packaging competence to meet future DP packaging needs by developing capabilities and assembly technologies for flip chip; fine pitch wirebonding and surface mount attach; area arrays; plastics; and 3-D packaging. Work will continue in certain technologies that enable multichip module applications, as well as package test structures (both ATC and smart MCM substrates). New emphasis will be placed on sensor and IMEMS packaging.

Keywords: Microelectronics, Packaging

404. **ADVANCED LITHOGRAPHY**
$1,000,000
DOE Contact: Bob Dewitt, (301) 903-3311
SNL Contact: Walter Bauer, (510) 294-2994

This project will develop the necessary technologies that result in all reflective lithography for design rules below 0.18 microns. These include prototype development laser plasma source, camera, optics, resists, masks, and precision motion control.

Keywords: Lithography

405. **IPP/SCT - MICROWAVE COMPONENTS**
$320,000
DOE Contact: Edwin E. Ives, (202) 586-4879
SNL Contact: Dennis Croessmann, (505) 845-9517

This CRADA project seeks to develop high-temperature superconducting thin-films with ferroelectrics to create tunable microwave filters. The tunable characteristics of the filters ease manufacturing tolerances and allow greater selectivity of operating frequency. The filters will be packaged with low-cost cryocoolers for use in communications base stations. Sandia and the collaborating NIS Institute will be responsible for optimizing the process for depositing the ferroelectic and superconducting materials and controlling their characteristics. The US industrial partner's contribution will be the integration and packaging of the films into commercial filters and other products.

Keywords: Superconductors, Microwave, Filters, NIS

406. **PHOSPHOR SUPPORT PROGRAM FOR FIELD EMISSION DISPLAYS**
$343,000
DOE Contact: Edwin E. Ives, (202) 586-4879
SNL Contact: E. Paul Royer, (505) 844-7385

The comprehensive understanding will be obtained through information from the following sources: (1) the measurement of the cathodoluminescent output from the phosphor powders; (2) the creation of phosphor screens from this powder using conventional settling and electrophoretic techniques, and an exploratory laser deposition technique producing thin film screens; (3) the measurement of the cathodoluminescence from the screens; (4) the cathodoluminescent output from the screens using laboratory FEDs, as opposed to the E-gun in (1) and (3); (4) aging and volatility studies of the screens; (5) surface morphology studies of the screens; (6) band structure and defect calculations of II-VI compounds

Keywords: Phosphor, Field Emission Displays

INSTRUMENTATION AND FACILITIES

407. **INTELLIGENT SYSTEMS FOR INDUCTION HARDENING**
$350,000
DOE Contact: Bob Dewitt, (301) 903-3311
SNL Contact: Dave Larson, (505) 843-4165

Sandia National Laboratories and the Saginaw Division of General Motors Corporation are working together to create intelligent systems for induction hardening processes. Induction hardening is a broadly used manufacturing process to add strength to specify regions of ferrous parts. The partners will develop advanced sensor technologies, process diagnostics and controls, computational modeling, and advanced architecture for induction hardening processes. Real-time process control and intelligent models for design will significantly reduce lead time for process modifications, as well as the time cost currently involved with machine change-over and set-up verification. Advanced induction hardening processes will improve manufacturing agility and will upgrade reliability because part-to-part variation can be minimized.

Keywords: Induction, Hardening

408. **SPECIALTY METALS PROCESSING CONSORTIUM**
$1,700,000
DOE Contact: Bob Dewitt, (301) 903-3311
SNL Contact: Dave Larson, (505) 843-4165

The Specialty Metals Processing Consortium (SMPC) is a group of U.S. Specialty Metals producers who have formed a consortium to perform joint research in the area of specialty metals production, processing, quality, and performance. To perform this research, in 1990 the SMPC has entered a partnership agreement with the U.S. Department of Energy (DOE), whose operations both include internal production of specialty metals and are dependent on a consistent domestic supply of high quality specialty metals, to conduct this research. The research is coordinated and managed by Sandia National Laboratories Materials and Processes Sciences Center and headquartered at the Liquid Metal Processing Laboratory in Albuquerque, New Mexico. Each member pays a $50,000 annual fee, which is matched by the DOE. Additionally, the membership contributes payment-in-kind of approximately $1M per year, which is also matched by the DOE. The SMPC benefits by not only the cooperation enabling a larger program, but also by the leveraging afforded by the range of advanced technologies available within the National Laboratory system. DOE (Defense Programs) benefits from the improvement to its internal manufacturing operations, improvement and support of its technology base, and the cultivation and maintenance of a stable domestic supply of high performance materials, often of custom compositions and with specialized requirements. Other DOE benefits include the application of melting science and technology to waste management, environmental re-rediation, and decontamination/decommissioning activities.

During the initial five-year program, the emphasis was placed on the development of a series of advanced diagnostic, control, and modeling tools which are enabling SMPC members and DOE production facilities to better characterize and optimize their processes. Several technologies were investigated, developed, and are in application in SMPC member facilities. Two U.S. Patents have been granted on SMPC-developed inventions, and an additional five applications have been filed. As the second five-year period begins, emphases identified include the reduction of melt-related defects, optimization of processes to improve ingot size and quality, development and incorporation of science-based models of material production and performance, and the integration of computational models and closed loop controls to enable virtual prototyping of processes and model-based selection and design of material production.

Keywords: Metals Processing, Consortium

409. **CATALYTIC MEMBRANE SENSORS**
$343,900
DOE Contact: M. J. Katz, (202) 586-5799
SNL Contact: Chuck E. Meyers, (505) 844-3459

We propose to develop a miniature, thin film, array of catalytic membrane sensors (CMS) that will significantly increase the number of compounds identifiable by a single sensor. The basic constructs of these multi-layer sensors will be a catalyst, sandwiched between two molecule-specific membranes deposited onto a sensor (either chemical or thermal). Our initial study will integrate the technology of membrane synthesis, catalytic reactivity and sensor technology presently in use at Sandia. Specifically, we will generate a H_2 selective membrane, deposited on the surface of a H_2 or thermal detector. This will then be followed by deposition of HTO and HTO-like catalyst onto the membrane resulting in a high surface area, ion exchangeable catalytic layer. A top-membrane would then be added that will allow for select-sized molecules to flow through. The novel use of a size specific membranes combined with a chemically specific catalyst in an array would provide a new level of selectivity for a single sensor. By ion exchange reactions, using a variety of metal cations, other catalytically specific surfaces can be generated. The systematic variation of the membrane, catalyst, and sensor will allow the system to be fine tuned to investigate a wide variety of different classes of compounds. Since thin film technology will be utilized, the overall size of the sensor will not be increased, however, its selectivity and sensitivity will be greatly enhanced. The technology behind these modified sensors will impact a number of areas including, defense related capabilities [weapon readiness (weapon degradation) and early battlefield chemical sensing], commercial applications [auto exhaust detection, chemical purification], and environmental chemical detection.

Keywords: Catalysis, Membranes, Sensors

410. **INTEGRATED THIN FILM STRUCTURES FOR IR IMAGING**
$410,200
DOE Contact: M. J. Katz, (202) 586-5799
SNL Contact: Chuck E. Meyers, (505) 844-3459

Uncooled pyroelectric IR imaging systems, such as night vision goggles, offer important strategic advantages in battlefield scenarios and reconnaissance surveys. Unfortunately, the current technology for fabricating these devices is limited by low throughput and high cost which ultimately limit the availability of these sensor devices.

We propose an alternative design for pyroelectric IR imaging sensors that utilizes a multilayer thin film deposition scheme to create a fully integrated thin film element on an active silicon substrate for the first time. This approach will combine a thin film pyroelectric imaging element with a thermally insulating SiO_2 aerogel thin film to produce a new type of uncooled IR sensor that offers significantly higher thermal, spatial, and temporal resolutions at a substantially lower cost per unit. The development of this type of IR sensor will require the characterization and optimization of the aerogel thin film and its surface morphology, identification and optimization of an appropriate pyroelectric imaging element, and overall integration of these components along with the appropriate planarization, etch stop, adhesion, electrode, and blacking agent thin film layers.

Keywords: Thin Films, IR Imaging

411. **MOLECULAR IMPRINTING IN AEROGELS FOR REMOTE SENSING OF CHEMICAL WEAPONS AND PESTICIDES**
$366,300
DOE Contact: M. J. Katz, (202) 586-5799
SNL Contact: Chuck E. Meyers, (505) 844-3459

Warfare agents, such as sarin, belong to a general class of phosphate and phosphonate esters that have a very broad range of activities including materials for nuclear weapons production, pesticides, genetic material, and biological cellular signals. Current methods to detect these agents are limited to laboratory analysis. An in-field, real-time sensor-based approach with remote sensing capability is highly desired.

We propose to design and develop highly sensitive and specific optical sensors for phosphate and phosphonate esters using molecular recognition sites in high surface area aerogels. Molecular recognition sites will be engineered using computer aided molecular design and generated via the powerful template imprinting technique in aerogels. The imprinting procedure will organize and orient guanidine functionality via self-assembly into a solid matrix to complimentary bind a phosphonate template molecule. The receptors will be formed in thin film and bulk aerogel matrices. Aerogels ideally provide a high surface area, high pore volume, robust material for sensor applications. The material will be designed with active fluorophores at the receptor site that will report on target molecule recognition by fluorescence signaling from complexation with the phosphonate guest. From these materials will be developed various toxic gas sensor motifs, such as visual detectors that monitor color changes, or extremely low level sensing applications that follow fluorescence lifetimes. Fiber optic microsensors, fabricated using Sandia thin film aerogel deposition techniques, will be tested for sensitivity and selectivity. We will also develop granular bulk aerogels for our smart pebbles concept. Application of this inconspicuous material to an area of interest will provide a remote sensing system for covert chemical warfare agent production facilities, battlefield alert for chemical weapons release, and agricultural pesticide application and runoff.

Keywords: Aerogel, Microsensor

412. **ANTIPODAL FOCUSING OF SHOCK ENERGY FROM LARGE ASTEROID IMPACTS ON EARTH**
$161,000
DOE Contact: M. J. Katz, (202) 586-5799
SNL Contact: Chuck E. Meyers, (505) 844-3459

We will continue our project to apply a combination of hydrocode simulation and seismic modeling to study the consequences of a large impact on the earth. In addition we will continue to apply the techniques that we developed and the knowledge we have gained from the impact of Comet Shoemaker-Levy 9 (SL9) on Jupiter to validate our models and to assess the effect of asteroid impacts on Earth's atmosphere. We will use the results of the observationally-validated impact models along with seismic simulations to further bolster our hypothesis that a large impact can influence the interior geophysical dynamics of the Earth. The inclusion SL9 modeling as part of this project takes advantage of the overwhelming amount of high-quality observational data collected by astronomers. Until the impact on Jupiter last year, all planetary impact models were based only on scaled laboratory experiments, computational simulations, theory, and the geologic record; there had never been a direct observation. The collision provided an historic opportunity to perform a "reality check" to test the various models, resulting in a major credibility boost for computational modeling in general, and in our models in particular.

Keywords: Shock Energy, Asteroid

413. **BIOCAVITY LASER MICROSCOPY/ SPECTROSCOPY OF CELLS**
$380,000
DOE Contact: M. J. Katz, (202) 586-5799
SNL Contact: Chuck E. Meyers, (505) 844-3459

Using vertical cavity surface-emitting laser technology developed at Sandia, we have invented a new biomedical laser sensor that can rapidly quantify size and shape of different kinds of living human cells for early detection of disease. This "biocavity laser" provides high contrast, coherent light images and spectra of cells and intracellular structures and has several critical advantages over conventional cell analysis methods. We have demonstrated that the biocavity laser can probe the human immune system (cell and nucleus shape in human lymphocytes), characterize genetic disorders (quantify sickled and normal red blood cell shapes), and size small (few micron) particles. Beyond these applications this intracavity laser sensor has shown potential for high speed analyses of liquids, gases, and particulates for environmental monitoring or for ultra sensitive detection of single molecules.

Keywords: Laser, Microscopy, Spectroscopy

414. **A NEW PARADIGM FOR NEAR REAL-TIME DOWNHOLE DATA ACQUISITION**
$100,000
DOE Contact: M. J. Katz, (202) 586-5799
SNL Contact: Chuck E. Meyers, (505) 844-3459

In many deep underground operations, it is difficult to establish a two-way data communications link between remote sensors and the surface data acquisition system. Yet, in most applications, knowing the downhole data is critical to the success of the operation. Tremendous improvements in efficiency or safety would be realized if the downhole data can be obtained at the surface easily and inexpensively. This project will prove the concept of acquiring near real-time downhole data using tools able to stay downhole indefinitely.

The proof of concept resulting from this project will establish a new paradigm in downhole telemetry that can greatly impact oil, gas, and geothermal production and drilling, as well as environmental drilling and monitoring. The capability will allow Sandia to lead industry to higher levels of safe and efficient downhole field operations.

Keywords: Data Acquisition, Oil/Gas Exploration

415. **UV SPECTROSCOPIC DETECTION AND IDENTIFICATION OF PATHOGENS**
$100,000
DOE Contact: M. J. Katz, (202) 586-5799
SNL Contact: Chuck E. Meyers, (505) 844-3459

Recent food poisoning incidents in the Pacific Northwest have highlighted the need for relatively inexpensive instrumentation that provides an automated detection capability for food pathogens. Similar instrumentation is also needed for nonproliferation treaty inspections which must detect the presence of biological agents at suspect production facilities. In this LDRD project we will develop a fundamental understanding of UV spectroscopic measurements that can be used to detect pathogens and to develop a prototype instrument for field measurements. Exploratory measurements carried out in collaboration with the University of New Mexico have already demonstrated the feasibility of UV fluorescence detection of protein, DNA, and E. coli. Our LDRD project will quantify the spectral signatures of pathogens and optimize our existing multivariate algorithm to distinguish pathogens from proteins, DNA strains, and interfering backgrounds. Low resolution spectra will be used to develop a database of spectral signatures that can be used to train our multivariate algorithm to recognize pathogens. In addition, high-resolution laser fluorescence and ionization spectra will be used to improve the sensitivity and specificity of our measurements. The project will evaluate the feasibility of developing a relatively inexpensive field-deployable prototype UV fluorometer that can be used to detect pathogens in DOE and USDA applications.

Keywords: UV Detection, Pathogens

416. **NOVEL LASER-BASED DIAGNOSTICS CAPABILITY FOR CHEMICAL SCIENCE**
$150,000
DOE Contact: M. J. Katz, (202) 586-5799
SNL Contact: Chuck E. Meyers, (505) 844-3459

An opportunity exists to assemble novel short-pulse laser technology to establish a new state-of-the-art in laser-based measurements for chemical science research. We propose to (1) develop techniques that use picosecond laser pulses (10-100 ps) to probe molecular energy transfer in the gas phase by novel laser-induced grating techniques, and (2) use the high laser intensity associated with the short pulse lasers to enhance the sensitivity of multiphoton processes (Resonant Enhanced Multi-photon Ionization, REMPI, and Resonant Four Wave Mixing Spectroscopies) that depend non-linearly on the laser intensity. The assembled capability will attract follow-on funding from BES Chemical Sciences that would form the basis of at least two new user laboratories associated with the DOE/BES Scientific Facilities Initiative.

Keywords: Laser, Diagnostic

417. **ADVANCED ANALYTICAL METHODS**
$1,058,000
DOE Contact: Bob Dewitt, (301) 903-3311
SNL Contact: J. M. Phillips, (505) 844-1071

This project consists of several tasks, each of which is a relatively independent analytical methods development activity. These include advanced microanalysis development, chemometrics, X-ray diffraction from thin films, sensor development, and X-ray tomography.

Keywords: X-ray, Microanalysis

418. **FIELD EMISSION SOURCE WITH PHOSPHOR SCREEN**
$269,000
DOE Contact: Edwin E. Ives, (202) 586-4879
SNL Contact: R. J. Walko, (505) 844-8652

The objective of the project is to develop a flat panel field emission display suitable for use in computers, test equipment, and anywhere a video display is currently used. The two major areas of investigation are the wedge-type field emitters developed at Sandia, and low voltage phosphors which are compatible with field emitters. SNL's field emitter design is based on a non-lithographic fabrication technique, which will be further developed to meet HP's needs. In the phosphor arena, we will attempt to use an electronically conductive adhesive deposited as a sol-gel film to adhere existing phosphors to the screen; and (2) we will attempt to deposit luminescent phosphor thin films from chemical solutions where purity can be maintained.

Keywords: Phosphor, Field Emission, Flat Panel Display

LAWRENCE LIVERMORE NATIONAL LABORATORY

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

419. **ENGINEERED NANOSTRUCTURE LAMINATES**
$2,000,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LLNL Contact: Troy W. Barbee, Jr., (510) 423-7796

Multilayers are man-made materials in which composition and structure are varied in a controlled manner in one dimension during synthesis. Individual layers are formed using atom by atom processes (physical vapor deposition) and may have thicknesses of from one monolayer (0.2 nm) to hundreds of monolayers (>100 nm). At this time more than 75 of the 92 naturally occurring elements have been incorporated in multilayers in elemental form or as components of alloys or compounds. In this work deposits containing up to 225,000 layers of each of two materials to form up to 500μ thick samples have been synthesized for mechanical property studies of multilayer structures.

These unique man-made materials have demonstrated extremely high mechanical performance as a result of the inherent ability to control both composition and structure at the near atomic level. Also, mechanically active flaws that often limit mechanical performance are controllable so that the full potential of the structural control available with multilayer materials is accessible. Systematic studies of a few multilayer structures have resulted in free-standing foils with strengths approaching those of whiskers, approximately 70 percent of theory. Also, new mechanisms for mechanically strengthening materials are accessible with nanostructure laminates.

Applications now under development include: coatings for aircraft gas turbine engines; EUV, soft X-ray and X-ray optics spectroscopy and imaging; high performance capacitors for energy storage; capacitor structures for industrial applications; high performance tribological coatings; strength materials; integrated circuit interconnects; machine tool coatings; projection X-ray lithography optics.

Keywords: Thin Films, Multilayer Technology

420. **SOL GEL COATINGS**
$335,000
DOE Contact: G. J. D'Alessio,
(301) 903-6688
LLNL Contact: I. M. Thomas,
(510) 423-4430 and J. Britten,
(510) 423-7653

We continue to investigate the preparation of multilayer sol-gel high reflection (HR) coatings using colloidal SiO_2 with either HfO_2 or ZrO_2. We have found that the incorporation of an organic polymer binder such as polyvinyl alcohol or polyvinyl pyrolidinone into the high index component has resulted in an increase in the damage threshold and a decrease in the number of layer pairs required for high reflection.

A laboratory size meniscus coater was evaluated and found to produce mirrors of high optical performance and adequate damage threshold. This is now the preferred method of application, and a large machine capable of producing Beamlet and NIF size mirrors is to be delivered in early FY 1994.

Keywords: Sol Gel Coatings, Meniscus Coater, HR Coatings

421. **KDP GROWTH DEVELOPMENT**
$900,000
DOE Contact: G. J. D'Alessio,
(301) 903-6688
LLNL Contact: J. J. DeYoreo,
(510) 423-4240

Potassium dihydrogen phosphate (KDP) and its deuterated analog (DKDP) are important nonlinear crystals used both for frequency conversion as well as for a large Pockels cell. These crystals are very expensive, due in part to the very long times required to grow large boules (2-3 years) and the cost of D_2O for growing DKDP. We are developing alternative growth techniques to dramatically increase the growth rate of these crystals.

We recently adopted a new growth technique with which we are growing both KDP and DKDP at 10 to 20 times the rates achieved with conventional methods. We have grown crystals up to almost 20cm on a side and have shown that crystals grown by this method are of exceptionally high quality. We are now working with crystallizers that are large enough to grow $50x50x50cm^3$ crystals. We will continue to grow crystals at the 10-15cm scale in order to determine optimum hydrodynamic and regeneration conditions, and to understand the effects of impurities and stresses in seed crystals on the stability of the growing crystal face.

Keywords: KDP, Nonlinear Crystals, Crystallization

422. **VICARIOUS NUCLEOPHILIC SUBSTITUTION CHEMISTRY**
$350,000[1]
DOE Contact: G. J. D'Alessio,
(301) 903-6688
LLNL Contact: R. L. Simpson,
(510) 423-0379

Vicarious nucleophilic substitution chemistry is being used to synthesize energetic materials. New explosive molecules are being synthesized. Alternate routes to existing molecules, such as TATB, have been developed.

Keywords: Examination, Explosive, Energetic, TATB

423. **CHEETAH THERMOCHEMICAL CODE**
$190,000[1]
DOE Contact: G. J. D'Alessio,
(301) 903-6688
LLNL Contact: R. L. Simpson,
(510) 423-0379

A thermochemical code for the prediction of detonation performance is being developed. In addition to detonation performance, thermochemical calculations of impetus and specific impulse for propellant applications may also be made.

Keywords: Examination, Explosive, Energetic, TATB

424. **EXPLOSIVES DEVELOPMENT**
$900,000[1]
DOE Contact: G. J. D'Alessio,
(301) 903-6688
LLNL Contact: R. L. Simpson,
(510) 423-0379

New explosives are being developed for hard target penetrators. The goals include insensitivity to shock loading and significantly higher energy density than that of currently available materials.

Keywords: Explosive

[1]General energetic materials-related input. This activity is jointly funded (50:50) by DOE DP and the DoD.

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

425. **INTERFACES, ADHESION, AND BONDING**
$460,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LLNL Contact: Wayne E. King, (510) 423-6547

Our experimental effort is producing results that are directly comparable with theoretical calculations. We are investigating planar metal/metal interfaces and metal/ceramic interfaces (in anticipation of improvements in the theory) of well defined misorientations. In order to span the entire range of length scales described above, macroscopic bicrystals a few millimeters thick, with interfacial areas on the order of a square centimeter, will be required. In order to obtain such bicrystals, we plan to employ the diffusion bonding approach. An ultra-high-vacuum diffusion bonding machine has been developed in parallel with this research project.

Keywords: Interfaces, Bonding, Electronic Structure

426. **LASER DAMAGE: MODELING AND CHARACTERIZATION**
$400,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LLNL Contact: M. R. Kozlowski, (510) 424-5637

We have been working to understand the damage mechanism in thin film coatings used on Nova and other ICF lasers, with the ultimate goal of improving the damage threshold in coatings for future laser systems. We have utilized atomic force microscopy (AFM) and focused ion-beam (FIB) cross sectioning to characterize laser damage as well as the laser conditioning process which allows coatings to sustain higher laser fluences. We have shown that pre-existing nodular defects are the initiation points for most laser damage. The laser conditioning process is associated with the gentle ejection of these nodules to produce benign pits.

We have modeled the laser induced electromagnetic fields at "typical" nodular defects in a simple quarter-wave dielectric mirror coating. The model results demonstrated that large field enhancements are produced by these defects, which are composed of the same dielectric material as the coating materials. We are not calculating the thermal-mechanical response of these defects. Work to date has only looked at the normal incidence illumination case. With recent electromagnetics code advancements, we will now be able to model the more interesting non-normal incidence case.

Keywords: Coatings, Atomic Force Microscopy, Laser Damage

427. **KDP CHARACTERIZATION**
$400,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LLNL Contact: J. J. DeYoreo, (510) 423-4240

We require very large, high quality crystals of potassium dihydrogen phosphate (KDP) and its deuterated analogue (DKDP) for present and advanced high power lasers in the ICF Program. The performance of these crystals is limited by strain which induces anomalous birefringence and wavefront distortion and by defects which result in laser-induced damage at low laser fluence. The level of internal strain and the laser damage threshold are the most important factors in determining the yield of useable plates from an "as-grown" boule. Our goal has been to identify the defects which are the source of strain and damage in KDP and DKDP, understand how these defects are generated, and how to avoid them during the growth process.

We are using optical scatterometry, spectroscopy, X-ray typography, crystal growth and chemical analysis to determine the distribution of defects in crystals and their relationship to the growth process. We have been able to relate strain to specific defects using these methods and are now investigating, *in situ*, the process of laser damage as well as laser and thermal annealing.

Keywords: KDP, Strain, Crystal

INSTRUMENTATION AND FACILITIES

428. **SCANNING TUNNELING MICROSCOPY (STM) AND ATOMIC FORCE MICROSCOPY (AFM)**
$250,00
DOE Contact: G. J. D'Alessio, (301) 903-6688
LLNL Contact: W. Siekhaus, (510) 422-6884

A large stage scanning probe microscope that can perform scanning tunneling as well as contact and non-contact atomic force microscopy on the surface of objects as large as 6" in diameter, a small stage modified so that it can perform non-contact AFM and STM as well as nano-indentation, and an ultra-high vacuum instrument that can perform non-contact AFM and STM measurements and STM spectroscopy (STS) are being used for the following studies:

- Uranium Hydriding - Understanding the early stages of uranium hydriding and the effect of surface impurities is of paramount importance in science based stockpile stewardship. The UHV STM/AFM is used to determine the effect of local impurities on uranium hydriding.

- Electronic Properties of Nano-scale Particles - Nm-scale clusters various materials, deposited by laser ablation and by evaporation in a noble gas atmosphere onto the basal plane of graphite are analyzed by STM to determine their size distribution and by optical spectroscopy and electron spectroscopy to determine their size-dependent optical properties and electronic structure.

- Dissolution Rate of Uranium Oxide - The dissolution of uranium oxide by ground is being determined by AFM on single crystal uranium oxide by monitoring the rate of recession of the U02 surface with reference to a gold marker.

- Combined Scanning Probe Microscopy/Nano-Indentation - Used to identify the local mechanical properties of composite materials such as fiber reinforced plastics, bone-, tooth- and arterial-tissue from healthy and diseased arteries.

Keywords: NDE, Chemical Reaction, Uranium Hydriding, Stockpile Stewardship, Uranium Oxide Dissolution, Nuclear Waste Disposal, Etching, Cluster, Nano-indentation, Mechanical Properties, Biomaterials, Tooth, Artery, Bone

429. **FATIGUE OF METAL MATRIX COMPOSITES**
$500,000
DOE Contact: Warren Chernock, (202) 586-7590
LLNL Contact: Donald Lesuer, (510) 422-9633

This project involves Lawrence Livermore National Laboratory, Oak Ridge National Laboratory and General Motors. The project is studying the mechanisms of high cycle fatigue in squeeze cast metal matrix composites. The life limiting microstructural features are being determined and the processing-structure-property correlations are being established. Models that can predict lifetimes will be developed.

Keywords: Materials Properties, Behavior, Characterization or Testing

430. **MATERIALS PRODUCED WITH DYNAMIC HIGH PRESSURE**
$400,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LLNL Contact: William Nellis, (510) 422-7200

This project produces novel materials (crystal structures, microstructures, and properties) using high shock pressures. The terms dynamic and shock are used synonymously in this context. Tuneable shock pressure pulses are produced by the impact of a projectile launched from a small two-stage light-gas gun. Shock pressures range from 0.01-1 Mbar, temperatures range from 50 up to a few 1000°C, strain rates on loading range above 10^8/s and quench rates on release of pressure are 10^{12} bar/s and 10^9 K/s in specimens which are recovered intact for investigation. A gas gun is used to achieve these high shock pressures. Specimens range from 1 micron to 3 mm thick and from 3 to 23 mm in diameter. The observed material structures are correlated with computational simulations to enhance understanding of the effects produced. For example, a computational model of the dynamic compaction of nanocrystalline Al particles was shown to be in good agreement with the structure of compacts produced experimentally. A wide variety of materials characterization measurements are made both before and after application of high dynamic pressures, including X-ray diffraction, TEM, SEM, magnetization, NMR, and neutron scattering. In the past year we have dynamically compacted nanocrystalline Al, ceramic, and magnetic powders, produced unusual glass in bulk and nanocrystalline Si in grain boundaries by shock compressing quartz single crystals, and investigated impacts in nature by studying structural effects in shocked minerals. This shock method can be used to produce nanocrystalline particles of many materials contained initially in single crystals.

Keywords: Shock Pressures, Gas Gun, Materials Characterization, Ceramics, Magnets, Nanocrystalline Si, Glass

431. **PROPERTIES OF HYDROGEN AT HIGH SHOCK PRESSURES AND TEMPERATURES**
$300,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LLNL Contacts: William Nellis, (510) 422-7200 and Neil Holmes, (510) 422-7213

The properties of hydrogen at high pressures and temperatures are a "Holy Grail" issue for laser fusion, condensed matter physics, and planetary physics. Hydrogen in the form of deuterium-tritium is the fuel in laser fusion targets; the metallization of hydrogen by electronic bandgap closure has been a key goal of condensed matter physics since the early part of this century: and Jupiter with its 300 Earth masses is 90 percent hydrogen at high pressures and temperatures. This project measures temperatures and electrical conductivities of cryogenic liquid hydrogen and deuterium shock-compressed to pressures up to 2 Mbar ($2x10^6$ bar) and temperatures up to 5000 K with a two-stage light-gas gun. These conditions are achieved by impact of projectiles accelerated to velocities up to 8 km/s. Shock temperatures up to 5000 K at 1 Mbar were measured by a fast optical spectrometer and show that hydrogen undergoes a continuous dissociative phase transition above 200 kbar. This continuous dissociation absorbs energy, which causes lower temperatures and higher densities in the Mbar shock pressure range than was thought previously.

Electrical conductivities were measured using metal electrodes at pressures in the range 1 to 2 Mbar at calculated temperatures of 2000 to 4000 K. A novel technique was used to produce just enough shock heating to excite just enough electronic carriers to be able to measure the electrical conductivity of hydrogen at Mbar pressures in the short time duration of the experiment. Ours are the only electrical conductivity measurements on condensed hydrogen at any pressure. We have, for the first time, metallized hydrogen at 1.4 Mbar and 3000 K in the fluid and determined the density dependence of the electronic bandgap in the molecular fluid phase. Our observed metallization pressure in the fluid is about one-half what was predicted for the solid at 0 K. Both molecular dissociation and electronic excitation (ionization) affect the hydrogen equation of state to make hydrogen more compressible than believed previously and, thus, facilitate laser fusion. We are the first to metallize hydrogen. Our improved hydrogen equation of state has produced an improved picture of the interior structure of Jupiter and we can now determine the electrical conductivity of hydrogen throughout the interior of Jupiter. The electrical conductivity determines the large magnetic field, which is about fifteen times larger than the Earth's.

Keywords: Shock Pressures, Shock Temperatures, Electrical Conductivities, Gas Gun, Hydrogen, Cryogenics, Equation of State, Dissociation, Metallization

432. **ATOMIC LEVEL EXPLOSIVE CALCULATIONS**
$400,000
DOE Contact: Maurice Katz, (202) 586-5799
LLNL Contacts: Larry Fried, (510) 422-7796

A package of atomic-level calculations has been assembled that will allow design of new explosive molecules. The package includes calculations of solid density, heat of formation, chemical stability and sensitivity. This package is being tried on various new postulated compositions in concert with feedback from three organic and inorganic synthesis chemists. The intent is to couple Molecular Design with actual synthesis routes at the start so that the final selected design will be something with a good chance of being made in the lab. The target is to provide 10 to 15 percent more detonation energy than CL-20 with no decrease in sensitivity.

Keywords: Energetic Materials, High Explosives, Molecular Design, Detonation

433. **METASTABLE SOLID-PHASE HIGH ENERGY DENSITY MATERIALS**
$535,000
DOE Contact: Maurice Katz, (202) 586-5799
LLNL Contacts: H. Lorenzana, (510) 422-8982 and M. Finger, (510) 422-6370

Conventional energetic materials such as propellants, explosives and fuel cells store energy within *internal* bonds of molecules. Recently, we predicted the existence of novel materials that are calculated to store two to four times the energy content per volume of existing explosives, a dramatic improvement in performance. Though the atomic components are similar to standard energetic materials, these new materials differ from conventional molecular systems in that they form infinite, three-dimensional networks of covalent bonds, otherwise known as "extended" solids. Every bond in these new systems is energetic; the result is a correspondingly larger storage of energy per volume. Specifically, pure nitrogen is calculated to be recoverable at ambient conditions as an energetic solid with three times the energy content of HMX, a very high performance explosive. Since these materials are predicted to exist at high pressures and high temperatures, we have developed the experimental capabilities for synthesizing and characterizing such compounds at megabar pressures.

Recently we have studied the properties of carbon monoxide (CO). We have verified the existence of a new extended solid (polymeric) phase of CO at about 50 kbar. This new materials is recoverable at ambient conditions, and is believed to be energetic. We have calculated the equation-of-state of various candidate structures for CO, but further experimental constraints are needed in the structure and bond nature. Accordingly, we have performed with our Raman measurements of absorption in the visible and infrared. This information, coupled with our Raman measurements, has provided important insights as to the character of the bonds present in this material. This year we have developed techniques for generating "large" samples of the extended-solid phase of CO at high pressures, as certain property characterizations require significant amounts of samples. With these larger samples we are now attempting to measure stoichiometry and energy content.

Keywords: Energetic Materials, High Energy Density Materials

434. **AFM INVESTIGATIONS OF CRYSTAL GROWTH**
$210,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LLNL Contact: J. J. DeYoreo, (510) 423-4240

The nanometer-scale morphology of crystalline surfaces exerts a strong control on materials properties and performance. While many researchers have studied vapor deposited metal and semiconductor surfaces grown far from equilibrium, few studies have given attention to the morphology of crystal surfaces grown from melts or solutions near equilibrium despite the fact that most bulk crystals are grown in this regime. Understanding the mechanisms of growth and the origin of defects in such crystals can impact materials performance in a number of fields including optics, electronics, molecular biology, and structural biology. We are using atomic force microscopy (AFM) to investigate the growth of single crystal surfaces from solution in order to determine the mechanism of growth, the kinetics of step advancement, the effect of impurities, and the origin of defects.

In 1995 we performed both *ex situ* and *in situ* AFM measurements on three systems, the ionic crystal KH_2PO_4 (KDP), the canonical solution grown crystal, and the protein crystal Canavalin, a prototypical macromolecular biological crystal and crystals of the Sattelite Tobacco Mosaic Virus (STMV). Our results have provided insight into the mechanisms of growth step kinetics and defect incorporation in these systems. In 1996 we will investigate the effect of impurities on step dynamics in these systems and begin to explore the process of biomineralization.

Keywords: Morphology, Crystal Surfaces, Atomic Force Microscopy

435. **SUPERPLASTIC FORMING OF STAINLESS STEEL AUTOMOTIVE COMPONENTS**
$150,000
DOE Contact: M. Michaelis, (202) 586-4105
LLNL Contact: J. W. Elmer, (510) 422-6543

Superplastic forming of automotive exhaust components is being investigated as a possible method for fabrication of low emission exhaust systems. Development of a superplastic stainless steels alloy that will meet the required fabrication and performance criteria is being performed. This alloy must be laser welded and superplastically formed to yield a component that maintains a high resistance to exhaust gas degradation during operation. To date welding and superplastic forming of a baseline stainless steel alloy has been demonstrated. New work will focus on continued development of superplastic stainless steel alloys, and testing of laser welded and superplastically formed exhaust system segments.

Keywords: Superplastic Forming, Stainless Steel Alloys, Laser Welding

436. **FORMABILITY AND JOINING ANALYSIS FOR SUPERPLASTIC PANEL DESIGN**
$360,000
DOE Contact: J. Van Fleet, (202) 586-5782
LLNL Contact: J. W. Elmer, (510) 422-6543 and D. J. Trummer, (510) 423-8848

The fabrication of internally stiffened aerospace panel components is being investigated through numerical modeling and experimental methods. These panels are fabricated by welding and superplastic forming of titanium and aluminum alloys. Numerical models are being developed by modifying the Nike 3D code to predict the superplastic pressure schedules and the placement of welds for optimum panel forming. The numerical models developed here will be used as a design tool to help reduce the cost and lead time required to fabricate these panels by conventional trial and error methods.

Keywords: Superplastic Forming, Numerical Modeling, NIKE-3D, Laser Welding, Titanium Alloys, Aluminum Alloys

437. **MICROSTRUCTURAL EVOLUTION IN WELDS**
$330,000
DOE Contact: Bharat Agrawal, (301) 903-2057
LLNL Contact: J. W. Elmer, (510) 422-6543 and Joe Wong, (510) 423-6385

Spatially Resolved X-ray Diffraction (SRXRD) is being used for *in-situ* mapping of phases during welding where severe temperature gradients, high peak temperatures and rapid thermal fluctuations occur as the heat source passes through the material. Real time spatially resolved diffraction during welding is accomplished using high brightness synchrotron radiation and is being used to map the phases that exist in the heat affect zone (HAZ) of welds. By combining the SRXRD phase map with a numerical model of the temperature field surrounding the weld, the kinetic parameters for phase transformations can be determined. These parameters can then be used to predict HAZ microstructural evolution for a wide range of welding conditions. The welding of commercially pure titanium is presently being investigated and modifications to our SRXRD experimental setup were performed by enclosing the weld in an environmental chamber to prevent oxidation during welding. Preliminary work is being performed on a technique that will allow the collection of diffraction patterns simultaneously from a row of points in order to reduce the number of measurements required to map the weld HAZ from n^2 to n. This technique uses imaging storage plates and micro-Soller slit assembly to provide spatial resolution.

Keywords: Synchrotron Radiation, X-ray Diffraction, In-Situ Experiments, Phase Mapping, Arc Welding, Titanium, Non-isothermal, Phase Transformation Kinetics

438. **URANIUM CASTING PROGRAM**
$1,000,000
DOE Contact: Marshall Sluyter, (301) 903-5491
LLNL Contact: Jeff Kass, (510) 422-4831

The uranium casting program is addressing the use of permanent molds for near net shape castings, controlled cooling for segregation and microstructure control and the effect of alloy additions and subsequent heat treatment on microstructure. Process modeling has played a key role in producing high quality castings in uranium and uranium alloys.

Keywords: Uranium Casting

439. **URANIUM SPIN FORMING**
$1,500,000
DOE Contact: Marshall Sluyter, (301) 903-5491
LLNL Contact: Jeff Kass, (510) 422-4831

Spin forming is being explored as a method to produce near net shape wrought uranium components. Process modeling has been useful in predicting stress/ strain distribution and spring back. Near net shape components have been produced.

Keywords: Spin Forming

440. **PLUTONIUM NEAR NET SHAPE CASTING**
$2,500,000
DOE Contact: Marshall Sluyter, (301) 903-5491
LLNL Contact: Jeff Kass, (510) 422-4831

Near net shape casting is being explored using permanent molds. High quality castings have been produced. Process modeling has played a significant role in defining conditions needed for solidification control.

Keywords: Shape Casting

441. **ELECTRON BEAM COLD HEARTH MELTING OF URANIUM**
$900,000
DOE Contact: Marshall Sluyter, (301) 903-5491
LLNL Contact: Jeff Kass, (510) 422-4831

An existing electron beam evaporation chamber has been modified to produce controlled solidification uranium alloy ingots. Scrap feeders of various types are being evaluated. High quality ingots which meet the applicable uranium alloy specification have been produced.

Keywords: Electron Beam Melting, Uranium

442. **NIF CAPSULE MANDREL R&D**
$600,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LLNL Contact: R. Cook, (510) 422-3117

This program has as its objective the development of 2 mm thin-walled plastic shells that will serve as the mandrel for the production of capsule targets for the National Ignition Facility (NIF). The mandrels must be extremely spherical (<1 μm out of round), have wall thickness uniformity better than 1 μm, and have a surface finish of less than 10 nm (rms over modes >9). Several routes are being explored.

Keywords: Polymers, Laser Fusion Targets, Microencapsulation, Microshells

443. **POLYIMIDE COATING TECHNOLOGY FOR ICF TARGETS**
$500,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LLNL Contacts: R. Cook, (510) 422-3117 and Steve Letts, (510) 422-4373

This program has as its objective the development of a vapor based, high strength polyimide coating technology that will allow us to produce a smooth, 150 to 200 μm polyimide ablator coating on a 2 mm diameter capsule target for the National

Ignition Facility (NIF). Such targets should be strong enough to hold the full DT fuel load (about 300 atm) at room temperature, allowing us important flexibility in fielding these capsules for ignition experiments.

Keywords: Polymers, Laser Fusion Targets, Polyimide, Ablator

444. **BERYLLIUM ABLATOR COATINGS FOR NIF TARGETS**
$600,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LLNL Contacts: D. Makowiecki, (510) 422-5794, R. McEachern, (510) 423-4734 and R. Cook, (510) 422-3117

This program has as its objective the development of sputter deposition techniques that will allow us to deposit 150 to 200 μm of a strong, smooth, Cu-doped Be ablator on a spherical plastic mandrel shell. These Be coated capsule targets have been shown by calculation to offer some important advantages as ignition targets for the National Ignition Facility (NIF).

Keywords: Beryllium, Laser Fusion Targets, Ablator, Sputter Deposition

LOS ALAMOS NATIONAL LABORATORY

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

445. **ACTINIDE PROCESSING DEVELOPMENT**
$1,350,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LANL (Contract No. W-7405-ENG-36) Contact: R. L. Gutierrez, (505) 665-3919

The aim of this project is the development and characterization of fabrication processes and the study of new processing technologies for plutonium. Research involves casting, thermo-mechanical working, and stability studies. Measurements of resistivity, thermal expansion, magnetic susceptibility, and formability are made to evaluate fabrication processes and alloy stability.

Keywords: Radioactive Materials, Plutonium Alloys, Ductility, Thermal Expansion, Electrical Resistivity, Stability

446. **PLUTONIUM OXIDE REDUCTION**
$150,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LANL (Contract No. W-7405-ENG-36) Contact: K. Axler, (505) 667-4045

The thermodynamics of interactions among the components used in the pyrochemical processing of plutonium are determined along with the relevant phase relations.

Keywords: Radioactive Materials, Plutonium, Thermodynamics, Phase Diagrams, Direct Oxide Reduction, Electrorefining, Molten Salt Extraction

447. **LOW DENSITY MICROCELLULAR PLASTIC FOAMS**
$200,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LANL (Contract No. W-7405-ENG-36) Contact: P. Apen, (505) 667-6887

Microstructural polyolefin foams with densities between 0.01 g/cc and 0.2 g/cc are manufactured by a nonconventional foaming process. Foams are both open and closed celled and have large surface areas. This process is being expanded to other polymeric materials for a wide variety of applications. Foams have cell sizes from 25μm down to the 1μm range, depending on the process. Composite foams are being produced with submicron cell sizes while maintaining structural properties.

Keywords: Foams, Polyolefins, Polyurethanes, Silicones, Polyesters

448. **PHYSICAL VAPOR DEPOSITION AND SURFACE ANALYSIS**
$300,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LANL (Contract No. W-7405-ENG-36) Contact: M. Scott, (505) 667-7557

Physical vapor deposition, one electron beam sputtering, and dual ion beam sputtering are employed to produce materials for structural applications, corrosion resistance, optical properties, and thin film transducers. Materials being developed include doped, *in situ* laminates of aluminum and Al_xO_y having high strength and smooth surface finish. Also included are ion assisted deposition and ion sputtering onto various substrates for corrosion resistance to gases and liquid plutonium, reflective and anti-reflective coatings for infrared, visible, ultraviolet and X-ray wavelengths. Novel photocathodes are being made and evaluated by these processes.

Keywords: Coatings and Films, Physical Vapor Deposition, Sputtering, Ion Plating, Corrosion, Nondestructive Evaluation

449. **CHEMICAL VAPOR DEPOSITION (CVD) COATINGS**
$150,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LANL (Contract No. W-7405-ENG-36)
Contacts: J. R. Laia and M. Trkula, (505) 667-0591

Chemical vapor deposition (CVD) techniques are used to deposit thin-film and bulk coatings of a wide variety of elements and compounds. Coatings are deposited by the following techniques: conventional flow-by, fluidized-bed, plasma-assisted, and chemical vapor infiltration. To support and enhance our basic CVD program, efforts are underway to study the fundamental nature of the CVD process, including *in situ* diagnostics in the gas phase just above the substrate and modeling efforts to predict gas flows, reactor design, and chemical behavior within the CVD systems. Another collaborative effort at Los Alamos is attempting to synthesize organometallic precursors to deposit coatings at temperatures <300°C. Substrates coated by the CVD technique range from particles 2.0 μm diameter to infiltrations of fabrics a square meter in area.

Applications include nuclear and conventional weapons, space nuclear reactor systems (fuels and structural components), inertial confinement fusion program, high temperature engine and structural components for advanced high-performance aircraft, hard/wear resistant coatings (tribological), corrosion resistant coatings, coatings of complex geometries, near-net-shape fabrication, heat-pipe structures, precision CVD of ultra-thin, freestanding shapes.

Keywords: Chemical Vapor Deposition, Coatings (metal and ceramic)

450. **POLYMERS AND ADHESIVES**
$430,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LANL (Contract No. W-7405-ENG-36)
Contact: D. A. Hemphill, (505) 667-8335

The objective of this project is to identify potential weapons engineering and physics applications for plastic and composite materials, select or develop appropriate materials, develop low cost fabrication techniques compatible with Integrated Contractor production capabilities, and characterize promising materials on a timely basis to provide optimum material choices for new weapons designs. Material or process development projects include: highly filled polymers, composite structural and spring components, cushioning materials, and high-explosive compatible adhesives, potting materials. This work will be compatible with all current and future ES&H guidelines.

Keywords: Adhesives, Composites, Plastics, Polymers, Weapons Design, Weapons Engineering, Integrated Contractors

451. **TRITIATED MATERIALS**
$175,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LANL (Contract No. W-7405-ENG-36)
Contact: J. R. Bartlit, (505) 667-5419

Advanced research and development efforts are focused on tritiated materials for tritium storage. New methods for preparing, fabricating, and containing such compounds are under investigation. We are also using laser-Raman techniques for *in situ* measurements of hydrogen-deuterium-tritium gas mixtures.

Keywords: Tritium, Tritiated Materials, Radioactive Materials

452. **SALT FABRICATION**
$800,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LANL (Contract No. W-7405-ENG-36)
Contact: D. Carstens, (505) 667-5849

Development and evaluation of new fabrication and containment processes for LiH and LiD. This includes preparation of device parts for WTS tests. Research topics include development of hot pressing, machining techniques for salt compacts.

Keywords: Tritium, Hydrides, Machining, Radioactive Materials, Near-Net-Shape Processing

453. **SLIP CASTING OF CERAMICS**
$300,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LANL (Contract No. W-7405-ENG-36)
Contact: D. S. Phillips, (505) 667-5128

We are slip casting many ceramics including alumina, zirconia-toughened alumina (ZTA), and magnesia. The technology uses colloidal chemistry and powder characterization techniques, along with materials engineering. Considerable progress was made in the development of ZTA ceramic alloys with a superior microstructure and improved thermal shock resistance. The scope of work has expanded to include frits and insulation materials, as well as dense crucibles.

Keywords: Ceramics, Microstructure, Strength, Transformation Toughened Ceramics, Thermal Shock

454. **PLASMA-FLAME SPRAYING TECHNOLOGY**
$300,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LANL (Contract No. W-7405-ENG-36)
Contact: R. Castro, (505) 667-5191

Free-standing shapes and metallic and ceramic coatings are fabricated by plasma spraying. Materials examined recently include Be, ^{238}U, $MoSi_2$ and ZrO_2. Applications include: radiochemical detectors; temperature-, oxidation-, and corrosion-resistant coatings; and electrically insulating coatings.

Keywords: Coatings, Metals, Ceramics, Plasma-Flame Spraying, High Temperature Service, Surface Characterization and Treatment

455. **RAPID SOLIDIFICATION TECHNOLOGY**
$500,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LANL (Contract No. W-7405-ENG-36)
Contact: P. Stanek, (505) 667-6914

RSR technologies such as melt spinning, splat cooling, and rapid solidification plasma spraying, are being developed to evaluate a range of RSR alloys, intermetallics and composites for defense and energy applications. Activities include alloy development, microstructural analysis, mechanical and physical properties testing, process development and modeling.

Keywords: Rapid Solidification, Low Pressure Plasma, Alloy Development, Composites, Intermetallics

456. **BULK CERAMIC PROCESSING**
$250,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LANL (Contract No. W-7405-ENG-36)
Contact: J. D. Katz, (505) 665-1424

Cold pressing and cold isostatic pressing, followed by sintering, are used to produce ceramic and metal components for various physics experiments and for plutonium processing. Materials fabricated include alumina, magnesia and boron.

In addition, a collaborative effort was established with the University of New Mexico Center for Micro-Engineered Ceramics to investigate the effect of 2.45 GHz microwave energy on the diffusion of cations in ceramic oxides. This research consists of both a theoretical and experimental component. The results have shown that although microwave enhanced diffusion of chromium in alumina does not exist, microwave sintering has been found to be a very effective engineering tool for densifying even large alumina ceramics.

Finally, considerable effort was devoted to developing methods for sintering, rather than hot pressing, boron carbide to achieve high density. This work involves a collaboration with the A.W.E. in the United Kingdom.

Keywords: Ceramics, Sintering, Microwave Sintering, Cold Pressing

457. **SYNTHESIS OF CERAMIC COATINGS**
$150,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LANL (Contract No. W-7405-ENG-36)
Contact: C. P. Scherer, (505) 665-3202

The objective of this effort is to synthesize ceramic films for liquid metal containment. One approach entails the use of organic and aqueous solvents to deposit erbia films, which are subsequently heat treated to densification. The second approach involves the *in situ* conversion of a metal surface to a nitride by precise heating in a nitrogen environment.

Keywords: Ceramic Coatings, Sol Gel, Nitration

MATERIALS STRUCTURE OR COMPOSITION

458. **ACTINIDE SURFACE PROPERTIES**
$700,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LANL (Contract No. W-7405-ENG-36)
Contact: J. M. Haschke, (505) 665-3342

Characterization of actinide metal, alloy and compound surfaces using the techniques of X-ray photoelectron spectroscopy, Auger analysis, ellipsometry and Fourier-transform infrared spectroscopy. Surface reactions, chemisorption, attack by hydrogen, and the nature of associated catalytic processes are being studied.

Keywords: Actinides, Hydrides, Surface Characterization and Treatment, Hydrogen Effects, Radioactive Materials

459. **NEUTRON DIFFRACTION OF PU AND PU ALLOYS AND OTHER ACTINIDES**
$237,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LANL (Contract No. W-7405-ENG-36)
Contact: A. C. Lawson, (505) 667-8844

Physical structure and properties of plutonium are being studied by pulsed neutron diffraction at the Manuel Lujan, Jr., Neutron Scattering Center (Los Alamos) and the Intense Pulsed Neutron Source (Argonne). A time-of-flight technique is used to measure diffraction at cryogenic and elevated temperatures.

Keywords: Alloys, Radioactive Materials, Transformation, Microstructure

460. **SURFACE, MATERIAL AND ANALYTICAL STUDIES**
$300,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LANL (Contract No. W-7405-ENG-36)
Contact: W. C. Danen, (505) 667-4686

Studies are underway in four key areas: surface and interfacial structures and properties, explosives dynamics, laser-based isotopic analysis, and metastable energetic materials. Current investigations in surface and interfacial studies include: surface modification, HTSC composition and structure, and the use of MeV ion beams. In explosives chemistry, we are using real-time optical- and mass-spectral methods to probe the early-time dynamics of detonation. Analytical studies have centered on the use of resonance ionization mass spectrometry to eliminate isobaric interferences in the measurement of high-dynamic range isotope ratio measurements. We continue to study the synthesis and characterization of a new class of high energy density materials consisting of atomically-thin multilayered composite materials.

Keywords: Surface, Explosives, Interfaces, Composite Materials

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

461. **MECHANICAL PROPERTIES OF PLUTONIUM AND ITS ALLOYS**
$450,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LANL (Contract No. W-7405-ENG-36)
Contact: R. L. Gutierrez, (505) 665-3919

The mechanical properties of plutonium and its alloys are related to the pre-test and post-test microstructures of the materials using optical and electron microscopy and X-ray, electron and neutron diffraction.

Keywords: Alloys, Radioactive Materials, Microstructures, Strength, Transformation

462. **PHASE TRANSFORMATIONS IN PU AND PU ALLOYS**
$450,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LANL (Contract No. W-7405-ENG-36)
Contact: R. L. Gutierrez, (505) 665-3919

Mechanisms and crystallography of thermally and mechanically induced allotropic transformations are studied with differential scanning calorimetry, optical and electron microscopy and electron and X-ray diffraction.

Keywords: Alloys, Radioactive Materials, Microstructure, Transformations

463. **PLUTONIUM SHOCK DEFORMATION**
$350,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LANL (Contract No. W-7405-ENG-36)
Contact: M. J. Reisfeld, (505) 667-8485

Plutonium and actinide alloys are subjected to shock deformation, recovered without further damage and examined to determine how the shock affected their microstructures and mechanical properties.

Keywords: Radioactive Materials, Plutonium Alloys, Microstructure, Strength

464. **NON-DESTRUCTIVE EVALUATION**
$550,000
DOE Contact: G. J. D'Alessio,
(301) 903-6688
LANL (Contract No. W-7405-ENG-36)
Contact: Thomas Claytor,
(505) 667-1973

Development of Nondestructive Evaluation Technology that produces quantitative estimates of material properties. Use of tomographic techniques to enhance radiographic inspection. Flash, cine-radiography, high speed video recorded optical and X-ray diagnostics of dynamic and ultra-fast events. Real-time radiography. Image enhancement of output results from all techniques. Development of ultrasonic inspection techniques.

Keywords: Nondestructive Evaluation, Radiography, Ultrasonic Microscopy, Tomography, Cine Radiography, Bonding Processes, Real-Time Radiography, Image Enhancement

465. **POWDER CHARACTERIZATION**
$50,000
DOE Contact: G. J. D'Alessio,
(301) 903-6688
LANL (Contract No. W-7405-ENG-36)
Contact: G. J. Vogt, (505) 667-5813

Synthesis and processing of ceramic or metal powders depends critically on the physical characterization of the starting powders being used. Typical starting powders include commercial powders of thoria, magnesia, alumina, tungsten, copper, tungsten carbide, and boron carbide. In the past year, considerable effort has been expended on characterizing palladium alloy powders. Physical properties of interest include particle size and distribution, surface area, bulk and packed densities, morphology, pore size and distribution, and zeta potential. The crystalline-phase composition of the starting powders and processed powders can be determined by X-ray diffraction.

Keywords: Ceramic Powder, Metal Powder, Particle Size, Superconducting Powder, X-ray Diffraction, Surface Area

466. **SHOCK DEFORMATION IN ACTINIDE MATERIALS**
$300,000
DOE Contact: G. J. D'Alessio,
(301) 903-6688
LANL (Contract No. W-7405-ENG-36)
Contact:
R. L. Gutierrez, (505) 665-3919

Measurement of shock-wave profiles in uranium, plutonium, and plutonium alloys. Use of soft-shock recovery test to examine the microstructural changes occurring during shock deformation. Measurement of spall strength in actinide materials and examination of fracture surfaces.

Keywords: Actinides, Shock Deformation, Microstructure, Spall Strength

467. **DYNAMIC MECHANICAL PROPERTIES OF WEAPONS MATERIALS**
$350,000
DOE Contact: G. J. D'Alessio,
(301) 903-6688
LANL (Contract No. W-7405-ENG-36)
Contact: G. Gray, (505) 667-5452

Measurements of dynamic stress-strain and fracture behavior of materials used for nuclear weapons. Development of plastic constitutive relations.

Keywords: Dynamic, Strength, Fracture, Microstructure

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

468. **TARGET FABRICATION**
$1,500,000
DOE Contact: G. J. D'Alessio,
(301) 903-6688
LANL (Contact No. W-7405-ENG-36)
Contact: L. Foreman, (505) 667-1846
LLNL Contact: W. Hatcher, (510) 422-1100
General Atomics Contact: Ken Schultz,
(619) 455-4304

ICF/AGEX targets are fabricated using PVD, CVD, precision micromachining, and polymer chemistry techniques. After the parts are fabricated, the components are assembled using a variety of techniques. These targets are used to provide laser materials interactions data for the inertial confinement fusion community.

Keywords: Inertial Fusion, Target Fabrication

469. **FILAMENT WINDER**
$100,000
DOE Contact: G. J. D'Alessio,
(301) 903-6688
LANL (Contract No. W-7405-ENG-36)
Contact: B. Benicewicz,
(505) 665-0101

The Entec filament winder in MST-7 Plastics is a 4-axis computer-programmed machine with a winding envelope extending up to 4 feet in diameter and 10 feet in length. It is being utilized to wind circumferential or helical cylinders, cones, spheres, and closed-end vessels from a variety of fibers including glass, kevlar, carbon, tungsten, and aluminum oxide. The applications cover a host of programs from within the Laboratory as well as from outside agencies.

Keywords: Filament Winding, Composites

470. **HIGH ENERGY DENSITY WELDING IN HAZARDOUS ENVIRONMENTS**
$800,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LANL (Contract No. W-7405-ENG-36)
Contact: G. Lewis, (505) 667-9663

High power Nd/YAG lasers combined with fiber optic beam delivery systems have been evaluated for welding applications in hazardous environments. Applications include the manufacture of nuclear weapons components and nuclear power reactor repair. High quality structural welds have been achieved without exposing the operators or the welding power supplies to the hazardous environment.

Keywords: Laser Welding, Fiber Optic Beam Delivery, Hazardous Environments, Nuclear Applications

471. **URANIUM SCRAP CONVERSION AND RECOVERY**
$1,500,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LANL (Contract No. W-7405-ENG-36)
Contact: Dan Knobeloch, (505) 667-4417

Maintain and develop technologies for conversion and recovery of uranium scrap. Maintain and upgrade facilities for processing enriched uranium and managing uranium inventories.

Keywords: Uranium, Uranium Scrap, Enriched Uranium, Recovery, Processing, Inventories

LABORATORY DIRECTED RESEARCH AND DEVELOPMENT

472. **ELECTRONICALLY CORRELATED MATERIALS AT AMBIENT AND EXTREME CONDITIONS**
$328,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36)
Contact: J. D. Thompson, (505) 667-6416

This coordinated program was aimed specifically at an in-depth description of the many-body ground state in correlated electron systems. This research examined heavy-electron compounds under extreme conditions of pressure, temperature, and magnetic field, thereby allowing unique insights into the correlated ground states.

Keywords: Heavy Electron Systems, Materials Under Extreme Conditions

473. **ORGANOMETALLIC CHEMICAL VAPOR DEPOSITION**
$248,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36)
Contact: D. C. Smith, (505) 667-2424

Most conventional metal halide based chemical vapor deposition processes take place at temperatures in excess of 800°C and produce corrosive gases (e.g., HCl, HF). Organometallic complexes as CVD precursors are a simple and powerful method for producing coatings at low temperatures, eliminating deleterious byproducts, and removing the halide from the process completely. In this effort, new routes to metal and metal carbide thin films from volatile organometallic precursors have been developed. Potential applications for these new low-temperature materials include: weapons diagnostics, oxidation protection coatings for polymers, barrier materials for use in nuclear fuels and high-temperature (>2000°C) environments, and coatings for solid propellants.

Keywords: Metal Thin Films, Metal Carbide Thin Films, Chemical Vapor Deposition

474. **POLYMER SORBENTS FOR HAZARDOUS METAL UPTAKE**
$164,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36)
Contact: B. Jorgensen, (505) 667-3619

Polymer sorbents with immobilized metal complexing agents are being developed for treatment of radioactive and mixed waste. The polymers are applicable to treatment of process streams, waste streams and environmental remediation. The polymers will remove hazardous metals and radionuclides from aqueous solutions. Two types of systems are being investigated. One of these is a water soluble polymer-supported extraction system for use in ultrafiltration technology and the other utilizes chelating resins. In each case, selective ligands are covalently bound to polymers and the polymers tested for metal ion uptake. Los Alamos is involved in the design, synthesis, and evaluation of actinide selective ligands in collaboration with several universities. Ligands developed in this program and other promising ligands are used in the polymer sorbents. The polymers are being tested on simulated waste mixtures and we hope to be able to test them on actual DOE radioactive waste.

Keywords: Metal Complexes, Radioactive Waste, Mixed Waste, Polymer Sorbents

475. **MICROSCOPIC MATERIALS MODELING: TEXTURES AND DYNAMICS**
$109,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36)
Contact: A. Bishop, (505) 667-6491

We applied analytical techniques developed in nonlinear science and simulation techniques using massively parallel computation to study textures and their dynamical consequences in areas of condensed matter and materials science. Specifically, we have (1) implemented a Langevin MD code on the CM-2 that allows for study of large 2D Josephson junction arrays and 2D magnets; (2) simulated spiral surface growth in the presence of Frank-Read dislocation sources; (3) developed a nonlinear-nonlocal elasticity formalism for 2D martensitic materials; (4) discovered a new "glassy" relaxation response for large arrays of Josephson junctions in the presence of thermal noise and structural disorder; (5) used collective coordinate and MC-MD techniques to analyze the classical anisotropic Heisenberg model and relate dynamics of vortices to recent experiments.

Keywords: Textures, Condensed Matter, Materials Science, CM-2, Frank-Read Dislocations, Josephson Junctions, Heisenberg Model

476. **SURFACE MODIFICATION OF MATERIALS**
$315,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36)
Contact: M. Nastasi, (505) 667-7007

A combination of surface processing techniques, including reactive and non-reactive physical vapor deposition (PVD), ion implantation alloying, ion beam and excimer laser mixing, have been used to synthesize intermetallic, ceramic, and composite coatings with amorphous and/or ultrafine-microstructures. The influence of synthesis variables on microstructural evolution and phase formation was evaluated using X-ray diffraction and transmission electron microscopy. Composition analysis was carried out using ion backscattering. The surface mechanical properties of these materials were evaluated for hardness and modulus using nanoindentation techniques and, in some instance, the friction and wear performance was also evaluated using a pin-on-disk tribometer.

Keywords: Physical Vapor Deposition, Ion Implantation, Ion Beam/Laser Mixing, Intermetallic Coatings, Ceramic Coatings, Composites

477. **INTEGRATION OF FUNDAMENTAL KNOWLEDGE IN PLASTICITY AND TEXTURES TO PROVIDE TECHNICAL TOOLS FOR MICROSCOPIC APPLICATIONS**
$290,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36)
Contact: U. F. Kocks, (505) 667-9323

The individual components of understanding that have been developed in basic research on mechanical properties are being integrated into a complete, coherent description of material behavior in plasticity. This involves the kinetics of flow and strain hardening, as well as texture development and the influence of textures on plastic anisotropy. Methods are established for determining the parameters required for applications of the model. User-friendly computer codes are maintained for the analysis of experimental textures, as well as for the prediction of current anisotropies on the basis of measured textures, and for the future development of texture and anisotropy during deformation through simulation of polycrystal plasticity. One aim is to foster development of a universal materials response package for incorporation into large engineering design codes for structures as well as processing. Conversely, these codes are used to derive properties of heterogeneous materials.

Keywords: Texture, Plastic Anisotropy, Plastic Deformation, Polycrystal Plasticity, Modeling

478. **HIGH RESOLUTION ELECTRON MICROSCOPY OF MATERIALS**
$350,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36)
Contact: T. E. Mitchell, (505) 667-0938

The high resolution electron microscopy (HREM) facility is based on a Philips CM30T microscope operating at 300 kV. Its point-to-point resolution of 1.9A makes it possible to obtain structure images of most materials at the atomic level. Image processing and enhancement procedures are being used to optimize the images obtained. Multi-slice image simulations on proposed structures are used to compare with experimental images and obtain information on atomic positions around defects such as dislocation and interfaces.

HREM is being used on a wide range of materials applications. These include interfaces in semiconductor multilayers, grain boundaries in high temperature superconductors, twin boundaries in molybdenum disilicide, interfaces between silicon carbide and silicon nitride, and dislocations in refractory oxides.

Keywords: High Resolution Electron Microscopy, Materials at the Atomic Level, Molybdenum Disilicide, Silicon Carbide/Silicon Nitride Interfaces, Refractory Oxides

479. **NANO-FABRICATION**
$255,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36)
Contact: Robert Day, (505) 667-2957

This project combines theory and experiment to investigate the limits of nano-fabrication technology. We are primarily using molecular dynamics (MD) to simulate the actions and interaction of materials at the nanometer size. MD is used to study the stability of nanofeatures and to simulate nanomachining.

Keywords: Nano-fabrication, Molecular Dynamics, Nanomachining

480. **THIN FILM MICRO-ELECTROCHEMICAL SENSOR DEVELOPMENT**
$210,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36)
Contact: F. H. Garzon, (505) 667-6643

The objective of this project is the development of solid state microelectrochemical sensors that are applicable to the monitoring of hazardous gases such as: chlorine containing solvent vapors, sulfur dioxide, and halogen gases.

Keywords: Chemical Sensors, Chlorinated Hydrocarbons, Sulfur Oxides, Halogen Gases

481. **LIQUID CRYSTAL THERMOSETS**
$200,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36)
Contact: B. C. Benicewicz, (505) 665-0101

Designing composite materials at the nano-scale or molecular level is predicted to lead to mechanical properties several orders of magnitude greater than current materials. In the area of organic polymer composites, it has been shown that increases in properties are possible, but the usefulness of such materials is limited because of phase separation of the immiscible liquid crystal reinforcement and isotropic matrix components. This effort is a study of a new concept to make stable molecular composites using high performance liquid crystal polymers and newly developed liquid crystal thermoset matrices.

Keywords: Liquid Crystal Polymers

482. **NEUTRON AND RESONANT X-RAY SCATTERING BY MATERIALS**
$350,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36)
Contact: A. C. Lawson, (505) 667-8844

The techniques of pulsed neutron scattering and resonant X-ray diffraction are used to study materials such as actinides, f-electron ferromagnets and structural materials.

Keywords: Neutron Scattering, X-ray Scattering, Actinides, Ferromagnets

483. **STRUCTURAL AND ELECTRONIC COMPETITIONS IN LOW-DIMENSIONAL MATERIALS**
$360,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36)
Contact: B. I. Swanson, (505) 667-5814

This represents a combined theoretical and experimental study of the structural and electronic properties of low-dimensional electronic materials as they are tuned to the phase boundary region between different broken symmetry states (charge-density-and spin-density-wave, CDW and SDW). Within the CDW/SDW phase boundary region, competitions arise between the ground and local states (doping, photoinduced) that give rise to large changes in the transport (electrical) and optical properties. Work to date has focused on (1) developing new approaches to chemically tuning these materials through the phase boundary region, (2) studies (theory and experiment) of weak CDW and SDW materials, and (3) studies of mixed-halide materials, where the properties of the dominant species can be used to control the structure and electronics of the doped species. Key findings to date include (1) a new approach to tuning these materials through a structural "template" effect, (2) many-body modeling of species near the phase boundary region that shows evidence for CDW/SDW transitions and complex new structures, and (3) observation of the quenching of the Peierls distortion and the CDW in

MX' segments of chains doped into a host MS lattice.

Keywords: Me Phase Boundary Tuning, Low-Dimensional Electronic Materials

484. **FUNDAMENTAL ASPECTS OF PHOTO-ELECTRON SPECTROSCOPY IN HIGHLY CORRELATED ELECTRONIC SYSTEMS**
$300,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36)
Contact: A. K. Arko, (505) 665-0758

Materials displaying strong electron-electron correlations continue to occupy condensed matter physicists, particularly in view of high T_c materials, where these correlations may be all important. Several variations of the Hubbard model are proposed as possible representations of this electronic structure. Photoelectron spectroscopy plays a major role in this research since it is one of the few experimental tools via which it is possible to observe the electronic structure directly without resorting to interpretation. We have performed numerous photoelectron spectroscopy tests on a large number of Ce- and Yb-based heavy fermions and compared the results to predictions of the model. Our single crystal data continue to indicate that the features usually identified as arising from the magnetic, or Kondo interaction, are much more logically described to first order as simple core levels.

Keywords: Photoemission Spectroscopy, Electronic Correlations

485. **DEVELOPMENT OF HIGH STRENGTH HIGH CONDUCTIVITY MATERIALS FOR HIGH MAGNETIC FIELD DEVICES**
$100,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36)
Contact: F. M. Mueller, (505) 667-9244

The project will cover the fabrication analysis and design of high strength high conductivity materials for pulsed magnet applications of relevance to NHMFL. New methods of fabrication will be considered based on the use of rapid solidification and cryogenic forming. An analysis of the materials will be conducted based on measurement of mechanical properties, characterization of the structure by SEM and TEM methods and measurement of the ratio of the electrical conductivity at 293K and 77K as a function of the material's thermal-mechanical history. Attempts will be made to link the results of the study directly to the needs of NHMFL in terms of both magnetic coil design and optimization of relevant fabrication methods.

Keywords: Conductive Materials, Magnetic Coil Designs

486. **LOW TEMPERATURE STM FOR STRUCTURAL AND SPECTROSCOPIC STUDIES OF HIGH TEMPERATURE SUPERCONDUCTORS AND OTHER ELECTRONIC MATERIALS**
$50,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36)
Contact: M. Hawley, (505) 665-3600

The STM is a powerful probe of the local density of states in the study of electronic materials. The extension of this capability to low temperatures creates an opportunity to apply this technique to such studies as phase transitions in low dimensional electronic materials and in superconductors, i.e., I-V gap measurements and vortex lattices. To this end, this program includes the design and construction of a variable low temperature STM for the study of these materials. Where possible, we will explore the utility of this technique in the study of changes in morphology of structural materials with lower temperature applications and to the fabrication of nanoscale features.

Keywords: Scanning Tunneling Microscope, Electronic Materials, Low Temperature Scanning

487. **MATERIALS WITH FINE MICROSTRUCTURES**
$365,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36)
Contact: R. B. Schwarz, (505) 667-8454

The refinement of the microstructure of multiphase alloys can lead to significant enhancements in the mechanical properties of engineered materials. One synthesis route for such materials is the consolidation of powders with fine microstructures. This program addresses both the problem of synthesizing powders with fine microstructures and the problem of consolidating these powders while preserving their fine microstructure.

Keywords: Multiphase Alloys, Microstructure, Powder Consolidation

488. **ION BEAM MATERIALS RESEARCH**
$330,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36)
Contact: C. J. Maggiore,
(505) 667-6133

The synthesis of any new material cannot proceed efficiently without the quantitative characterization of the composition and structure of the material actually fabricated. The use of MeV ions is a well understood means of quantitative analysis and is routinely available at the IBML (Ion Beam Materials Laboratory). However, the continued development of new materials with better defined structure and composition on a finer scale has placed more stringent requirements on existing analytical methods. The objective of this program is to extend the analytical range and applicability of the IBML to the classes of new synthetic materials of current technological interest. Samples will be prepared by a variety of collaborators that are suitable for studying the fundamental limitations of multiple straggling on depth resolution using ion beams, improving sensitivity limits for light elements in complex samples using prompt and delayed nuclear reaction analysis, and bulk detection of hydrogen.

Keywords: Ion Beam Characterization

489. **TEXTURE STUDIES OF HIGHLY DEFORMED COMPOSITE MATERIALS**
$192,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36)
Contact: A. C. Larson, (505) 667-2942

Recently scientists have become interested in creating composite materials, such as high Tc-superconductors encased in silver wire and then deformed to prepare a tape, aluminum with SiC whiskers embedded in the aluminum matrix and copper metal containing tungsten wires. These composite materials are an effort to prepare materials displaying an optimal combination of the properties of the component materials. It is important to recognize that, in the deformation of two-phase systems, two processes become of importance: (a) the development of accommodation strain or arrays of geometrically necessary dislocations around the particles of the more rigid phase and (b) a change in the patterns of the flow in each phase due to the presence of the other phase. The occurrence of these processes is dependent on the relative fractions of the phases. We propose to study the relationships among the phases present in a composite by examination of the texture or orientation distribution of the crystallites in each phase.

Keywords: Silicon Carbide Whisker Reinforced Aluminum, Tungsten Wire Reinforced Copper, Two Phase Deformation

490. **PRESSURE DEPENDENCY OF THE STRUCTURE OF HIGH EXPLOSIVES: NITROMETHANE**
$192,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36)
Contact: R. B. VonDreele,
(505) 667-3630

This program examines the structural changes as a function of pressure for nitromethane and correlates them with the pressure dependence of solid state ionization processes proposed as an explosion front propagation mechanism.

Keywords: Nitromethane, Pressure Dependencies, Explosive Front Propagation Mechanisms

491. **NEUTRON REFLECTION STUDIES OF THIN FILM AND MULTILAYER STRUCTURES**
$300,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36)
Contact: M. R. Fitzsimmons,
(505) 665-4045

The purpose of this research program is to understand magnetism in thin film and multilayer structures using polarized neutron reflection (PNR). In order to obtain meaningful measurements of the magnetic structures and properties of surfaces and interfaces, the capability to manufacture thin films and multilayers, while PNR measurements are made, is essential. Such a capability—a first for a neutron source—will be developed. Topics to be explored by this research program are: two-dimensional magnetism, the kinetics of diffusion within multilayers, diffusion-induced changes of the magnetic properties of multilayers, the correlation between the magnetic properties of surfaces and interfaces with their roughness, and the design of improved super-mirrors for neutron applications.

Keywords: Magnetic Properties of Thin Films, Polarized Neutron Diffusion in Multilayers

492. NEUTRON REFLECTIVITY STUDIES OF IN SITU CORROSION OF METAL SURFACES
$145,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36)
Contact: G. S. Smith, (505) 665-2842

Corrosion of metallic surfaces have been studied for many years by several techniques. These studies have looked at the problem of corrosion both as a problem to be eradicated and as a useful end to the electroplating process. Never before has anyone been able to look at the microscopic details of composition as well as surface roughness at the metal-electrolyte interface. This program uses neutron reflectometry to study these features.

Keywords: Corrosion, Neutron Reflectometry

493. THE DYNAMICS OF AMORPHOUS MATERIALS
$330,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36)
Contact: R. A. Robinson, (505) 667-3626

This research program studies the vibrational and magnetic dynamics of amorphous materials, using inelastic neutron scattering. While atomic and magnetic fluctuations are well understood as collective excitations (e.g., phonons, magnons) in single crystals, much less is understood in amorphous materials. The materials to be studied include silica, porous silica aerogels, a metallic glass and metglas.

Keywords: Vibration Dynamics, Magnetic Dynamics, Silica, Silica Aerogels, Metallic Glasses

494. ADVANCED MATERIAL SCIENCE ALGORITHMS FOR SUPERCOMPUTER ARCHITECTURES
$75,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36)
Contact: J. E. Gubernatis, (505) 667-6727

This project is concerned with exploiting the potential new computer architectures offer to improving the understanding and modeling of material properties and behavior through computer simulation. The focus is on developing the simulation ability to study flux line dynamics, noise, melting, and pinning in London and Ginzburg-Landau phenomenological models of thin films on high temperature superconducting materials. The emphasis of the program is also on parallizing the world-line quantum Monte Carlo method and developing procedures to extract dynamical information from imaginary-time quantum Monte Carlo data.

Keywords: High Temperature Superconducting Materials, London Phenomenological Models, Ginzburg-Landau Phenomenological Models

495. METAL VAPOR SYNTHESIS IN ORGANOMETALLIC CHEMISTRY
$235,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36)
Contact: J. G. Watkin, (505) 667-4546

This program will employ the rare synthetic technique of metal vapor synthesis (MVS) to prepare a series of organometallic complexes of middle- and late-transition metals and lanthanides. Applications include catalytic processes and/or organic synthesis. The technique of metal vapor synthesis has been employed to prepare many examples of low-valent early transition metal complexes which have been shown to exhibit high reactivity, but the technique has rarely been applied to the later transition metals such as Rh, Ir, Pd, Pt and the lanthanides.

Keywords: Metal Vapor Synthesis, Lanthanides

496. SEPARATION CHEMISTRY OF TOXIC METALS
$250,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36)
Contact: P. H. Smith, (505) 667-1604

The goal of this research is to develop a new class of chelators for toxic metals which have the capacity to bind two species and where the binding of one substrate affects the binding of the second. In the process we hope to gain a fundamental understanding of the key parameters which govern toxic metal ion selective binding as it relates to separations chemistry. We will synthesize and evaluate a class of chelators which add a new dimension to coordination chemistry, namely cooperative/antagonistic binding. The chemistry involves the development and synthesis of ditopical receptors which contain two binding sites in close proximity to each other. In systems with cation and anion sites, the simultaneous binding of both a cation and an anion can enhance the overall binding constants relative to either one binding alone.

Keywords: Cooperative/Antagonistic Binding Sites, Chelates, Ditopical Receptors

497. **POLYMERS FOR INTEGRATED OPTICAL INTERCONNECTS**
$266,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36)
Contact: B. Laurich, (505) 665-0333

The recent discovery of electroluminescent polymers opens up, for the first time, the possibility of using optical interconnects for conventional silicon integrated circuits. If this capability can be realized, it will have a tremendous impact on the architecture and performance of the complex computing and communications systems.

Keywords: Electroluminescent Polymers, Integrated Optical Interconnects

498. **HIGH TEMPERATURE MATERIALS SYNTHESIS WITHOUT HEAT: OXIDE LAYER GROWTH ON ELECTRONIC MATERIALS USING HIGH KINETIC ENERGY ATOMIC SPECIES**
$164,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36)
Contact: M. A. Hoffbauer, (505) 667-4878

This research program examines high temperature materials synthesis using high kinetic energy atomic species instead of heat. Emphasis is being placed on the direct growth of oxide and nitride insulating layers on compound semiconducting electronic materials such as GaAs where we have already shown the unprecedented formation of oxide layers that are thick, uniform, and of extremely high quality. Research into this novel material synthesis process with the aim of producing and demonstrating device-quality oxide layers is being emphasized. Application of this materials synthesis technology to space-based manufacturing technology is also being pursued.

Keywords: Ceramic Oxides, Ceramic Nitrides, Insulating Layers, KE Atomic Heating

499. **DYNAMIC DEFORMATION OF ADVANCED MATERIALS**
$855,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36)
Contact: G. T. Gray, (505) 667-5452

Composites, metal or ceramic matrix, and advanced materials, such as intermetallics, are receiving increasing attention due to their higher specific strengths, stiffness, and high temperature properties. Advanced composites also allow other physical properties besides mechanical properties to be custom tailored to specific applications. Increased utilization of these material classes under dynamic loading conditions requires an understanding of the relationship between high-rate/shock-wave response as a function of microstructure if predictive material behavior capabilities are to be attained. This program is a multidisciplinary effort to investigate the influence of microstructure, anisotropy, orientation, and structural ordering on the high-strain-rate and shock-wave deformation behavior of advanced composites and intermetallics. The long-term objective is to provide high quality experimental measurements on advanced materials to facilitate the development of predictive computational models.

Keywords: High-Strain Rate Deformation, Shock-Wave Deformation, Composites, Intermetallics

500. **STRAIN MEASUREMENTS IN INDIVIDUAL PHASES OF MULTI-PHASE MATERIALS**
$130,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36)
Contact: J. A. Goldstone, (505) 667-3629

Employment of metal matrix and ceramic composites in high-technology aerospace applications or as lighter (more economic) material in the auto industry requires the development of analytical methods capable of predicting the durability, debonding, and damage tolerance during the mechanical and thermal loads expected during service. Neutron diffraction has been used to measure residual stress in composites, steels, and compacted powders. We wish to extend our capability by acquiring a stress rig with a furnace to make in situ measurements of material response. This will permit measurements on technologically important materials under conditions close to service. Preliminary studies will address an Al/TiC composite (under consideration for automotive use) and $MoSi_2$.

Keywords: Neutron Diffraction, Aluminum/Titanium Carbide Composites, Molybdenum Disilicide Composites

501. **ARTIFICIALLY STRUCTURED NONLINEAR OPTIC AND ELECTRO-OPTIC MATERIALS**
$465,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36)
Contact: B. I. Swanson, (505) 667-5814

New artificially structured materials that are optimized for nonlinear optic (NLO) and electro-optic applications will be synthesized, characterized, and modeled. Materials based on two new synthetic strategies will be pursued.

Chromophores with optical absorptions tuned to the red and near-IR portion of the spectrum will be directly attached to optical surfaces through the use of covalent bonding of self-assembled (CBSA) mono- and multilayers. The second strategy is based on the construction of single hetero-junctions or multiple hetero-junctions in super-lattice materials where charge separation across the junctions results in optimal NLO and electro-optic properties. The overall goal is to further develop these two synthetic approaches through a combined synthesis, characterization, and theory effort where materials modeling, benchmarked by observed physical properties, is used to guide rational synthesis of advanced materials.

Keywords: Nonlinear Optic Materials, Electro-Optic Materials, Superlattice Materials

502. **STRUCTURAL PHASE TRANSITIONS IN NON-STOICHIOMETRIC OXIDES**
$275,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36)
Contact: A. Migliori, (505) 667-2515

Structural phase transitions (SPT) have profound effects on mechanical, magnetic, and electronic properties. In Stoichiometric compounds, SPTs are well understood and produce the magnetism in ferrites and the ferroelectricity in piezoelectric oxides that make these materials so important. However, for non-stoichiometric compounds, the situation is very far from clear, and the puzzles are not merely academic. For example, the high T_c perovskite $La_{2-x}Sr_xCuO_4$ undergoes a second-order SPT from a tetragonal to an orthorhombic structure upon cooling through $T_s(x)$. As T_s is approached from either direction, one shear modulus collapses, making the material mechanically partially unstable, a non-trivial consequence for applications. The surprise is that this collapse begins 100K above T_s, not at 2K predicted by the best theoretical approach. Resonant Ultrasound Spectroscopic (RUS) studies of this and other SPTs reveal additional and subtle problems with current theory, not observed with any other experimental problem. Lack of just this sort of observation has stymied the theory of SPTs in heavily doped crystals because a simple observation of modulus collapse cannot distinguish between several competing possibilities. An understanding of the effects of doping on material properties near SPTs is of extreme fundamental interest and is crucial for a very broad spectrum of applications; recent observations by us suggest that only LANL's unique RUS capability can provide the necessary clues.

Keywords: Resonant Ultrasound Spectroscopy, Structural Phase Transitions

503. **STRONGLY CORRELATED ELECTRONIC MATERIALS**
$495,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36)
Contact: K. S. Bedell, (505) 665-047

New, novel materials have a number of extra-ordinary and often unexpected properties and, it is likely, they will play a major role in the high-technology electronic materials of the future. To better design materials for specific applications it is necessary to understand the microscopic origins of their novel physical characteristics. To relate the microscopic models of these strongly correlated systems to specific materials properties requires the extension of and the development of new many-body techniques. This program provides the basic science component for a number of new initiatives that include the Presidential initiative in materials science, the Advanced Computing Laboratory (ACL), the use of novel electronic materials for device applications, the National High Magnetic Field Laboratory (NHMFL), the UC Los Alamos INCOR program in high temperature superconductivity (HTS), and the Program in Correlated Electron Theory.

Keywords: High-Temperature Electronic Materials, Electronic Correlations

504. **PLASMA IMMERSION ION IMPLANTATION FOR SEMICONDUCTOR FILM GROWTH**
$261,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36)
Contact: M. Tuszewski, (505) 667-3566

An interdisciplinary team of plasma and semi-conductor physicists will develop a novel plasma implanter for thin film growth on semiconductors with unprecedented control. The scientific objectives of this project are: (1) construction of a compact, inexpensive, and high-throughput implanter based on an inductive plasma source and on e plasma immersion ion implantation (PIII) technique; (2) extension of the PIII technique to higher frequencies, lower voltages, and higher dose rates; (3) characterization, optimization, and control of the plasma species concentrations and impurities; (4) generation of semiconductor dielectrics and alloys for new electronics device technologies.

Keywords: Plasma Ion Implantation, Semiconducting Materials

505. **ANALYSIS OF STRUCTURE AND ORIENTATION OF ADSORBED POLYMER IN SOLUTION SUBJECT TO DYNAMIC SHEAR STRESS**
$172,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36)
Contact: S. Baker, (505) 667-6069

Polymer based separation techniques rely on the ability of a binding portion of the polymer to interact with a specific molecule in a solution flowing past the polymer. The location of the binding site within or out of the entangled polymer chains is thus crucial to the effectiveness of these methods. For this reason, the details of flow induced deformation of the polymer chains is important in such applications as exclusion chromatography, waste water treatment, ultra-filtration, enhanced oil recovery and microbial adhesion. Few techniques exist to examine the structure and orientation of polymeric materials, and even fewer to examine systems in a dynamic fluid flow. The goal of this program is to understand the molecular structure and orientation of adsorbed polymers with and without active binding ligands as a function of solvent shear rate, solvent ower, polymer molecular weight, surface polymer coverage, and heterogeneity of the surface polymer chains by neutron reflectometry in a newly Designed shear cell. Geometrical effects on binding of molecules in the flow will also be studied subject to the same parameters.

Keywords: Polymer Molecules, Neutron Reflectometry, Flow Induced Deformation

506. **DEVELOPMENT OF PAIR DISTRIBUTION FUNCTION ANALYSIS OF MESO-STRUCTURAL DETAILS IN SINGLE CRYSTAL PEROVSKITES AND NANOCRYSTALLINE MATERIALS**
$170,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36)
Contact: G. H. Kwei, (505) 667-8840

It has become increasingly evident that structural coherence in the CuO_2 planes of high-Tc super-conducting (HTSC) materials over some intermediate length scale (in the nanometer range) is important to superconductivity. Significant progress has been made in understanding these structural instabilities using pair distribution function analysis of powder diffraction data. However, PDF diffraction data on single crystals is required, both because of the greater amount of information in the latter and because of the much greater sample quality that is available in single crystals. The goal of this program is to develop analysis techniques for obtaining PDF's from single crystal diffraction data and to use these techniques to study structural instabilities and structural coherence in HTSC and other interesting materials. PDF techniques are also planned for studying mesostructural features in nanocrystalline materials.

Keywords: Powder Diffraction Analysis, High Temperature Superconductors, Mesostructural Nanocrystals

507. **NEUTRON SCATTERING AS A PROBE OF THE STRUCTURE OF LIQUID CRYSTAL POLYMER-REINFORCED COMPOSITE MATERIALS**
$180,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36)
Contact: R. P. Hjelm, (505) 665-2372

The goal of this program is to obtain nanoscale and molecular level information on the mechanism of reinforcement 9n crystal polymer-reinforced composites, and to realize the production of molecularly-reinforced LCP composites. Small-angle neutron scattering methods are proposed to study the structures on length scales ranging from 10-1000 Å. The goal of the small-angle scattering measurements is to understand the morphology of separation of the reinforcing and matrix phases as a function of composition, mixing, temperature and other process conditions. This information will be correlated with mechanical properties to achieve a better understanding of the molecular mechanism of reinforcement.

Keywords: Small-Angle Neutron Scattering, Polymer Composites

508. **STRAIN MEASUREMENTS IN INDIVIDUAL PHASES OF MULTI-PHASED MATERIALS DURING THERMOMECHANICAL LOADING: LANSCE NEUTRON SCATTERING EXPERIMENT SUPPORT**
$318,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36)
Contact: J. A. Goldstone, (505) 667-3629

Employment of metal matrix and ceramic composites in high-technology aerospace applications or as lighter (more economic) material, in the auto industry requires the development of analytical methods capable of predicting the durability, debonding, and damage tolerance during the mechanical and thermal loads expected during service. Neutron diffraction has been used to measure residual stress in composites, steels and compacted powders. We wish to extend our capability by acquiring a stress rig with a furnace to make in situ measurements of material response. This will permit measurements on technologically important materials under conditions close to service. Preliminary studies will address an Al/TiC composite (under consideration for automotive use) and $MoSi_2$.

Keywords: Neutron Diffraction, Metal Matrix Composites, Ceramic Matrix Composites

509. **A NEW APPROACH TO TEXTURE MEASUREMENTS: ODF DETERMINATION BY RIETVELD REFINEMENT**
$73,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36)
Contact: R. B. VonDreele, (505) 667-3630

This program centers on the development of the experimental procedures and the mathematical treatment needed to produce an orientation distribution function (ODF) directly from full diffraction patterns from a sample in a limited number of orientations.

Keywords: Texture Measurement, Orientation Distribution Function, Diffraction Patterns

510. **APPLICATIONS OF FULLERENES IN NUCLEAR TECHNOLOGY**
$360,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36)
Contact: D. K. Veirs, (505) 667-9291

The major focus of our research efforts is in the use of fullerene-based materials in the solution to problems in the nuclear research and industry. Fullerene encapsulation of nuclear waste is of interest in the storage of high-level nuclear waste. Fullerene-encapsulated uranium or plutonium may be very stable with respect to the environment and may provide a safe and efficient way of disposing of nuclear waste. The metal-in-fullerene aspect or metal-doped fullerene compounds in conjunction with the high thermal stability and low density of fullerene suggests the fabrication of efficient, high-yield targets for the production of radioactive beams. It is likely that a target composed fullerene, upon proton-induced fission or spallation of the uranium, will allow the efficient release of the fission or spallation products for the purpose of producing radioactive nuclear beams. We propose to explore the production of actinide fullerides and to develop the relevant technology to generate and separate them for these purposes.

Keywords: Fullerenes, Encapsulation, Nuclear Waste, Uranium, Plutonium

511. **CERAMIC OXIDE FOAMS FOR SEPARATION**
$400,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36)
Contact: P. C. Apen, (505) 665-7513

Ceramic oxide foams and novel foam structures are playing an important role in environmental R&D, specifically in the areas of chemical separations and filtration for removal of heavy metals and particulates from contaminated waste streams and effluent. This program focusses on the investigation of virgin oxide and surface-modified oxide foams in environmental remediation applications. Processes for the preparation and modification of porous ceramic structures will be developed and the products characterized for functionality in the separation of heavy metal and toxic particulates from waste streams.

Keywords: Silica Foams, Silica Sol-Gels, Heavy Metal Ligands, Metal Ion Chelating Agents

512. **MATERIALS MODELING PROJECT**
$125,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36)
Contact: R. LeSar, (505) 665-0420

This program involves the modeling of laser-assisted deposition processes with an emphasis on laser/solid interactions, plasma chemistry and dynamics, nucleation and growth, and the theoretical design of novel materials. The modeling will also involve analytical studies of strain-induced diffusion along specific interfaces and Monte Carlo studies of diffusion in polycrystalline materials. The goal of the program is to link this work with a micromechanical fracture model.

Keywords: Laser-Assisted Deposition Processes, Micromechanical Fracture Models, Plasma Chemistry

513. **SYNTHESIS AND OPTICAL CHARACTERIZATION OF NOVEL FULLERENE-BASED COMPOSITES**
$50,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36)
Contact: J. M. Robinson, (505) 665-4834

This program takes an interdisciplinary approach to develop and study a novel family of fullerene-based organic and inorganic composites for applications as photodiodes and photovoltaic devices. The emphasis of the program is on "proof of principle" for the synthesis of new composite materials which will guide further synthetic refinements. A novel "host-guest" chemistry will result in two new classes of materials. The first class utilizes sol-gel chemistry to incorporate fullerenes into optically transparent hosts that are processable into thick glass monoliths or thin film waveguides. The principal role of the host is to protect the fullerene guests from environmental degradation, and to provide a low loss transparent medium for light transmission. The second class of materials is based on fullerene/conjugated polymer composites.

Keywords: Fullerene Composites, Photodiodes, Photovoltaic Devices, Sol-Gels

TECHNOLOGY TRANSFER INITIATIVE

514. **A PILOT PROGRAM: CHEMICAL VAPOR DEPOSITION OF DIAMOND IN A FLUIDIZED-BED FOR CUTTING TOOL AND TRIBOLOGICAL APPLICATIONS**
$250,000
DOE Contact: W. P. Chernock, (202) 586-7590
LANL (Contract No. W-7405-ENG-36)
Contact: David Carroll, (505) 667-2145

A program to develop and commercialize a process to generate high-quality diamond coatings for machine tools.

Keywords: Diamond Coatings, Chemical Vapor Deposition, Cutting Tools, Tribology

515. **ADVANCED BERYLLIUM PROCESSING**
$632,000
DOE Contact: W. P. Chernock, (202) 586-7590
LANL (Contract No. W-7405-ENG-36)
Contact: Loren Jacobson, (505) 667-5151

A program to produce beryllium powders and rolled beryllium sheet using improved manufacturing techniques that minimize worker exposure and reduce the environmental consequences of beryllium processing.

Keywords: Beryllium Processing, Beryllium Alloy Processing, Centrifugal Atomization

516. **AUTOMATED PULSED LASER DEPOSITION SYSTEM**
$130,000
DOE Contact: W. P. Chernock, (202) 586-7590
LANL (Contract No. W-7405-ENG-36)
Contact: Ross Muenchausen, (505) 665-4949

A program to design an automated pulsed laser deposition system to deposit high-temperature superconducting thin films.

Keywords: Pulsed-Laser-Deposition, High-Temperature Superconducting Films

517. **PLASMA SOURCE ION IMPLANTATION FOR THE AUTOMOTIVE INDUSTRY**
$1,326,000
DOE Contact: W. P. Chernock, (202) 586-7590
LANL (Contract No. W-7405-ENG-36)
Contact: Donald Rej, (505) 665-1883

A program to develop a production-scale plasma-source ion implantation system for improving the surface properties of auto parts.

Keywords: Plasmas, Ion Implantation, Tool Hardening

518. **PROCESSING MODELING AND CONTROL FOR U.S. STEEL INDUSTRY**
$1,195,000
DOE Contact: W. P. Chernock, (202) 586-7590
LANL (Contract No. W-7405-ENG-36)
Contact: Brian Lally, (505) 667-9954

A program to develop new process models and control systems for the U.S. Steel Industry.

Keywords: Steel, Electric-Arc-Furnace, Scrap Steels

OFFICE OF FOSSIL ENERGY

	FY 1996
Office of Fossil Energy - Grand Total	$6,713,000
Office of Advanced Research	$6,713,000
Fossil Energy AR&TD Materials Program	$6,713,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$2,720,000
Coating Process Development for Cr-Nb Alloys	120,000
Procurement of Advanced Austenitic and Aluminide Alloys	50,000
Development of Iron Aluminides	105,000
Development of Cr-Nb Alloys	200,000
High-Strength Iron Aluminide Alloys	78,000
Low-Aluminum Content Iron-Aluminum Alloys	50,000
Mo-Si Alloy Development	78,000
Development of Improved and Corrosion Resistant Surfaces for Fossil Power System Components	60,000
Commercial-Scale Melting and Processing of Low-Aluminum Content Alloys	50,000
Development of a Modified 310 Stainless Steel	143,000
Application of Advanced Austenitic Alloys to Fossil Power System Components	80,000
Influence of Processing on Microstructure and Properties of Aluminides	175,000
Investigation of Electrospark-Deposited Coatings for Protection of Materials in Sulfidizing Atmospheres	100,000
Technology Transfer of Electrospark-Deposited Coatings for Protection of Materials in Sulfidizing Atmospheres	80,000
Fabrication of Fiber-Reinforced Composites by Chemical Vapor Infiltration and Deposition	150,000
Compliant Oxide Coating Development	100,000
Development of Oxidation/Corrosion-Resistant Composite Materials and Interfaces	150,000
Optimization of the Chemical Vapor Infiltration Technique for Ceramic Composites	50,000
Transport Properties of Ceramic Composites	110,000
Modeling of Fibrous Preforms for CVD Infiltration	50,000
Corrosion Protection of SiC-Based Ceramics with CVD Mullite Coatings	100,000
Feasibility of Synthesizing Oxide Films on Ceramic and Metal Substrates	75,000
Ceramic Coating and Native Oxide Scales Evaluation	80,000
Metal Dusting Study	PYF[1]
Carbon Fiber Composite Molecular Sieves	267,000
Carbon Materials Equipment	30,000
Activation of Carbon Fiber Composite Molecular Sieves	64,000
Characterization of Coal and Coal Extracts	PYF[1]
Production of Aluminum Reduction Electrodes from Solvent-Extracted Coal-Derived Carbon Feedstocks	PYF[1]
Exploration of Coal-Based Pitch Precursors for Ultra-High Thermal Conductivity Graphite Fibers	PYF[1]
Development of Carbon-Carbon Composites from Solvent-Extracted Pitch	PYF[1]
Conversion of Pitches and Cokes from Solvent-Extracted Materials	PYF[1]
Carbon Fiber Composite Molecular Sieves Technology Transfer	50,000
Development of Precursors for Production of Graphites and Carbon Products	PYF[1]
Production of Yarn From VLS Whiskers	PYF[1]
Radio-Wave Nano-Phase Silicon Nitride and Silicon Carbide Processes	75,000

[1]PYF denotes that funding for this activity, active in FY 1996, was provided from prior year funds.

OFFICE OF FOSSIL ENERGY (continued)

	FY 1996
Office of Advanced Research (continued)	
Fossil Energy AR&TD Materials Program (continued)	
Materials Properties, Behavior, Characterization or Testing	$1,753,000
Investigation of the Weldability of Polycrystalline Iron Aluminides	75,000
Aqueous Corrosion of Iron Aluminides	PYF[1]
Evaluation of the Intrinsic and Extrinsic Fracture Behavior of Iron Aluminides	68,000
Investigation of Iron Aluminide Weld Overlays	30,000
Fireside Corrosion Tests of Candidate Advanced Austenitic Alloys, Coatings, and Claddings	100,000
Joining Techniques for Advanced Austenitic Alloys	50,000
Fatigue and Fracture Behavior of Cr-Nb Alloys	20,000
Corrosion and Mechanical Properties of Alloys in FBC and Mixed-Gas Environments	270,000
Mechanically Reliable Coatings and Scales for High-Temperature Corrosion Resistance	PYF[1]
High Temperature Environmental Effects on Iron Aluminides	170,000
Investigation of Moisture-Induced Embrittlement of Iron Aluminides	75,000
Corrosion Protection of Ultrahigh Temperature Intermetallic Alloys	200,000
Oxide Dispersion Strengthened (ODS) Iron Aluminides	275,000
Materials Support for HITAF	PYF[1]
Joining of Ceramics	50,000
Support Services for Ceramic Fiber-Ceramic Matrix Composites	50,000
Development of Nondestructive Evaluation Methods and Effects of Flaws on the Fracture Behavior of Structural Ceramics	270,000
Fracture Behavior of Advanced Ceramic Hot-Gas Filters	PYF[1]
Ceramic Catalyst Materials	50,000
Device or Component Fabrication, Behavior or Testing	$1,803,000
Materials and Components in Fossil Energy Applications Newsletter	50,000
Compilation and Editing of Book on Materials Behavior in Coal Liquefaction Plants	11,000
Ceramic Fiber Filter Technology	75,000
Development of Microwave-Heated Diesel Particulate Filters	PYF[1]
Development of Ceramic Membranes for Gas Separation and Fuel Cells	380,000
Furnace Equipment	100,000
High-Temperature Heat Exchanger and Hot-Gas Filter Development	172,000
Investigation of the Mechanical Properties and Performance of Ceramic Composite Components	135,000
Solid State Electrolyte Systems	655,000
ODS Fe_3Al Tubes for High-Temperature Heat Exchangers	PYF[1]
Porous Iron Aluminide Alloys	PYF[1]
Iron Aluminide Filters for IGCCs	53,000
Iron Aluminide Filters for PFBCs	45,000
Corrosion Resistance of Iron Aluminides in CS_2 Environments	27,000

[1]PYF denotes that funding for this activity, active in FY 1996, was provided from prior year funds.

OFFICE OF FOSSIL ENERGY (continued)

	FY 1996
Office of Advanced Research (continued)	
Fossil Energy AR&TD Materials Program (continued)	
Thermal and Mechanical Analysis of a Ceramic Tubesheet	PYF[1]
Ceramic Tubesheet Design Analysis	PYF[1]
Dense Ceramic Tube Development	100,000
Instrumentation and Facilities	$ 437,000
Management of the Fossil Energy AR&TD Materials Program	400,000
General Technology Transfer Activities	35,000
Gordon Research Conference Support	2,000

OFFICE OF FOSSIL ENERGY

The Office of Fossil Energy responsibilities include management of the Department's fossil fuels (coal, oil and natural gas) research and development program. This research is generally directed by the Office of Coal Technology (OCT), the Office of Gas and Petroleum Technology, and the Office of Advanced Research and Special Technologies in support of the National Energy Strategy Goals for Increasing Energy Efficiency, Securing Future Energy Supplies, Respecting the Environment, and Fortifying our Foundations. Three specific fossil energy goals are currently being pursued:

- The first is to secure liquids supply and substitution. This goal targets the enhanced production of domestic petroleum and natural gas, the development of advanced, cost-competitive alternative fuels technology, and the development of coal-based, end-use technology to substitute for oil in applications traditionally fueled by liquid and gaseous fuel forms.
- The second is to develop power generation options with environmentally superior, high-efficiency technologies for the utility, industrial, and commercial sectors. This goal targets the development of super-clean, high-efficiency power generation technologies.
- The third is to pursue a global technology strategy to support the increased competitiveness of the U.S. in fossil fuel technologies, to maintain world leadership in our fossil fuel technology base, and provide expanded markets for U.S. fuels and technology. This crosscutting goal is supported by the activities in the above two technology goals.

OFFICE OF ADVANCED RESEARCH

FOSSIL ENERGY AR&TD MATERIALS PROGRAM

Fossil Energy (FE) materials-related research is conducted under an Advanced Research and Technology Development (AR&TD) Materials subactivity and is an integral part of the R&D conducted by the Office of Advanced Research and Special Technologies. The AR&TD Materials program includes cross-cutting research to obtain a fundamental understanding of materials and how they perform in fossil-based process environments and the development of new classes of generic materials that will allow the development of new fossil energy systems or major improvements in existing systems. The present program is focused on ceramics (composite structural ceramics, catalyst supports, solid state electrolytes, membranes, and ceramic filters), new alloys (aluminides, filters, advanced austenitic steels, and coatings and claddings), corrosion research, and technology development and transfer.

The AR&TD research is carried through development and technology transfer to industry. Special emphasis is given to technology transfer to ensure that the materials will be available for subsequent fossil commercial applications. This also enhances U.S. technological competitiveness not only in the fossil area but in the materials industry in general and other technology application areas as well. The research is conducted in industry, universities, not-for-profit agencies, and national laboratories. This widespread participation also helps maintain the U.S. materials technology capabilities.

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

519. **COATING PROCESS DEVELOPMENT FOR Cr-Nb ALLOYS**
$120,000
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: R. R. Judkins, (423) 574-4572
Ohio State University Contact: R. A. Rapp, (614) 292-6178

Cr-Nb alloys are being developed for high temperature service, but require protection from high temperature environments, such as oxidation. Previously developed $MoSi_2$-base coatings have shown some promise for protecting Nb, and the principles learned may have applicability for protective coatings of Cr-Nb. The purpose of this work is to examine the protection of Cr-Nb alloys with either silicides or aluminides.

Keywords: Alloys, Aluminizing, Chromizing, Corrosion, Coatings

520. **PROCUREMENT OF ADVANCED AUSTENITIC AND ALUMINIDE ALLOYS**
$50,000
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: R. R. Judkins, (423) 574-4572

This task provides funds for the procurement of alloys necessary for alloy development and testing activities of the AR&TD Materials Program.

Keywords: Alloys, Aluminides, Austenitic

521. **DEVELOPMENT OF IRON ALUMINIDES**
$105,000
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: G. M. Goodwin, (423) 574-4809

The objective of this task is to develop low-cost and low-density intermetallic alloys based on Fe_3Al with an optimum combination of strength, ductility, weldability, and corrosion resistance for use as components in advanced fossil energy conversion systems. Emphasis is on the development of iron aluminides for heat recovery applications in coal gasification systems.

Keywords: Alloys, Aluminides, Intermetallic Compounds

522. **DEVELOPMENT OF Cr-Nb ALLOYS**
$200,000
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: C. T. Liu, (423) 574-4459

The objective of this task is to develop high-strength, corrosion-resistant intermetallic alloys for use as hot components in advanced fossil energy conversion and power generation systems. The successful development of these alloys is expected to improve the thermal efficiency of fossil energy conversion systems through increased operating temperatures and to increase the service life of hot components exposed to corrosive environments at elevated temperatures (1000°C). The work is focused on *in situ* composite alloys based on the $Cr-Cr_2Nb$ system.

Keywords: Alloys, Chromium-Niobium, Corrosion, Intermetallic Compounds

523. **HIGH-STRENGTH IRON ALUMINIDE ALLOYS**
$78,000
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: C. G. McKamey, (423) 574-6917

The objective of this task is to use microalloying techniques to further develop the Fe_3Al-based alloys. Emphasis is on producing a low-cost, low-density, precipitation-strengthened Fe_3Al-based intermetallic alloy with improved high-temperature creep resistance while maintaining an optimum combination of room- temperature and high-temperature (600-700°C) tensile properties, weldability, and corrosion resistance for use as structural components of advanced fossil energy conversion systems.

Keywords: Alloys, Aluminides, Microalloy

524. **LOW-ALUMINUM CONTENT IRON-ALUMINUM ALLOYS**
$50,000
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: V. K. Sikka, (423) 574-5112

The objective of this task is to develop a conventionally-fabricable low-cost and lower density iron-aluminum-based alloy with a good combination of strength, ductility, weldability, and corrosion resistance for use as components in advanced fossil energy systems. Initial emphasis is on the development of iron-aluminum alloys for heat-recovery applications in coal gasification systems.

Keywords: Alloys, Iron-Aluminum

525. **Mo-Si ALLOY DEVELOPMENT**
$78,000
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: C. T. Liu, (423) 574-4559

The objective of this task is to develop new-generation corrosion-resistant Mo-Si alloys for use as hot components in advanced fossil energy conversion and power generation systems. The successful development of Mo-Si alloys is expected to improve the thermal efficiency and performance of fossil energy systems through increased operating temperature and to increase the service life of hot components exposed to corrosive environments at high temperatures (to

1600°C). The initial effort is devoted to Mo_5Si_3-base alloys containing boron additions.

Keywords: Alloys, Molybdenum, Silicon

526. **DEVELOPMENT OF IMPROVED AND CORROSION RESISTANT SURFACES FOR FOSSIL POWER SYSTEM COMPONENTS**
$60,000
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: V. K. Sikka, (423) 574-5112

A Cooperative Research and Development Agreement (CRADA) has been established with ABB Combustion Engineering for the development of corrosion-resistant surface protection for fossil power systems.

Keywords: Alloys, Iron-Aluminum, Corrosion, Technology Transfer

527. **COMMERCIAL-SCALE MELTING AND PROCESSING OF LOW-ALUMINUM CONTENT ALLOYS**
$50,000
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: V. K. Sikka, (423) 574-5112

The purpose of this activity is the preparation and evaluation of castings of low-aluminum content, iron-aluminum alloys. The castings will be prepared in several types of molds including: (1) graphite, (2) sand, and (3) investment. Castings will be prepared primarily from the air-induction-melted material. Selected graphite and investment castings will also be prepared from the vacuum-induction-melted material. The graphite and sand castings will be prepared at ORNL and will also be procured from the commercial foundries. The castings will be evaluated for porosity, grain structure, mechanical properties, and weldability. The mechanical property evaluation will consist of Charpy impact, tensile, and creep testing.

Keywords: Alloys, Iron-Aluminum, Melting, Casting

528. **DEVELOPMENT OF A MODIFIED 310 STAINLESS STEEL**
$143,000
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: R. W. Swindeman, (423) 574-5108

The purpose of this task is to evaluate structural alloys for improved performance of high-temperature components in advanced combined-cycle and coal-combustion systems.

Keywords: Materials, Mechanical Properties, Austenitics, Hot-Gas

529. **APPLICATION OF ADVANCED AUSTENITIC ALLOYS TO FOSSIL POWER SYSTEM COMPONENTS**
$80,000
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: R. W. Swindeman, (423) 574-5108

A Cooperative Research and Development Agreement (CRADA) has been established with ABB Combustion Engineering for the development of advanced austenitic alloys for fossil power systems.

Keywords: Alloys, Austenitics, Technology Transfer

530. **INFLUENCE OF PROCESSING ON MICROSTRUCTURE AND PROPERTIES OF ALUMINIDES**
$175,000
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: I. G. Wright, (423) 574-4451
Idaho National Engineering Laboratory Contact: R. N. Wright, (208) 526-6127

The purpose of this program is to determine the influence of processing on the properties of alloys based on the intermetallic compound Fe_3Al. Thermomechanical processing of these alloys is pursued to improve their properties. The response of the microstructure to elevated temperature deformation and subsequent annealing is characterized in terms of the establishment of equilibrium phases and equilibrium degree of long-range order. The role of dislocation and antiphase boundary structures in enhancing ductility of Fe_3Al is investigated. The tensile properties are determined at room and elevated temperature and related to the microstructure. Reaction synthesis is investigated as a novel joining method and as a process to fabricate porous iron aluminides for filter applications. Oxide dispersion strengthened alloys, fabricated by reaction synthesis, are developed for improved high temperature strength. Compositions of the Fe_3Al alloys and details of the processing are determined in collaboration with the program at Oak Ridge National Laboratory (ORNL).

Keywords: Aluminides, Processing, Microstructure

531. **INVESTIGATION OF ELECTROSPARK-DEPOSITED COATINGS FOR *PROTECTION OF MATERIALS IN* SULFIDIZING ATMOSPHERES**
$100,000
DOE Contacts: F. M. Glaser, (301) 903-2784
and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact:
R. R. Judkins, (423) 574-4572
Pacific Northwest National Laboratory
Contact: R. N. Johnson,
(509) 375-6906

The purpose of this task is to examine the use of the electrospark deposition coating process for the application of corrosion-, erosion-, and wear-resistant coatings to candidate heat exchanger (including superheater and reheater) alloys. Materials to be deposited may include MCrAl, MCrAlY, highly wear-resistant carbides, and other hardsurfacing materials.

Keywords: Coatings, Materials, Deposition

532. **TECHNOLOGY TRANSFER OF ELECTRO-SPARK DEPOSITED COATINGS FOR PROTECTION OF MATERIALS IN SULFIDIZING ATMOSPHERES**
$80,000
DOE Contacts: F. M. Glaser, (301) 903-2784
and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact:
I. G. Wright, (423) 574-4451
Pacific Northwest National Laboratory
Contact: R. N. Johnson,
(509) 375-6906

The purpose of this task is to transfer to industry the electrospark deposition coating process technology for the application of corrosion-, erosion-, and wear-resistant coatings to candidate heat exchanger [including superheater and reheater] alloys.

Keywords: Coatings, Materials, Deposition

533. **FABRICATION OF FIBER-REINFORCED COMPOSITES BY CHEMICAL VAPOR INFILTRATION AND DEPOSITION**
$150,000
DOE Contacts: F. M. Glaser, (301) 903-2784
and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact:
D. P. Stinton, (423) 574-4556

The purpose of this task is to develop a process for the fabrication of fiber-reinforced ceramic composites having high fracture toughness and high strength. This process utilizes a steep temperature gradient and a pressure gradient to infiltrate low-density fibrous structures with gases, which deposit solid phases to form the matrix of the composite. Further development of this process is needed to fabricate larger components of more complex geometry, and to optimize infiltration for shortest processing time, greatest density and maximum strength.

Keywords: Composites, Fiber-Reinforced,
Ceramics

534. **COMPLIANT OXIDE COATING DEVELOPMENT**
$100,000
DOE Contacts: F. M. Glaser, (301) 903-2784
and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact:
D. P. Stinton, (423) 574-4556

Monolithic SiC heat exchangers and fiber-reinforced SiC-matrix composite heat exchangers and filters are susceptible to corrosion by alkali metals at elevated temperatures. Protective coatings are currently being developed to isolate the SiC materials from the corrodents. Unfortunately, these coatings typically crack and spall when applied to SiC substrates. The purpose of this task is to determine the feasibility of using a compliant material between the protective coating and the substrate. The low-modulus compliant layer could absorb stresses and eliminate cracking and spalling of the protective coatings.

Keywords: Ceramics, Oxides, Coatings

535. **DEVELOPMENT OF OXIDATION/ CORROSION-RESISTANT COMPOSITE MATERIALS AND INTERFACES**
$150,000
DOE Contacts: F. M. Glaser, (301) 903-2784
and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact:
D. P. Stinton, (423) 574-4556

Fiber-reinforced SiC-matrix composites have been observed to fail in fossil energy applications for two reasons. First, the mechanical properties of composites deteriorate under stressed oxidation because oxidants such as steam penetrate cracks formed in the SiC matrix and react with the carbon or boron nitride interface. The mechanical properties of composites may degrade because of corrosion due to sodium species typically present in fossil systems. Therefore, the purposes of this task are to first, develop fiber-matrix interfaces that are resistant to oxidation and yet optimize the mechanical behavior of composites, and second, to develop protective overcoats or oxide matrices that are resistant to oxidation and corrosion.

Keywords: Composites, Ceramics,
Fiber-Reinforced, Interfaces

536. **OPTIMIZATION OF THE CHEMICAL VAPOR INFILTRATION TECHNIQUE FOR CERAMIC COMPOSITES**
$50,000
DOE Contacts: F. M. Glaser, (301) 903-2784 andM. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: D. P. Stinton, (423) 574-4556
University of Tennessee Contact: Peter Liaw, (423) 974-6356

This project is focused on an optimization of the forced chemical vapor infiltration technique for fabrication of ceramic matrix composites (CMCs) using process models. In particular, a process model developed at the Georgia Tech Research Institute shall be thoroughly investigated. Experimental verification of the process model shall be conducted in light of microstructural characterization using both destructive and nondestructive evaluation techniques. An optimized process for manufacturing CMCs shall be demonstrated. Moreover, mechanistic understanding regarding the effects of processing parameters on microstructural features, and fatigue and fracture behavior of CMCs shall be provided.

Keywords: Composites, Fiber-Reinforced, Ceramics

537. **TRANSPORT PROPERTIES OF CERAMIC COMPOSITES**
$110,000
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: D. P. Stinton, (423) 574-4556
Georgia Institute of Technology Contact: T. L. Starr, (404) 894-0579

The purpose of this research effort is to conduct a theoretical and experimental program to identify new compositions and processing methods to improve the physical and mechanical properties of selected fiber-reinforced ceramics. The ceramic matrix material is amorphous fused silica or modified silica glass, and the focus is the development of fiber-reinforced silica. Parameters studied include: (1) differences in elastic modulus between matrix and fiber, (2) differences in thermal expansion, (3) nature of interfacial bond, (4) densification of matrix, (5) nature of fiber fracture/pull-out, (6) fiber diameter and fiber length-to-diameter ratio, (7) fiber loading, and (8) fiber dispersion and orientation. A model will be developed based on the information generated in the experimental phase of the program.

Keywords: Ceramics, Composites, Fiber-Reinforced

538. **MODELING OF FIBROUS PREFORMS FOR CVD INFILTRATION**
$50,000
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: D. P. Stinton, (423) 574-4556
Georgia Institute of Technology Contact: T. L. Starr, (404) 894-0579

The purpose of this project is to conduct a theoretical and experimental program to develop an analytical model for the fabrication and infiltration of fibrous preforms. The analytical model will: (1) predict preform structure (density, porosity, fiber orientation, etc.) based on fabrication technique and fundamental fiber parameters (diameter, aspect ratio, etc.), and (2) predict permeation and heat conduction through the preform structure and, thus, predict the CVD infiltration performance.

Keywords: Ceramics, Composites, Modeling

539. **CORROSION PROTECTION OF SiC-BASED CERAMICS WITH CVD MULLITE COATINGS**
$100,000
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: D. P. Stinton, (423) 574-4556
Boston University Contact: Vinod Sarin, (617) 353-6451

This project involves the growth of dense mullite coatings on SiC-based substrates by chemical vapor deposition. SiC and SiC-based composites have been identified as the leading candidate materials for stringent elevated temperature applications. At moderate temperatures and pressures, the formation of a thin self-healing layer of SiO_2 is effective in preventing catastrophic oxidation by minimizing the diffusion of O_2 to the substrate. The presence of impurities can increase the rate of passive oxidation by modifying the transport rate of oxygen through the protective scale, can cause active oxidation via formation of SiO which accelerates the degradation process, or can produce compositions such as Na_2SO_3 which chemically attack the ceramic via rapid corrosion. There is therefore a critical need to develop adherent oxidation/corrosion-resistant, and thermal-shock-resistant coatings that can withstand such harsh environments. Mullite has been identified as an excellent candidate material due to its desirable properties of toughness, corrosion resistance, and a good coefficient of thermal expansion match with SiC.

Keywords: Ceramics, Coatings

540. **FEASIBILITY OF SYNTHESIZING OXIDE FILMS ON CERAMIC AND METAL SUBSTRATES**
$75,000
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: D. P. Stinton, (423) 574-4556
Lawrence Berkeley Laboratory Contact: Ian Brown, (510) 486-4174

The objective of this project is the study of the feasibility of synthesizing metal oxide ceramic films on ceramic and metal substrates. This feasibility will be demonstrated by use of plasma-based deposition and ion mixing techniques. The films shall be characterized for properties such as composition, structure, hardness, high temperature oxidation resistance, adhesion to the substrate, and stability to high temperature cycling. The value of intermediate transition or buffer layers, composed of materials with suitably matched thermal expansion characteristics and atomically graded interfaces, as a technique for improving the high temperature survivability of the films, shall be explored. Samples shall be formed on substrates of various shapes and sizes, including perhaps on the inside and outside of pipes, as well as on small flat coupons. The issue of deposition onto and atomic mixing into substrates which are insulating shall be addressed experimentally. The work is divided into two parts: (1) Al_2O_3 films on alumina-forming alloy substrates, and (2) oxides on SiC.

Keywords: Ceramics, Films, Oxides

541. **CERAMIC COATING AND NATIVE OXIDE SCALES EVALUATION**
$80,000
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contacts: P. F. Tortorelli, (423) 574-5119

The purpose of this work is to generate the information needed for the development of improved (slow growing, adherent, sound) protective oxide coatings and scales. The specific objectives are to systematically investigate the relationships among substrate composition and surface oxide structure, adherence, soundness, and micromechanical properties, (2) use such information to predict scale and coating failures, and (3) identify and evaluate compositions and synthesis routes for producing materials with damage-tolerant scales and coatings.

Keywords: Coatings, Corrosion

542. **METAL DUSTING STUDY**
PYF[1]
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contacts: P. F. Tortorelli, (423) 574-5119

The objective of this task is to establish the potential risk of operating problems due to carbon deposition and metal dusting in advanced coal gasification processes and to identify methods for avoiding carbon deposition. The work involves a literature search, compilation of a bibliography of relevant articles, and a summary of the current state of knowledge.

Keywords: Coatings, Corrosion

543. **CARBON FIBER COMPOSITE MOLECULAR SIEVES**
$267,000
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: T. D. Burchell, (423) 576-8595

Hydrogen recovery technologies are required to allow the upgrading of heavy hydrocarbons to transport fuels, thus reducing the amount of carbon rejected during the conversion of fossil resources into hydrocarbon products. The purpose of this work is to develop carbon molecular sieves (CMS) starting with porous carbon fiber composites (CFC) manufactured from petroleum pitch derived carbon fibers. The carbon fiber composite molecular sieves (CFCMS) will be utilized in pressure swing adsorption units for the efficient recovery of hydrogen from synthesis gas, refinery purge gases, and for other gas separation operations associated with hydrogen recovery.

Keywords: Carbon Fibers, Sieves, Composites

544. **CARBON MATERIALS EQUIPMENT**
$30,000
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: T. D. Burchell, (423) 576-8595

This task provides funds for the procurement of major equipment items , necessary for AR&TD Materials Program activities.

Keywords: Equipment

[1]PYF denotes that funding for this activity, active in FY 1996, was provided from prior year funds.

545. **ACTIVATION OF CARBON FIBER COMPOSITE MOLECULAR SIEVES**
$64,000
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: R. R. Judkins, (423) 574-4572
University of Kentucky Contact: Frank Derbyshire, (606) 257-0305

A novel monolithic adsorbent carbon, manufactured from carbon fibers, has been invented jointly by researchers at Oak Ridge National Laboratory (ORNL) and the University of Kentucky Center for Applied Energy Research. The novel material, referred to as a carbon-fiber composite molecular sieve (CFCMS) is fabricated at ORNL in the Carbon Materials Technology Group. The purpose of this activity is to activate samples of the CFCMS and to perform subsequent analyses of the surface area, pore width distributions, and micropore volume. Activities are directed toward an understanding of the relationships between the activation process and the micro- or mesopore structure that develops.

Keywords: Carbon Fibers, Sieves, Composites

546. **CHARACTERIZATION OF COAL AND COAL EXTRACTS**
PYF[1]
DOE Contacts: F. M. Glaser, (301) 903-2784 andM. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: R. R. Judkins, (423) 574-4572
University of Tennessee Contact: E. L. Fuller, (423) 974-6356

The objective of this work is to characterize coal and coal extracts and to assist Oak Ridge National Laboratory in the research activities connected with the Cooperative Research Partnership on Carbon Products and the Non Fuel Uses of Coal. Work involves the characterization of coal and coal extracts obtained form West Virginia University. Activation and reactivity studies of carbon materials, including carbon fiber composite molecular sieves, shall be performed. Analysis of the pore structures of activated carbons, including carbon fiber composite molecular sieves, shall be performed.

Keywords: Carbon Fibers, Sieves, Composites

547. **PRODUCTION OF ALUMINUM REDUCTION ELECTRODES FROM SOLVENT-EXTRACTED COAL-DERIVED CARBON FEEDSTOCKS**
PYF[1]
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: R. R. Judkins, (423) 574-4572
Alcoa Aluminum Company Contact: Dave Belitskus, (412) 337-4812

This research is directed toward the objective of producing aluminum reduction electrodes from solvent-extracted coal-derived carbon feedstocks obtained from West Virginia University (WVU) and Koppers Industries, Inc.

Keywords: Carbon, Feedstocks, Coal-Derived

548. **EXPLORATION OF COAL-BASED PITCH PRECURSORS FOR ULTRA-HIGH THERMAL CONDUCTIVITY GRAPHITE FIBERS**
PYF[1]
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: R. R. Judkins, (423) 574-4572
Amoco Performance Products, Inc. Contact: G. V. Deshpande, (770) 772-8200

The preparation of high-performance carbon (graphite) fibers requires a mesophase pitch precursor. Traditionally, in the USA, this has been derived from a petroleum precursor. Overseas suppliers have, however, developed high-performance fibers from coal derived precursors. Amoco Performance Products' goal is to explore coal-based pitch precursors' utility for use in ultra-high thermal conductivity graphite fibers.

Keywords: Carbon, Fibers, Graphite, Precursors

[1]PYF denotes that funding for this activity, active in FY 1996, was provided from prior year funds.

549. **DEVELOPMENT OF CARBON-CARBON COMPOSITES FROM SOLVENT-EXTRACTED PITCH**
PYF[1]
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: R. R. Judkins, (423) 574-4572
Fiber Materials, Inc. Contact: Cliff Baker, (207) 282-5911

The manufacture of carbon-carbon composites for use in the aerospace industry has been heavily reliant on petroleum and coal tar pitches as matrix precursors. It is of great importance to strategic materials production for the Department of Defense that a stable, long-lived source of pitch be developed. Consequently, Fiber Materials, Inc. will work with staff members at the Oak Ridge National Laboratory and at West Virginia University to develop carbon-carbon composite materials from pitches derived from coal via a solvent extraction process. The objectives of this project shall be twofold. First, FMI shall use solvent extracted pitch to develop carbon-carbon composites with similar or improved properties over those currently manufactured from Allied 15V coal tar or Ashland A-240 petroleum pitches. Second, FMI shall develop improved, lower-cost composites from improved solvent extracted pitches supplied by WVU.

Keywords: Carbon, Composites, Pitch

550. **CONVERSION OF PITCHES AND COKES FROM SOLVENT-EXTRACTED MATERIALS**
PYF[1]
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: R. R. Judkins, (423) 574-4572
Koppers Industries, Inc. Contact: R. McHenry, (412) 826-3989

The closure of by-product coke ovens has caused the domestic production of coal tar pitch to decline at 3 percent to 4 percent per annum during the mid-1990s. This reduction has directly affected Koppers' capability to produce required quantities of quality binder and impregnating pitches used in the aluminum and commercial carbon and graphite industries. Moreover, the other major constituent of carbon anodes and graphites is a coke, usually produced from petroleum pitch precursors, 50 percent of which are imported. The objectives of this research are to develop dependable domestic coal-based raw materials for the production of: binder pitches for aluminum cell anodes and commercial carbon and graphite products; impregnating pitches for commercial carbon and graphite products and specialty materials; oils for wood treatment and carbon black production; chemicals for phthalic anhydride and other products; and metallurgical and foundry grade cokes.

Keywords: Coke, Pitch, Conversion

551. **CARBON FIBER COMPOSITE MOLECULAR SIEVES TECHNOLOGY TRANSFER**
$50,000
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: T. D. Burchell, (423) 576-8595

Hydrogen and methane gas recovery technologies are required to: (1) allow the upgrading of heavy hydrocarbons to transport fuels, thus reducing the amount of carbon rejected during crude oil refining and (2) to improve the yield and process economics of natural gas wells. The purpose of this work is to develop carbon fiber composite molecular sieves (CFCMS) from porous carbon fiber composites manufactured from solvent extracted coal tar pitch derived carbon fibers. The work will be performed in collaboration with other members of the Cooperative Research Partnership on Carbon Products and the Non Fuel Uses of Coal.

Keywords: Consortium, Carbon Products

552. **DEVELOPMENT OF PRECURSORS FOR PRODUCTION OF GRAPHITES AND CARBON PRODUCTS**
PYF[1]
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: R. R. Judkins, (423) 574-4572
UCAR Carbon Company Contact: Irv Lewis, (216) 676-2203

The manufacture of graphite utilizes cokes and pitches derived from petroleum refining by-products and by-product coke ovens. These include isotropic and anisotropic cokes, binder, and impregnant pitches. Assuring feedstock quality is of great importance to the graphite industry. Therefore, a stable long-lived source of feedstock pitch (and hence coke) would be of considerable benefit to the industry. Consequently, UCAR Carbon Company Inc. shall work with staff members at the Oak Ridge National Laboratory and at the West Virginia University to develop suitable precursor pitches, binders, impregnants,

---

[1]PYF denotes that funding for this activity, active in FY 1996, was provided from prior year funds.

and cokes for the production of graphites and other carbon products.

Keywords: Carbon Products, Precursors, Graphites

553. **PRODUCTION OF YARN FROM VLS WHISKERS**
PYF[1]
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: D. P. Stinton, (423) 574-4556

In order to exploit the superior thermomechanical properties of fibrils produced by the Vapor-Liquid-Solid (VLS) Process, the feasibility of scaled-up production of the SiC fibril will be demonstrated in this activity. Through time-series study and computer simulation, the parameters affecting the growth process and properties of the fibrils will be examined.

Keywords: Whiskers, Fibers, Ceramic

554. **RADIO-WAVE NANO-PHASE SILICON CARBIDE AND SILICON NITRIDE PROCESSES**
$75,000
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: R. R. Judkins, (423) 574-4572
Sandia National Laboratories Contact: R. J. Buss, (505) 844-3504

This program examines the use of radio-frequency plasma discharges as a synthetic route to nanometer-size silicon carbide and silicon nitride particles.

Keywords: Nanophase, Silicon Nitride, Silicon Carbide

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

555. **INVESTIGATION OF THE WELDABILITY OF POLYCRYSTALLINE IRON ALUMINIDES**
$75,000
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: R. W. Swindeman, (423) 574-5108
Colorado School of Mines Contact: G. R. Edwards, (303) 273-3773

The purpose of this project is the investigation of the weldability of polycrystalline aluminides. The major thrust of the project is to determine the role of microstructure in the intergranular cracking of aluminides, with special emphasis on weld cracking susceptibility. The weldability of polycrystalline Fe_3Al-X alloys is being evaluated, and the weldability is correlated with composition, phase equilibria, grain size and morphology, domain size, and degree of long-range order.

Keywords: Joining, Welding

556. **AQUEOUS CORROSION OF IRON ALUMINIDES**
PYF[1]
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: I. G. right, (423) 574-4451
University of Tennessee Contact: R. A. Buchanan, (423) 974-4858

The objective of this project is to investigate: (1) evaluation of the effects of surface conditions on the corrosion and embrittlement of Fe-Al alloys, and (2) corrosion fatigue properties of Fe-Al alloys.

Keywords: Alloys, Aluminides, Corrosion, Stress

557. **EVALUATION OF THE INTRINSIC AND EXTRINSIC FRACTURE BEHAVIOR OF IRON ALUMINIDES**
$68,000
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: I. G. Wright, (423) 574-4451
West Virginia University Contact: B. R. Cooper, (304) 293-3423

The purpose of this activity is the evaluation of the intrinsic and extrinsic fracture behavior of iron aluminides and the study of atomistic simulations of defect concentrations, dislocation mobility, and solute effects in Fe_3Al. The work also involves an experimental study of environmentally-assisted crack growth of Fe_3Al at room and at elevated temperatures. The combined modeling and experimental activities are expected to elucidate the mechanisms controlling deformation and fracture in Fe_3Al in various environments.

Keywords: Alloys, Aluminides, Fracture

[1]PYF denotes that funding for this activity, active in FY 1996, was provided from prior year funds.

558. **INVESTIGATION OF IRON ALUMINIDE WELD OVERLAYS**
$30,000
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: R. W. Swindeman, (423) 574-5108
Lehigh University Contact: J. N. DuPont, (610) 758-3942

The objective of this activity is the investigation of iron aluminide weld overlays. Specific tasks include: (1) filler wire development, (2) weldability, (3) oxidation and sulfidation studies, (4) erosion studies, (5) erosion-corrosion studies, and (6) field exposures.

Keywords: Alloys, Aluminides, Overlay, Welding, Joining

559. **FIRESIDE CORROSION TESTS OF CANDIDATE ADVANCED AUSTENITIC ALLOYS, COATINGS, AND CLADDINGS**
$100,000
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: R. W. Swindeman, (423) 574-5108
Foster Wheeler Development Corporation Contact: J. L. Blough, (201) 535-2355

The purpose of this project is to provide comprehensive corrosion data for selected advanced austenitic tube alloys in simulated coal ash environments. ORNL- modified alloys and standard comparison alloys have been examined. The variables affecting coal ash corrosion and the mechanisms governing oxide breakdown and corrosion penetration are being evaluated. Corrosion rates of the test alloys are determined as functions of temperature, ash composition, gas composition, and time.

Keywords: Austenitics, Alloys, Corrosion

560. **JOINING TECHNIQUES FOR ADVANCED AUSTENITIC ALLOYS**
$50,000
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: R. W. Swindeman, (423) 574-5108
University of Tennessee Contact: C. D. Lundin, (423) 974-5310

Weldability is an important consideration in the selection of a suitable alloy for the fabrication of boiler components such as superheaters and reheaters. It is often a challenge to select joining materials and establish procedures that will allow advanced materials to function at their full potential. The purpose of this research is to examine important aspects of newly developed austenitic tubing alloys intended for service in the temperature range 550 to 700°C.

Keywords: Alloys, Austenitics, Joining, Welding

561. **FATIGUE AND FRACTURE BEHAVIOR OF Cr-Nb ALLOYS**
$20,000
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: I. G. Wright, (423) 574-4451
University of Tennessee Contact: Peter Liaw, (423) 974-6356

The objective of this research shall be to characterize the fatigue and fracture behavior of Cr_2Nb-based alloys and other intermetallic materials at ambient and elevated temperatures in controlled environments. These studies are expected to lead to mechanistic understanding of the fatigue and fracture behavior of these alloys. Fatigue tests shall be conducted for the purpose of evaluating crack initiation and fatigue life of Cr_2Nb-based alloys as well as other intermetallic alloys. The fatigue properties shall be evaluated as functions of test environment, cyclic frequency and test temperature. Additional tensile tests will be required to characterize the fracture behavior of these structural alloys. Mechanical tests shall be performed to determine the fatigue and fracture behavior of Cr_2Nb-based alloys. The microstructure of the alloys shall be characterized and correlated with the mechanical properties.

Keywords: Fracture, Fatigue, Alloys

562. **CORROSION AND MECHANICAL PROPERTIES OF ALLOYS IN FBC AND MIXED-GAS ENVIRONMENTS**
$270,000
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: I. G. Wright, (423) 574-4451
Argonne National Laboratory Contact: K. Natesan, (708) 252-5103

The purposes of this task are to: (1) evaluate the corrosion mechanisms for chromia- and alumina-forming alloys in mixed-gas environments, (2) develop an understanding of the role of several microalloy constituents in the oxidation/sulfidation process, (3) evaluate transport kinetics in oxide scales as functions of temperature and time, (4) characterize surface scales that are resistant to sulfidation attack, and (5) evaluate the role of deposits in corrosion processes.

Keywords: Corrosion, Gasification, Creep Rupture, Fluidized-Bed Combustion

563. **MECHANICALLY RELIABLE COATINGS AND SCALES FOR HIGH-TEMPERATURE CORROSION RESISTANCE**
PYF[1]
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: R. R. Judkins, (423) 574-4572
Argonne National Laboratory Contact: K. Natesan, (708) 252-5103

This project involves the development of mechanically reliable coatings and scales for high-temperature corrosion resistance. ANL shall systematically generate the knowledge required to establish a scientific basis for design and synthesis of improved (slow growing, adherent, sound) protective oxide coatings and scales on high temperature materials, without compromising the requisite bulk material properties. In addition, ANL shall provide information on the performance of advanced candidate materials from the standpoint of corrosion resistance and residual mechanical properties, after exposure in simulated combustion environments typical of indirectly-fired gas turbines. The work shall emphasize corrosion evaluation of materials in air, salt, and coal/ash environments at temperatures between 1000° and 1400°C, and measurement of residual toughness properties of the materials after corrosion.

Keywords: Corrosion, Coatings, Scales

564. **HIGH-TEMPERATURE ENVIRONMENTAL EFFECTS ON IRON ALUMINIDES**
$170,000
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: P. F. Tortorelli, (423) 574-5119

The purpose of this task is to evaluate the high-temperature corrosion behavior of iron-aluminum alloys as part of the effort to develop highly corrosion-resistant iron-aluminide alloys and coatings for fossil energy applications. A primary objective is to investigate the resistance of the alloys to mixed-oxidant (oxygen-sulfur-chlorine-carbon) environments that arise in the combustion or gasification of coal. This includes the determination of the influence of sulfur and other reactive gaseous species on corrosion kinetics and oxide microstructures and the effects of alloying additions and oxide dispersoids on sulfidation and oxidation resistance.

Keywords: Corrosion, Aluminides, Mixed-Gas, Scales

565. **INVESTIGATION OF MOISTURE-INDUCED EMBRITTLEMENT OF IRON ALUMINIDES**
$75,000
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: I. G. Wright, (423) 574-4451
Rensselaer Polytechnic Institute Contact: N. S. Stoloff, (518) 276-6371

The purpose of this work is to study hydrogen embrittlement of iron aluminide alloys. Moisture in air can significantly reduce the room-temperature tensile ductility of Fe_3Al-based alloys by combining with the aluminum in the alloys to form atomic hydrogen. The atomic hydrogen diffuses rapidly into the material causing embrittlement. Experiments are being conducted on selected Fe_3Al alloys that will lead to an understanding of the phenomenon. The work focuses on the effects of moisture on relevant mechanical properties such as fatigue and tensile strengths, and correlates important microstructural variables such as degree of order, grain size, and phases present with the alloy's susceptibility to embrittlement.

Keywords: Aluminides, Embrittlement, Moisture

566. **CORROSION PROTECTION OF ULTRAHIGH TEMPERATURE INTERMETALLIC ALLOYS**
$200,000
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: P. F. Tortorelli, (423) 574-5119

The objective of this task is to develop high-strength, corrosion-resistant intermetallic alloys for use as hot components in advanced fossil energy conversion and combustion systems. The successful development of these alloys is expected to improve the thermal efficiency of fossil energy conversion systems through increased operating temperatures and to increase the service life of hot components exposed to corrosive environments at elevated temperatures (1000°C). The initial effort will be devoted to in situ composite alloys based on the $Cr-Cr_2Nb$ system.

Keywords: Corrosion, Chromium-Niobium, Mixed-Gas, Scales

[1]PYF denotes that funding for this activity, active in FY 1996, was provided from prior year funds.

567. **OXIDE DISPERSION STRENGTHENED (ODS) IRON ALUMINIDES**
$275,000
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: I. G. Wright, (423) 574-4451

The purpose of this task is to develop fabrication procedures for making oxide dispersion-strengthened (ODS) iron-aluminum alloys based on Fe_3Al. The suitability of the procedures is measured in terms of the high-temperature oxidation and sulfidation resistance and creep strength of the ODS alloys compared with Fe_3Al alloys fabricated by conventional ingot and powder processes.

Keywords: Aluminides

568. **MATERIALS SUPPORT FOR HITAF**
PYF[1]
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: K. Breder, (423) 574-5089

This task involves the measurement of selected mechanical and physical properties of structural ceramics which are proposed for use in the construction of the High Temperature Advanced Furnace (HITAF) air heater design being developed under the Combustion 2000 Program. The purpose of the research is to evaluate candidate structural ceramics for this application by studying the fast fracture and fatigue (both dynamic and interrupted static) properties at temperatures from 1100 to 1400°C in air, their corrosion behavior, property uniformity of components and long term degradation of ceramic properties due to exposure in prototype HITAF systems.

Keywords: Furnace, Materials, HITAF

569. **JOINING OF CERAMICS**
$50,000
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: D. P. Stinton, (423) 574-4556
Idaho National Engineering Laboratory Contact: B. H. Rabin, (208) 526-0058

The purpose of this project is to explore and develop joining techniques for silicon carbide fiber-reinforced silicon carbide ceramics produced by chemical vapor infiltration and deposition (CVID). The research goals include identifying appropriate joining methods, establishing experimental procedures for fabricating joints, and characterizing the structure and properties of joined materials. An understanding of the factors that control joint performance is sought through studies of the relationships among processing variables, joint microstructures, and mechanical properties. Additional funds for this project are provided by the DOE Pittsburgh Energy Technology Center.

Keywords: Ceramics, Joining, Technology Transfer

570. **SUPPORT SERVICES FOR CERAMIC FIBER-CERAMIC MATRIX COMPOSITES**
$50,000
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: D. P. Stinton, (423) 574-4556
University of North Dakota Energy and Environmental Research Center Contact: J. P. Hurley, (701) 777-5159

This task will review and, if appropriate, propose modifications to plans, materials, and tests planned by researchers on the AR&TD Materials Program in work to test materials for coal-fueled energy systems. The changes shall be suggested in order to make the corrosion experiments more reflective of the actual conditions that will be encountered by the materials in the energy systems. UNDEERC shall accomplish this task by reviewing the major advanced energy system projects being funded by the DOE, and by working with the company's technical monitor and staff to prepare a summary of the expected corrosion problems. Both gasification and combustion systems will be included. Ceramic materials in two subsystems will be the focus of this work: (1) hot gas cleanup systems and (2) high-temperature heat exchangers. UNDEERC shall review and suggest improvements to materials testing procedures that are used to determine material behavior when used in hot-gas cleanup or heat exchanger applications. A limited amount of computer modeling and laboratory experimentation shall be a part of this effort.

Keywords: Composites, Ceramics, Fibers

[1]PYF denotes that funding for this activity, active in FY 1996, was provided from prior year funds.

571. **DEVELOPMENT OF NONDESTRUCTIVE EVALUATION METHODS AND EFFECTS OF FLAWS ON THE FRACTURE BEHAVIOR OF STRUCTURAL CERAMICS**
$270,000
DOE Contacts: F. M. Glaser, (301) 903-2784
and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact:
D. P. Stinton, (423) 574-4556
Argonne National Laboratory Contacts:
W. A. Ellingson, (708) 252-5068 and
J. P. Singh, (708) 252-5123

The purpose of this project is to study and develop acoustic and radiographic techniques and possible novel techniques such as nuclear magnetic resonance, to characterize structural ceramics with regard to presence of porosity, cracking, inclusions, amount of free silicon, and mechanical properties, and to establish the type and character of flaws that can be found by nondestructive evaluation (NDE) techniques. Both fired and unfired specimens are being studied to establish correlations between NDE results and failure of specimens.

Keywords: Nondestructive Evaluation, Ceramics, Flaws, Fracture

572. **FRACTURE BEHAVIOR OF ADVANCED CERAMIC HOT-GAS FILTERS**
PYF[1]
DOE Contacts: F. M. Glaser, (301) 903-2784
and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact:
D. P. Stinton, (423) 574-4556
Argonne National Laboratory Contacts:
J. P. Singh, (708) 252-5123

The purpose of this project is to study the fracture behavior of ceramic hot-gas filters. ANL shall evaluate mechanical/physical properties and microstructure, identify critical flaws and failure modes, and correlate mechanical/physical properties with microstructure and critical flaws to provide much needed information for selection of materials and optimization of fabrication procedures for hot-gas ceramic filter modules. As part of the information base, requirements for strength and fracture toughness of the filter material shall be established from stress and fracture mechanics analyses of typical filters subjected to loadings expected during operation and pulse-cleaning cycles.

Keywords: Ceramics, Flaws, Fracture, Failure

[1]PYF denotes that funding for this activity, active in FY 1996, was provided from prior year funds.

573. **CERAMIC CATALYST MATERIALS**
$50,000
DOE Contacts: F. M. Glaser, (301) 903-2784
and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact:
R. R. Judkins, (423) 574-4572
Sandia National Laboratories Contact:
A. G. Sault, (505) 844-8723

The purpose of this research is to investigate the role of ceramic material properties in the catalytic activity of a novel class of catalytic supports, known as hydrous titanium oxides (HTO). Catalysts prepared on these materials show particular promise as economically and environmentally attractive alternatives to present commercial catalysts for the direct liquefaction of coal. In these studies, improved understanding and control of the synthesis process is being pursued in order to tailor the composition, molecular structure, microporosity, and physical/mechanical properties of the HTO thin films. The effects of altered structure, composition, and other material properties of the thin film ceramic support material on catalytic activity are being assessed.

Keywords: Ceramics, Catalysts

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

574. ***MATERIALS AND COMPONENTS IN FOSSIL ENERGY APPLICATIONS* NEWSLETTER**
$50,000
DOE Contacts: F. M. Glaser, (301) 903-2784
and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact:
I. G. Wright, (423) 574-4451

The purpose of this task is to publish a periodic (bimonthly) joint DOE-Electric Power Research Institute (EPRI) newsletter to address current developments in materials and components in fossil energy applications. Matching funding is provided by EPRI.

Keywords: Materials, Components

575. **COMPILATION AND EDITING OF BOOK ON MATERIALS BEHAVIOR IN COAL LIQUEFACTION PLANTS**
$11,000
DOE Contacts: F. M. Glaser, (301) 903-2784
and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact:
R. R. Judkins, (423) 574-4572

The purpose of this task is to publish a report of work, which assessed the selection and performance of the materials of construction in direct-coal-liquefaction process plants. One part of this task was to document the results of the study. The second part involved establishing a computerized information system on materials performance and design selection for direct-coal-liquefaction processes. This database was intended to complment the larger and more comprehensive Department of Energy Liquefaction Technology Data Base at the former Pittsburgh Energy Technology Center.

Keywords: Materials, Components, Liquefaction

576. **CERAMIC FIBER FILTER TECHNOLOGY**
$75,000
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: M. A. Janney, (614) 424-4281

The purpose of this effort is to develop the fabrication technology necessary to make ceramic-fiber based filters for a variety of filtration applications of interest to the Fossil Energy community.

Keywords: Filters, Ceramics, Fibers

577. **DEVELOPMENT OF MICROWAVE-HEATED DIESEL PARTICULATE FILTERS**
PYF[1]
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: M. A. Janney, (423) 574-4281

The purpose of this research, which derives from our work on ceramic filters for coal systems, is to help develop microwave-heated diesel engine particulate filter/burner devices. The goal is to develop materials that will perform both as filter and heater in such a device. A Cooperative Research and Development Agreement (CRADA) between Lockheed Martin Energy Systems and the Cummins Engine Company is in place that supports this work, CRADA No. ORNL93-0172. We propose to develop a ceramic composite structure of SiC-coated ceramic fiber that can be used as a diesel engine particulate filter. For commercial usage a particulate filter must: (1) filter carbon particles from high temperature diesel exhaust gas at an acceptable (low) backpressure; (2) survive thousands of thermal transients caused by regeneration (cleaning) of the filter by oxidizing the collected carbon; (3) be durable and reliable over the life of the filter, which is in excess of 300,000 miles (10,000 hours of operation); and (4) provide a low overall operating cost which is competitive with other filtering techniques.

Keywords: Ceramics, Microwave Processing

578. **DEVELOPMENT OF CERAMIC MEMBRANES FOR GAS SEPARATION AND FUEL CELLS**
$380,000
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: R. R. Judkins, (423) 574-4572
Oak Ridge K-25 Site Contact: D. E. Fain, (423) 574-9932

The purpose of this activity is to fabricate inorganic membranes for the separation of gases at high temperatures and/or in hostile environments, typically encountered in fossil energy conversion processes such as coal gasification. This work is performed in conjunction with a separate research activity that is concerned with the development and testing of the ceramic membranes.

Keywords: Ceramics, Membranes, Filters, Separation

579. **FURNACE EQUIPMENT**
$100,000
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: R. R. Judkins, (423) 574-4572
Oak Ridge K-25 Site Contact: D. E. Fain, (423) 574-9932

This task provides funds for the procurement of major equipment items , necessary for AR&TD Materials Program activities.

Keywords: Equipment

580. **HIGH-TEMPERATURE HEAT EXCHANGER AND HOT-GAS FILTER DEVELOPMENT**
$172,000
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: D. P. Stinton, (423) 574-4556
Pennsylvania State University Contact: R. E. Tressler, (814) 865-7961

This project addresses the development of ceramic heat exchanger materials with chromia surface treatments for corrosion resistance. High chromia-content refractories have been demonstrated to be resistant to corrosion by coal slags. This project will focus on improving the corrosion resistance of ceramics by incorporating chromia into the surface layers. This work has two principal parts: (1) screening analysis of candidate ceramic

[1]PYF denotes that funding for this activity, active in FY 1996, was provided from prior year funds.

hot-gas filter materials, and (2) internal pressure testing of ceramic tubes exposed to coal combustion environments.

Keywords: Ceramics, Corrosion, Filters

581. **INVESTIGATION OF THE MECHANICAL PROPERTIES AND PERFORMANCE OF CERAMIC COMPOSITE COMPONENTS**
$135,000
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: D. P. Stinton, (423) 574-4556
Virginia Polytechnic Institute Contact: K. L. Reifsnider, (703) 231-5259

The purpose of this project is to develop a test system and test methods to obtain information on the properties and performance of ceramic composite materials. The work involves a comprehensive mechanical characterization of composite engineering components such as tubes, plates, shells, and beams subjected to static and cyclic multiaxial loading at elevated temperatures for extended time periods.

Keywords: Ceramics, Composites, Mechanical Properties, Testing

582. **SOLID STATE ELECTROLYTE SYSTEMS**
$655,000
DOE
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: R. R. Judkins, (423) 574-4572
Pacific Northwest Laboratory Contact: L. R. Pederson, (509) 375-2579

The purpose of this project is to develop functional ceramic materials that will ultimately lead to the broader, cleaner, and more efficient utilization of fossil fuels, particularly coal and natural gas. This project is composed of three principal tasks:

(1) Stability of Solid Oxide Fuel Cell Materials - The purpose of this task is to evaluate the stabilities of materials and interfaces in SOFCs in order to identify features that would limit system performance.

(2) Mixed Oxygen Ion/Electron-Conducting Ceramics for Oxygen Separation - Compositions and physical forms are being developed that simultaneously conduct oxygen ions and electrons. Such mixed conducting ceramics can function as highly selective oxygen separation membranes, allowing high purity oxygen to be separated from air.

(3) Proton-Conducting Solid Electrolytes - This task will develop perovskite compositions and physical forms, which will be used as the electrolyte in small-scale solid oxide fuel cells operating at intermediate temperatures.

Keywords: Fuel Cells, SOFC

583. **ODS Fe_3Al TUBES FOR HIGH-TEMPERATURE HEAT EXCHANGERS**
PYF[1]
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: I. G. Wright, (423) 574-4451
PM Hochtemperatur-Metall. GmbH Contact: Dieter Sporer, 011-43-5672-70-2923

The goal of the work is to produce tubes of Fe_3Al-0.5 wt. percent Y_2O_3 which have properties suitable for application as heat transfer surfaces in very high-temperature heat exchangers. The alloy is produced by a powder metallurgical (mechanical alloying) process, the main purpose of which is to obtain a uniform distribution of sub-micron Y_2O_3 particles in the Fe_3Al matrix. The required high-temperature creep strength is derived largely by developing very large, elongated grains which are effectively pinned by the oxide dispersion. Development of the necessary grain structure is dependent on the characteristics of the mechanically-alloyed powder, and on thermomechanical processing of the consolidated powder.

Keywords: Aluminide, Tubes, Heat Exchangers

584. **POROUS IRON ALUMINIDE ALLOYS**
PYF[1]
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: R. R. Judkins, (423) 574-4572
Oak Ridge K-25 Site Contact: D. E. Fain, (423) 574-9932

This project is directed to the development of porous iron aluminide structures for applications such as hot-gas filters.

Keywords: Filters, Aluminides

[1]PYF denotes that funding for this activity, active in FY 1996, was provided from prior year funds.

585. **IRON ALUMINIDE FILTERS FOR IGCCs**
$53,000
DOE Contacts: F. M. Glaser, (301) 903-2784
and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact:
P. F. Tortorelli, (423) 574-5119

The purpose of this project is to provide technical support to the Pall Corporation in its development of porous sintered iron-aluminide filters for hot-particle removal from product streams in coal gasification systems. The ORNL role is to provide specialized expertise in the areas of corrosion analysis, microstructural characterization, alloy selection, and processing based on extensive experience with iron aluminides and materials performance in fossil energy systems. ORNL's contribution via this project should aid the success and timely completion of Pall's development and demonstration efforts.

Keywords: Filters, Aluminides

586. **IRON ALUMINIDE FILTERS FOR PFBCs**
$45,000
DOE Contacts: F. M. Glaser, (301) 903-2784
and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact:
P. F. Tortorelli, (423) 574-5119

The goal of this project is to determine the suitability of particular iron aluminides as materials of construction for hot-gas filters in advanced first- and second-generation PFBCs.

Keywords: Filters, Aluminides

587. **CORROSION RESISTANCE OF IRON ALUMINIDES IN CS_2 ENVIRONMENTS**
$27,000
DOE Contacts: F. M. Glaser, (301) 903-2784
and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact:
P. F. Tortorelli, (423) 574-5119

The purpose of this effort is to examine he corrosion behavior and resistance of iron alunminides in CS_2 environments. Results from this study will determine if the application of iron aluminides as materials of construction for CS_2 production systems should be pursued.

Keywords: Corrosion, Aluminides

588. **THERMAL AND MECHANICAL ANALYSIS OF A CERAMIC TUBESHEET**
PYF[1]
DOE Contacts: F. M. Glaser, (301) 903-2784
and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact:
R. W. Swindeman, (423) 574-5108
Mallett Technology Contact: R. H. Mallett,
(919) 406-1500

A transport combustor is being commissioned at the Southern Services facility in Wilsonville, Alabama, to provide a gaseous product for the assessment of hot-gas filtering systems. These hot-gas filtration systems will include granular-bed and barrier filter concepts. Filters will be evaluated for carbonizer and gasifier gaseous products. In addition, a pressurized fluidized-bed combustor (PFBC) will be installed to burn the carbonizer product, and a hot gas filter will be installed in the PFBC gas stream. Compositions of the gas streams will range from oxidizing to reducing, and the partial pressures of oxygen and sulfur will vary substantially. Temperatures of the gas streams will range from 840 to 980°C (or higher). One of the barrier filters under consideration incorporates a ceramic tubesheet to support the candle filters. This system, to be designed and built by Industrial Filter & Pump Manufacturing Company (IF&PM) is unique and may offer distinct advantages over metal/ceramic systems that have been tested extensively in other EPRI/DOE projects. To gain an insight that could prove to be useful in the scaleup of a commercial-size, all-ceramic system, work will be undertaken to develop a design methodology applicable to the thermal-mechanical analysis of the all-ceramic system.

Keywords: Ceramics, Tubesheet

589. **CERAMIC TUBESHEET DESIGN ANALYSIS**
PYF[1]
DOE Contacts: F. M. Glaser, (301) 903-2784
and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact:
R. W. Swindeman, (423) 574-5108

The purpose of this task is to perform thermal and mechanical analyses of critical regions in a ceramic tubesheet support for barrier filters in a hot gas cleanup vessel designed for use in gasifier, carbonizer, and pressurized fluidized bed combustion gas streams.

Keywords: Ceramics, Tubesheet

[1]PYF denotes that funding for this activity, active in FY 1996, was provided from prior year funds.

590. **DENSE CERAMIC TUBE DEVELOPMENT**
$100,000
DOE Contacts: F. M. Glaser, (301) 903-2784
and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact:
D. P. Stinton, (423) 574-4556

The goal of this project is to demonstrate that composite materials of high interest to the fossil energy community can be fabricated by chemical vapor infiltration (CVI). Earlier work demonstrated that composites could be fabricated in simple geometries (thick-walled plates). However, more complex geometries were identified as important in a recent Continuous Fiber Ceramic Composite (CFCC) Initiative report. Potentials applications for CFCCs include air heaters or recuperators, heat exchangers, catathermal or porous combustors, components for filtration systems, gas turbine components (primarily combustors), and radiant homer tubes. Nearly all of these applications require tubular composites; therefore, the process will be developed for the fabrication of tubular shapes.

Keywords: Ceramics, Tubesheet

INSTRUMENTATION AND FACILITIES

591. **MANAGEMENT OF THE FOSSIL ENERGY AR&TD MATERIALS PROGRAM**
$400,000
DOE Contacts: F. M. Glaser, (301) 903-2784
and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact:
R. R. Judkins, (423) 574-4572

The overall objective of the Fossil Energy Advanced Research and Technology Development (AR&TD) Materials program is to conduct a fundamental, long-range research and development program that addresses, in a generic way, the materials needs of fossil energy systems and ensures the development of advanced materials and processing techniques. The purpose of this task is to manage the Fossil Energy AR&TD Materials program in accordance with procedures described in the Program Management Plan approved by DOE. This task is responsible for preparing the technical program implementation plan for DOE approval; submitting budget proposals for the program; recommending work to be accomplished by subcontractors, other national laboratories, and by Oak Ridge National Laboratory (ORNL); placing and managing subcontracts for fossil energy materials development at industrial research centers, universities, and other government laboratories; and for reporting the progress of the program.

Keywords: Management, Materials Program

592. **GENERAL TECHNOLOGY TRANSFER ACTIVITIES**
$35,000
DOE Contacts: F. M. Glaser, (301) 903-2784
and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact:
R. R. Judkins, (423) 574-4572

The task provides funds for the initiation of technology transfer activities to identify and develop relationships with industrial partners for the transfer of AR&TD Materials Program technologies to industry.

Keywords: Technology Transfer

593. **GORDON RESEARCH CONFERENCE SUPPORT**
$2,000
DOE Contacts: F. M. Glaser, (301) 903-2784
and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact:
R. R. Judkins, (423) 574-4572

The task provides funds to support the annual Gordon Research Conference.

Keywords: Technology Transfer

DIRECTORY

J. D. Achenbach
Department of Civil Engineering
Northwestern University
Evanston, IL 60201
(312) 491-5527

Iqbal Ahmad
Associate Professor
Far East Liaison Office
ONR/AFOSR/ARO
7-23-17, Roppongi
Minato-ku, Tokyo 106
(03) 3401-8924, 3423-1374

L. F. Allard
ORNL
P.O. Box 2008
Bldg. 4515, MS 064
Oak Ridge, TN 37831
(615) 574-4981

Richard Anderson
Kroftt-Brakston International, Inc.
5836 Sunrise Avenue
Claendon Hills, IL 60514
(708) 655-3207

P. Angelini
ORNL
P.O. Box 2008
Bldg. 4515, MS 6065
Oak Ridge, TN 37830-6065
(615) 574-4565

C. Arnold, Jr.
Division 1811
Sandia National Laboratories
Albuqeurque, NM 87185
(505) 844-8728

T. W. Arrigoni
U.S. Dept. of Energy
P.O. Box 10940
Pittsburgh, PA 15236
(312) 972-4450

J. S. Arzigian
Division 1815
Sandia National Laboratories
Albuquerque, NM 87185
(505) 844-2465

R. A. Assink
Division 1811
Sandia National Laboratories
Abuquerque, NM 87185
(505) 844-6372

D. G. Austin
1060 Sun Valley Drive
Annapolis, MD 21401
(410) 626-7826

V. Saimasarma Avva
N. Carolina State Univ.
Grahm Hall #8
Greensboro, NC 27411
(919) 379-7620

Walter C. Babcock
Bend Research, Inc.
64550 Research Road
Bend, OR 97701-8599
(503) 382-4100

Murray Bailey
NASA Lewis Research Center
MS 77-6
21000 Brookpark Road
Cleveland, OH 44135
(216) 433-3416

Samuel J. Barish
ER-16/GTN
U.S. Dept. of Energy
Washington, DC 20545
(301) 903-3054

W. Barnett
NE-53/FORS
U.S. Dept. of Energy
Washington, DC 20585
(301) 903-3097

Harold N. Barr
Hittman Mat. & Med. Components, Inc.
9190 Red Branch Road
Columbia, MD 21045
(301) 730-7800

Bulent Basol
Internl. Solar Electric Tech., Inc.
8635 Aviation Boulevard
Inglewood, CA 90301
(310) 216-4427

J. L. Bates
Pacific Northwest Laboratories
P.O. Box 999
Richland, WA 99352
(509) 375-2579

S. Bauer, Division G314
Sandia National Laboratory
P.O. Box 5800
Albuquerque, NM 87185
(505) 846-9645

M. B. Beardsley
Caterpillar, Inc.
100 N.E. Adams Street
Peoria, IL 61629
(309) 578-8514

R. L. Beatty
ORNL
P.O. Box 2008
Bldg. 4508, MS 088
Oak Ridge, TN 37831
(615) 574-4536

B. Beaudry
Ames Laboratory
Iowa State University
Ames, Iowa 50011
(515) 294-1366

P. F. Becher
ORNL
P.O. Box 2008
Bldg. 4515, 068, Room 275
Oak Ridge, TN 37831-6088
(615) 574-5157

David J. Beecy
FE-72/FORS
U.S. Dept. of Energy
Washington, DC 20585
(301) 903-2787

James A. Begley
Packer Engineering, Inc.
200 Fleet Street
Pittsburgh, PA 15220
(412) 921-6441

Mohamad M. Behravesh
Nuclear Plant Corrosion Control
Electric Power Research Institute
3412 Hillview Avenue
Palo Alto, CA 94303
(415) 855-2388

R. G. Behrens
LANL
Los Alamos, NM 87545
(505) 667-8327

William L. Bell
TDA Research, Inc.
12345 West 52nd Avenue
Wheat Ridge, CO 80033
(303) 940-2301

John Benner
Solar Electric Conversion Div.
NREL
1617 Cole Blvd.
Golden, CO 80401
(303) 231-1396

Dave Benson
NREL
1617 Cole Blvd
Golden, CO 80401
(303) 384-6462

Clifton G. Bergeron
University of Illinois
105 South Goodwin Avenue
204 Ceramics Building
Urbana, IL 61801
(217) 333-1770

Sam Berman
Bldg. 90, Rm. 3111
Lawerence Berkeley Laboratory
University of California
Berkeley, CA 94720
(415) 486-5682

Theodore M. Besmann
Metals and Ceramics Division
Oak Ridge National Laboratory
P.O. Box 2008
Oak Ridge, TN 37831
(615) 574-6852

Fritz Bien
Spectral Sciences, Inc.
99 South Bedford Street, #7
Burlington, MA 01803-5169
(617) 273-4770

L. Blair
Los Alamos National Lab
P.O. Box 1663
Los Alamos, NM 87545
(505) 667-6250

David W. Bobrek
Blasch Precision Ceramics
99 Cordell Road
Schenectady, NY 12304
(518) 372-9416

J. Bockris
Texas A&M University
College Station, TX 77843-3255
(713) 845-5335

Robert Boettner
EE-112/FORS
U.S. Dept. of Energy
Washington, DC 20585
(202) 252-9136

W. D. Bond
Oak Ridge National Laboratory
P.O. Box 2008
Bldg. 7920, 384, Room 0014
Oak Ridge, TN 37831-6088
(615) 574-7071

J. A. M. Boulet
University of Tennessee
310 Perkins Hall
Knoxville, TN 37996
(615) 974-8376

R. J. Bourcier
Division 1832
Sandia National Laboratories
Albuquerque, NM 87185
(505) 844-6638

H. K. Bowen
Dept. of Mat. Science & Eng.
MIT
77 Massachusetts Avenue
Cambridge, MA 02139
(617) 253-6892

D. J. Bradley
Pacific Northwest National Laboratory
Richland, WA 99352
(509) 375-2587

R. A. Bradley
ORNL
P.O. Box 2008
Bldg. 4515
Oak Ridge, TN 37831-6067
(615) 574-6094

Joyce M. Brien
Research International, Inc.
18706-142nd Avenue, NE
Woodinville, WA 98072
(206) 486-7831

C. R. Brinkman
ORNL
P.O. Box 2008
Bldg. 4500-S, MS 154
Oak Ridge, TN 37831
(615) 574-5106

Leslie Bromberg
Plasma Fusin Center
MA Institute of Tech.
Cambridge, MA 02139
(617) 253-6919

S. E. Bronisz
LANL
Los Alamos, NM 87545
(505) 667-4665

J. A. Brooks
Division 8312
Sandia National Laboratories
Livermore, CA 94550
(415) 422-2051

K. L. Brower
Division 1110
Sandia National Laboratories
Abuquerque, NM 87185
(505) 844-6131

Alexander Brown
Chesapeake Composites Corporation
239 Old Churchman's Road
New Castle, DE 19720
(302) 324-9110

Ian G. Brown
Lawrence Berkeley Laboratory
Berkeley, CA 94720
(510) 486-4147

J. J. Brown, Jr.
Materials Engineering
Virginia Polytechnic Inst.
Blacksburg, VA 24061
(703) 961-6777

N. E. Brown
Division 1821
Sandia National Laboratories
Albuquerque, NM 87185
(505) 844-2747

J. Budny
Busek Company
19 Kearney Road
Needham, MA 92194
(617) 449-3929

S. T. Buljan
GTE Laboratories, Inc.
40 Sylvan Road
Waltham, MA 02254
(617) 890-8460

R. F. Bunshah
Mat. Science & Eng. Dept.
Univ. of CA, Los Angeles
6532 Boelter Hall
Los Angeles, CA 90024
(213) 825-2210

Richard Burrows
NASA Lewis Research Center
21000 Brookpark Road
MS 77-6
Cleveland, OH 44135
(216) 433-3388

R. J. Buss
Division 1812
Sandia National Laboratories
Albuquerque, NM 87185
(505) 844-7494

Kenneth R. Butcher
Selee Corporation
700 Shepherd Street
Hendersonville, NC 28792
(704) 697-2411

J. F. Butler
Aurora Technologies Corporation
7408 Trade Street
San Diego, CA 92121-2410
(619) 549-4645

Oral Buyukozturk
MIT
77 Massachussetts Avenue
Cambridge, MA 02139
(617) 253-7186

E. Buzzeli
Westinghouse R&D Center
1310 Beulah Rd
Pittsbugh, PA 15235
(412) 256-1952

Elton Cairns
Lawrence Berkeley Laboratory
University of California
Berkeley, CA 94720
(415) 486-5028

Juan Carbajo
ORNL
P.O. Box Y
Oak Ridge, TN 37831
(615) 574-3784

R. W. Carling, Div. 8313
Sandia National Laboratories
Livermore, CA 94550
(415) 422-2206

P. T. Carlson
Oak Ridge National Laboratory
P.O. Box 2008
Oak Ridge, TN 37831
(615) 574-6094

J. P. Carr
FE-14/GTN
U.S. Dept. of Energy
Washington, DC 20545
(301) 903-6519

D. W. Carroll
LANL
Los Alamos, NM 87545
(505) 667-2145

D. H. W. Carstens
LANL
Los Alamos, NM 87545
(505) 667-5849

G. M. Caton
ORNL
P.O. Box 2008
Bldg. 4515
Oak Ridge, TN 37831-6065
(615) 574-7782

Ken Chacey
EM-34/GTN
U.S. Dept. of Energy
Washington, DC 20545
(301) 903-7186

A. T. Chapman
Georgia Institute of Technology
Georgia Tech Research Institute
Atlanta, GA 30332-0420
(404) 894-4815

Yok Chen
ER-131/GTN
U.S. Dept. of Energy
Washington, DC 20585
(301) 903-3428

Lalit Chhabildas
Org. 1433 Mail Stop 0821
P.O. Box 5800
Sandia National Laboratory
Albuquerque, NM 87185
(505) 844-4147

Russell Chou
Materials Research Center
Lehigh University
Bethlehem, PA 18015
(215) 861-4235

D. C. Christensen
LANL
Los Alamos, NM 87545
(505) 667-2556

Richard Christensen
LLNL
University of California
P.O. Box 808
Livermore, CA 94550
(415) 422-7136

L. Christophorou
ORNL
P.O. Box 2008
Bldg. 4500S, 122, Rm. H156
Oak Ridge, TN 37831
(615) 574-6199

Russel J. Churchill
American Research Corp. of Va.
642 First Street
P.O. Box 3406
Radford, VA 24143-3406
(703) 731-0836

M. J. Cieslak
Division 1833
Sandia National Laboratories
Albuquerque, NM 87185
(505) 846-7500

D. E. Clark
Materials Technology Div
Idaho National Eng. Laboratory
Idaho Falls, ID 83415
FTS 583-2627

Robert Clark
Sandia National Laboratory
Albuquerque, NM 87185
(505) 844-6332

S. K. Clark
Dept. of Mech. Eng. & App. Mech.
University of Michigan
Ann Arbor, MI 48109
(313) 764-4256

David Clarke
Univ. of California
Materials Department
Engineering III
Santa Barbara, CA 93106
(805) 893-8275

A. H. Claver
Battelle-Columbus Labs
505 King Avenue
Columbus, OH 43201
(614) 424-4377

Michael O. Cloninger
Yucca Mountain Project
DOE Nevada Operations Office
P.O. Box 98518
Las Vegas, NV 89195-8518
(702) 794-7847

R. L. Clough
Sandia National Laboratories
Albuquerque, NM 87185
(505) 844-3492

Joe K. Cochran, Jr.
School of Ceramic Eng.
Georgia Inst. of Technology
Atlanta, GA 30332
(404) 894-2851

Marvin M. Cohen
ER-533/GTN
U.S. Dept. of Energy
Washington, DC 20545
(301) 903-4253

Robert Cook
LLNL
University of California
P.O. Box 808
Livermore, CA 94550
(415) 422-6993

lastair N. Cormack
NYS College of Ceramics
Alfred University
Alfred, NY 14802
(607) 871-2180

J. E. Costa
Division 8314
Sandia National Laboratories
Livermore, CA 94550
(415) 422-2352

Bruce Cranford
EE-222/FORS
U.S. Dept. of Energy
Washington, DC 20585
(202) 586-9496

Frederick A. Creswick
ORNL
P.O. Box 2009
Oak Ridge, TN 37831
(615) 574-2009

James V. Crivello
Department of Chemistry
Rensselaer Polytechnic Institute
Troy, NY 12180-3590
(518) 276-6825

Gary M. Crosbie
Ceramics Research
Ford Motor Company
P.O. Box 2053
Dearborn, MI 48121-2053
(313) 327-1208

Randy Curlee
ORNL
P.O. Box 2008
Oak Ridge, TN 37831
(615) 576-4864

M. J. Curry
Plastics Inst. of America
Stevens Inst. of Tech.
Castle Point Station
Hoboken, NJ 07030
(201) 420-5552

David I. Curtis
NE-60/NR
U.S. Dept of Energy
(703) 603-5565

Steinar Dale
ORNL
P.O. Box 2008
Bldg. 5500, 366, Room A217
Oak Ridge, TN 37831
(615) 574-4829

G. J. D'Alessio
DP-242/GTN
U.S. Dept. of Energy
Washington, DC 20585
(301) 903-6688

S. J. Dapkunas
National Institute of Standards
and Technology
Gaithersburg, MD 20899
(301) 975-6119

John Davis
McDonnell Douglas Astro. Co.
Fusion Energy Program
P.O. Box 516, Bldg 278
St. Louis, MO 63166
(314) 234-4826

Robert F. Davis
Dept. of Materials Eng.
North Carolina State University
232 Riddick Lab, Box 7907
Raleigh, NC 27695
(919) 737-3272

Victor Der
ER-531/FORS
U.S. Dept. of Energy
Washington, DC 20585
(301) 903-5736

R. Diegle
Division 1841
Sandia National Labs
Albuquerque, NM 87185
(505) 846-3450

R. Diercks
Mat. Science & Tech. Div.
Argonne National Labs
9700 South Cass Ave
Argonne, Illinois 60439
(312) 972-5032

Joseph A. Dodson
Space Power, Inc.
621 River Oaks Parkway
San Jose, CA 95134
(408) 434-9500

Larry A. Dominey
Covalent Associates, Inc.
10 State Street
Woburn, MA 01801
(617) 938-1140

A. D. Donaldson
Materials Technology Div.
Idaho National Eng. Lab
Idaho Falls, ID 83415
(208) 526-2627

Alan Dragoo
ER-131, G236/GTN
U.S. Dept. of Energy
Washington, DC 20585
(301) 903-4895

Elaine Drew
Supercon, Inc.
830 Boston Turnpike
Shrewsbury, MA 01545
(508) 842-0174

W. D. Drotning
Division 1824
Sandia National Laboratories
Albuquerque, NM 87185
(505) 844-7934

T. J. Drummond
Division 1150
Sandia National Laboratories
Albuquerque, NM 87185
(505) 844-9677

Jerry Duane
Director of Implementation & Deploy.
EE-223/FORS
U.S. Dept. of Energy
Washington, DC 20585
(202) 586-7448

C. Michael Dube
Dynamics Technology, Inc.
22939 Hawthorne Blvd., #200
Torrance, CA 90505
(213) 373-0666

George Duda
ER-72/FORS
U.S. Dept. of Energy
Washington, DC 20585
(301) 903-3651

C. Duffy
LANL P.O. Box 1663
Los Alamos, NM 87545
(505) 843-5154

Keith F. Dufrane
Battelle-Columbus Labs
505 King Avenue
Columbus, OH 43201
(614) 424-4618

E. M. Dunn
GTE Laboratories, Inc.
40 Sylvan Road
Waltham, MA 02254
(617) 466-2312

Sunil Dutta
NASA Lewis Research Center
21000 Brookpark Road, MS 49-3
Cleveland, OH 44135
(216) 433-3282

Christopher A. Ebel
Norton Company
Goddard Road
Northboro, MA 01532-1545
(617) 393-5950

James J. Eberhardt
EE-34/FORS
U.S. Dept. of Energy
Washington, DC 20585
(202) 586-5377

G. R. Edwards
Colorado School of Mines
Golden, CO 80401
(303) 273-3773

Mr. Paul Eggerstedt
Ind. Filter & Pump Man. Co.
5900 Ogden Avenue
Cicero, IL 60650
(708) 656-7800

W. A. Ellingson
Argonne National Laboratories
Mat. Science Div., Bldg. 212
9700 South Cass
Argonne, Illinois 60439
(312) 972-5068

Mr. Norbert B. Elsner
Hi-Z Technology, Inc.
6373 Nancy Ridge Drive
San Diego, CA 92121-2247
(619) 535-9343

James Ely, Thermophys. Prop.
Ctr. for Chemical Engineering
National Eng. Laboratory
NIST
Boulder, CO 80303
(303) 320-5467

Gerald Entine
Radiation Monitoring Devices, Inc.
44 Hunt Street
Watertown, MA 02172
(617) 926-1167

Mike Epstein
Battelle-Columbus Labs
505 King Avenue
Columbus, OH 43201
(614) 424-6424

R. H. Ericksen
Division 1813
Sandia National Laboratories
Albuquerque, NM 87185
(505) 844-8333

Albert Evans
ER-13/GTN
U.S. Dept. of Energy
Washington, DC 20585
(301) 903-3427

Bob Evans
NASA Lewis Research Center
21000 Brookpark Road, MS 77-6
Cleveland, OH 44135
(216) 433-3400

John Fairbanks
EE-322/FORS
U.S. Dept. of Energy
Washington, DC 20585
(202) 586-8066

P. D. Fairchild
ORNL
P.O. Box Y
Bldg. 9102-2, 001, Room 0210
Oak Ridge, TN 37831
(615) 574-2009

D. A. Farkas
Virginia Polytechnic Institute
and University
Blacksburg, VA 24061
(703) 961-4742

Cynthia K. Farrar
Montec Associates, Inc.
P.O. Box 4182
Butte, MT 59702
(406) 494-2596

G. C. Farrington
University of Pennsylvania
Philadelphia, PA 19104
(215) 898-8337

W. Feduska
Westinghouse Electric Corp.
R&D Center
1310 Beulah Road
Pittsburgh, PA 15235
(412) 256-1951

Robert S. Feigelson
Center for Materials Research
Stanford University
Stanford, CA 94305
(415) 723-4007

Mattison K. Ferber
ORNL
P.O. Box 2008
Building 4515
Oak Ridge, TN 37831-6064
(615) 576-0818

Nicholas Fiore
Carpenter Technology Corp.
101 West Bern Street
P.O. Box 14662
Reading, PA 19612
(215) 371-2556

Ronald J. Fiskum
EE-422/FORS
U.S. Dept. of Energy
Washington, DC 20585
(202) 586-9130

Timothy J. Fitzsimmons
ER-131, G-236/GTN
U.S. Dept. of Energy
Washington, DC 20585
(301) 903-9830

J. E. Flinn
Materials Technology Div.
Idaho National Eng. Laboratory
Idaho Falls, ID 83415
(208) 526-8127

P. S. Follansbee
LANL
Los Alamos, NM 87545
(505) 667-8021

D. M. Follstaedt
Division 1110
Sandia National Laboratories
Albuquerque, NM 87185
(505) 844-2102

F. Forsyth
Brookhaven National Lab
Upton, NY 11973
(516) 282-4676

Christopher A. Foster
Cryogenic Applications F, Inc.
450 Bacon Springs Lane
Clinton, TN 37716
(615) 435-5433

Earle Fowler
ER-226/FORS
U.S. Dept. of Energy
Washington, DC 20585
(301) 903-4801

Mark Frei
EM-34/FORS
U.S. Dept. of Energy
Washington, DC 20585
(301) 903-7201

Ehr-Ping Huang Fu
Thermal Science
EE-232/FORS
U.S. Dept. of Energy
Washington, DC 20585
(202) 586-1493

P. W. Fuerschbach
Division 1833
Sandia National Laboratories
Albuquerque, NM 87185
(505) 846-2464

E. R. Fuller
National Institute of Standards
and Technology
Gaithersburg, MD 20899
(301) 921-2942

F. D. Gac
LANL/MS G771
Los Alamos, NM 87545
(505) 667-5126

G. F. Gallegos
LLNL
University of California
P.O. Box 808
Livermore, CA 94550
(415) 422-7002

Yogendra S. Garud
S. Levy, Inc.
3425 South Bascom Avenue
Campbell, CA 95008
(408) 377-4870

F. P. Gerstle, Jr.
Sandia National Laboratories
Albuquerque, NM 87185
(505) 844-4304

C. P. Gertz
Yucca Mountain Project Mgr.
U.S. Dept. of Energy
P.O. Box 98518
Las Vegas, NV 89193
(702) 794-7920

Larry Gestaut
Eltech Systems Corp.
Painsville, OH 44077
(216) 357-4041

E. R. Gilbert
Pacific Northwest National Laboratory
Richland, WA 99352
(509) 375-2533

A. Glass
KMS Fusion
3621 South State Road
Ann Harbor, MI 48106
(313) 769-8500

R. Glass
LLNL
University of California
P.O. Box 808
Livermore, CA 94550
(415) 423-7140

Leon Glicksman
MIT
77 Massachussetts Avenue
Cambridge, MA 02139
(617) 253-2233

Martin Glicksman
Rensselear Polytechnic Inst.
Materials Research Ctr. - 104
8th Street
Troy, NY 12180-3690
(518) 276-6721

F. D. Gmeindl
METC
P.O. Box 880
Morgantown, WV 26505
(304) 291-4751

Neil J. Goldfine
Jentek Sensors, Inc.
1616 Soldiers Field Road
Boston, MA 02135
(617) 254-5552

John Goldsmith
EE-332/FORS
U.S. Dept. of Energy
Washington, DC 20585
(202) 586-8171

Robert L. Goldsmith
CeraMem Corporation
12 Clematis Avenue
Waltham, MA 02154
(617) 899-0467

Gerald Goldstein
ER-74/GTN
U.S. Dept. of Energy
Washington, DC 20545
(301) 903-5348

Mark Goldstein
Quantum Group, Inc.
11211 Sorrento Valley Road
San Diego, CA 92121
(619) 457-3048

B. Goodman
NREL
1617 Cole Blvd
Golden, CO 80401
(303) 231-1005

S. H. Goods
Divison 8314
Sandia National Laboratories
Livermore, CA 94550
(415) 422-3274

Paul D. Gorsuch
Space Systems Division
General Electric Company
P.O. Box 8555
Philadelphia, PA 19101
(215) 354-5047

R. J. Gottschall
ER-13/FORS
U.S. Dept. of Energy
Washington, DC 20585
(301) 903-3427

Fred S. Goulding
Instrumentation Division
Lawerence Berkeley Laboratory
Berkeley, California 94720
(415) 486-6432

R. A. Graham
Division 1130
Sandia National Laboratories
Albuquerque, NM 87185
(505) 844-1931

Anton C. Greenwald
Spire Corporation
One Patriots Park
Bedford, MA 01730-2396
(617) 275-6000

N. Grossman
NE-42/FORS
U.S. Dept. of Energy
Washington, DC 20585
(301) 903-3745

Dieter M. Gruen
Materials Science Division
Argonne National Laboratory
9700 South Cass Avenue
Argonne, IL 60439
(708) 252-3513

T. R. Guess
Division 1812
Sandia National Laboratories
Albuquerque, NM 87185
(505) 844-5604

Marvin E. Gunn
EE-14/FORS
U.S. Dept. of Energy
Washington, DC 20585
(202) 586-2826

M. Gurevich
EE-332/FORS
U.S. Dept. of Energy
Washington, DC 20585
(202) 586-6104

Adi R. Guzdar
Foster-Miller, Inc.
350 Second Avenue
Waltham, MA 02154
(617) 890-3200

John P. Gyeknyesi
NASA Lewis Research Center
2100 Brookpark Road, MS 49-7
Cleveland, OH 44135
(216) 433-3210

J. S. Haggarty
MIT
77 Massachussetts Avenue
Cambridge, MA 02139
(617) 253-2129

Kathleen Hain
EM-54/FORS
U.S. Dept. of Energy
Washington, DC 20585
(301) 903-7917

Phil Haley
Allison Turbine Operations
P.O. Box 420
Indianapolis, IN 46206-0420
(317) 230-2272

John M. Halstead
SOHIO Engineered Materials
P.O. Box 1054
Niagara Falls, NY 14302
(716) 278-2330

David G. Hamblen
Advanced Fuel Research, Inc.
87 Church Street
P.O. Box 380379
East Hartford, CT 06138-0379
(203) 528-9806

Edward P. Hamilton
American Superconductor Corp.
2 Technology Drive
Westboro, MA 01581
(508) 836-4200

Michael T. Harris
Chemical Tech. Div.
Oak Ridge National Lab
P.O. Box 2008
Oak Ridge, TN 37831
(615) 574-5962

Pat Hart
Pacific Northwest Labs
P.O. Box 999
Richland, WA 99352
(504) 375-2906

R. W. Haskell
GE Research Laboratory
P.O. Box 8
Schenectady, NY 12301
(518) 385-4226

Debbie Haught
EE-34/FORS
U.S. Dept. of Energy
Washington, DC 20585
(202) 586-2211

Jeff Hay
Chem.-Mat. Science Div.
Los Alamos National Lab
Los Alamos, NM 87545
(505) 843-2097

A. K. Hays
Division 1831
Sandia National Labs
Albuquerque, NM 87185
(505) 844-9996

Norman L. Hecht
University of Dayton
300 College Park, KL165
Dayton, OH 45469-0001
(513) 229-4343

Richard L. Heestand
ORNL
P.O. Box 2008
Bldg. 4508, 083, Room 128
Oak Ridge, TN 37831
(615) 574-4352

Kamithi Hemachalam
Intermagnetics General Corp.
1875 Thomaston Avenue
Waterbury, CT 06704
(203) 753-5215

Timothy Henderson
KMS Fusion, Inc.
Ann Arbor, MI 48106
(313) 769-8500

Mary T. Hendricks
Alabama Cryogenic Engineering, Inc.
P.O. Box 2470
Huntsville, AL 35804
(205) 536-8629

Carolyn J. Henkens
Andcare, Inc.
2810 Meridian Parkway
Suite 152
Durham, NC 27713
(919) 544-8220

Carl Henning
Lawrence Livermore Nat. Lab
P.O. Box 5511
Livermore, CA 94550
(415) 532-0235

Thomas P. Herbell
NASA Lewis Research Center
21000 Brookpark Road, 105-1
Cleveland, OH 44135
(216) 433-3246

Carl B. Hilland
DP-28/GTN
U.S. Dept. of Energy
Washington, DC 20545
(301) 903-3687

G. Duncan Hitchens
Lynntech, Inc.
7610 Eastmark Drive
Suite 105
College Station, TX 77840
(409) 693-0017

Kai-Ming Ho
Inst. for Physical
Research and Technology
Ames Labatory
Ames, IA 50011
(515) 294-1960

J. M. Hobday
METC
P.O. Box 880
Morgantown, WV 26505
(304) 291-4347

D. M. Hoffman
Lawrence Livermore Nat. Lab
University of California
P.O. Box 808
Livermore, CA 94550
(415) 422-7759

E. E. Hoffman
U.S. Dept. of Energy
P.O. Box 2001
Oak Ridge, TN 37831-8600
(615) 576-0735

G. J. Hooper
EE-324/FORS
U.S. Dept. of Energy
Washington, DC 20585
(202) 586-4153

Linda L. Horton
Oak Ridge National Laboratory
Box 2008, Bldg. 4500-S
Oak Ridge, TN 37831-6118
(615) 574-5081

E. Philip Horwitz
Chemistry Division
Argonne National Laboratory
9700 South Cass Avenue
Argonne, IL 60439
(708) 252-3653

Charles R. Houska
Dept. of Materials Eng.
Holden Hall
Virginia Polytechnic Institute
Blacksburg, VA 24061
(703) 961-5652

Stephen M. Hsu
Center for Materials Science
National Measurements Lab
NIST
Gaithersburg, MD 20899
(301) 975-6119

W. J. Huber
METC
P.O. Box 880
Morgantown, WV 26505
(304) 291-4663

Donald R. Huffman
Dept. of Physics
University of Arizona
Tucson, AZ 85721
(602) 621-4804

Robert A. Huggins
Dept. of Mat. Science & Eng.
Peterson 550I
Stanford University
Stanford, CA 94305
(415) 497-4110

Arlon Hunt
Lawrence Berkeley Laboratory
University of California
Berkeley, CA 94720
(415) 486-5370

Thomas K. Hunt
Advanced Modular Power Systems, Inc.
4667 Freedom Drive
Ann Arbor, MI 48108
(313) 677-4260

George F. Hurley
Chemistry-Materials Sci. Div.
Los Alamos National Laboratory
Los Alamos, NM 87545
(505) 667-9498

Gerald C. Huth
Univ. of Southern California
Inst. for Phys. & Imag. Sci.
4676 Admiralty Way
Marina del Rey, CA 90292
(213) 822-9184

Mallika D. Ilindra
Sumi Tech, Inc.
3006 McLean Court
Blacksburg, VA 24060
(703) 552-8334

D. David Ingram
Universal Energy Systems, Inc.
4401 Dayton-Xenia Road
Dayton, OH 45432
(513) 426-6900

L. K. Ives
National Institute of Standards
and Technology
Gaithersburg, MD 20899
(301) 921-2843

Jan S. Iwanczyk
Xsirius, Inc.
1220 Avenida Acaso
Camarillo, CA 93012
(805) 484-8300

David A. Jackson
Energy Photovoltaics, Inc.
276 Bakers Basin Road
Lawrenceville, NJ 08648
(609) 587-3000

Jonah Jacob
Science Research Lab, Inc.
15 Ward Street
Somerville, MA 02143
(617) 547-1122

N. S. Jacobson
NASA Lewis Research Center
21000 Brookpark Road
Cleveland, OH 44135
(216) 433-5498

Radha Jalan
ElectroChem, Inc.
400 West Cummings Park
Woburn, MA 01801
(617) 932-3383

Mark A. Janney
ORNL
P.O. Box 2008
Bldg. 4515, 069, Room 228
Oak Ridge, TN 37831-6088
(615) 574-4281

J. L. Jellison
Division 1833
Sandia National Laboratories
Albuquerque, NM 87185
(505) 844-6397

M. M. Jenior
EE-332/FORS
U.S. Dept. of Energy
Washington, DC 20585
(202) 586-2998

J. E. Jensen
CVI Inc.
P.O. Box 2138
Columbus, OH 43216
(614) 876-7381

Carl E. Johnson
Chemical Technology Division
Argonne National Laboratory
9700 Cass Ave, Bldg. 205
Argonne, IL 60439
(312) 972-7533

Curtis A. Johnson
GE Research Laboratory
P.O. Box 8
Bldg. 31 #3C7
Schenectady, NY 12301
(518) 387-6421

D. L. Johnson, Chairman
Dept. of Mat. Science & Eng.
2145 Sheridan Road, Rm 1034
Northwestern University
Evanston, IL 60201
(312) 492-3537

D. Ray Johnson
ORNL, Metals & Ceramics Div.
P.O. Box 2008
Bldg. 4515, 066, Room 206
Oak Ridge, TN 37831-6088
(615) 576-6832

R. J. Johnson
Hanford Eng. Dev. Lab.
P.O. Box 1970
Richland, WA 99352
(509) 376-0715

T. Johnson
Bldg. 205
9700 South Cass Avenue
Argonne, IL 60439
(312) 972-5964

H. Jones
GA Technologies
P.O. Box 81608
San Diego, CA 92138
(615) 455-2360

Robert Jones
Los Alamos National Lab.
P.O. Box 1663, M/S J577
Los Alamos, NM 87545
(505) 667-6441

Robert A. Jones
DP-28/GTN
U.S. Dept. of Energy
Washington, DC 20545
(301) 903-4236

Ram Kachare
M/S 238-343
Flat Plate Solar Array Project
Jet Propulsion Laboratory
Pasadena, CA 91109
(213) 354-4583

Neil Kaminar
Solar Eng. Applications Corp.
P.O. Box 62246
Sunnyvale, CA 94088
(408) 986-9231

Chris Kang
EE-142/FORS
U.S. Dept. of Energy
Washington, DC 20585
(202) 586-4563

M. J. Kania
ORNL
P.O. Box 2008
Bldg. 3525, 390, Room 109
Oak Ridge, TN 37831
(615) 576-4856

Landis Kannberg
Pacific Northwest Lab
Battlelle Blvd.
P.O. Box 999
Richland, WA 99352
(509) 375-3919

Michael E. Karpuk
TDA Research, Inc.
12345 West 52nd Avenue
Wheat Ridge, CO 80033
(303) 940-2301

M. E. Kassner
Oregon State University
Dept. Of Mechanical Engineering
Rogers 204
Corvallis, OR 97331-5001
(503) 737-7023

Carlos Katz
Cable Technology Lab
P.O. Box 707
New Brunswick, NJ 08903
(201) 846-3220

Joel Katz
LANL
P.O. Box 1663/MS G771
Los Alamos, NM 87545
(505) 665-1424

Robert N. Katz
Worcester Polytechnical Inst.
Dept. of Mechanical Eng.
100 Institute Street
Worcester, MA 01609
(508) 831-5336

Larry Kazmerski
Solar Electric Conv. Div.
NREL
1617 Cole Blvd.
Golden, CO 80401
(303) 231-1115

M. R. Keenan
Division 1813
Sandia National Laboratories
Albuquerque, NM 87185
(505) 844-6631

J. R. Keiser
ORNL
P.O. Box 2008
Bldg. 4500-S, 156, Room 0734
Oak Ridge, TN 37830
(615) 574-4453

Rudolf Keller
EMEC Consultants
4221 Roundtop Road
Export, PA 15632
(412) 325-3260

Paul T. Kerwin
NASA Lewis Research Center
21000 Brookpark Road, MS 77-6
Cleveland, OH 44135
(216) 433-3409

Lawrence W. Kessler
Sonoscan, Inc.
530 East Green Street
Bensenville, IL 60106
(213) 766-7088

Han Kim
GTE Labs
40 Sylvan Road
Waltham, MA 02254
(617) 466-2742

Christopher N. King
Planar Systems, Inc.
1400 Northwest Compton Drive
Beaverton, OR 97006
(503) 690-1100

Richard King
EE-131/FORS
U.S. Dept. of Energy
Washington, DC 20585
(202) 586-1693

J. H. Kinney
LLNL
University of California
P.O. Box 808
Livermore, CA 94550
(415) 422-6669

G. S. Kino
Edward Ginzton Laboratory
Stanford University
Stanford, CA 94305
(415) 497-0205

Thomas Kitchens
ER-7/GTN
U.S. Dept. of Energy
Washington, DC 20585
(301) 903-3426

E. E. Klaus
Penn State
Room 108, Fenske Laboratory
Univ Park, PA 16802
(814) 865-2574

Paul Klemmens
University of Connecticut
Box U-46
Storrs, CT 06268
(203) 486-3134

S. J. Klima
NASA Lewis Research Center
MS 106-1
21000 Brookpark Road
Cleveland, OH 44135
(216) 433-6020

J. A. Knapp
Division 1110
Sandia National Laboratories
Albuquerque, NM 87185
(505) 844-2305

G. A. Knorovsky
Division 1833
Sandia National Laboratories
Albuquerque, NM 87185
(505) 844-1109

Timothy R. Knowles
Energy Science Labs, Inc.
6888 Nancy Ridge Drive
San Diego, CA 92121-2232
(619) 552-2034

C. C. Koch
Materials Eng. Department
North Carolina State University
Raliegh, NC 27650
(919) 737-2377

Victor R. Koch
Covalent Associates, Inc.
10 State Street
Woburn, MA 01801
(617) 938-1140

D. Krajcinovic
Dept. of Civil Eng.,
Mechanics & Metallurgy
University of Illinois
Chicago, IL 60680
(312) 996-7000

K. G. Kreider
National Institute of Standards
and Technology
Washington, DC 20234
(301) 921-3281

L. E. Kukacka
Brookhaven National Laboratory
Upton, NY 11973
(516) 282-3065

David Kurtz
Advanced Technology Materials, Inc.
7 Commerce Drive
Danbury, CT 06810
(203) 794-1100

S. R. Kurtz
Division 1811
Sandia National Laboratories
Albuquerque, NM 87185
(505) 844-5436

Richard J. Lagow
Department of Chemistry
The Univ. of Texas at Austin
Austin, TX 78712
(512) 471-1032

C. M. Lampert
Lawerence Berkeley Laboratory
University of California
Berkeley, CA 94720
(415) 486-6093

A. Landgrebe
EE-32/FORS
U.S. Dept. of Energy
Washington, DC 20585
(202) 586-1483

P. M. Lang
NE-45/FORS
U.S. Dept. of Energy
Washington, DC 20585
(301) 903-3313

James Lankford
Southwest Research Inst.
6220 Culebra Road
P.O. Drawer 28510
San Antonio, TX 78284
(512) 684-5111

Herbert J. Larson
Caterpillar, Inc.
Building F
100 N.E. Adams
Peoria, IL 61629
(309) 578-6549

R. LaSala
EE-122/FORS
U.S. Dept. of Energy
Washington, DC 20585
(202) 586-4198

W. N. Lawless
CeramPhysics, Inc.
921 Eastwind Drive, Suite 110
Westerville, OH 43081
(614) 882-2231

Ed LeBaker
ARACOR
425 Lakeside Drive
Sunnyvale, CA 94086
(408) 733-7780

Robert LeChevalier
U.S. Dept. of Energy
San Fransisco Oper. Office
1333 Broadway
Oakland, CA 94612
(415) 273-6362

S. R. Lee
U.S. Dept. of Energy
P.O. Box 10940
Pittsburgh, PA 15236
(412) 675-6137

Franklin D. Lemkey
United Tech. Research Ctr.
Silver Lane
East Hartford, CT 06108
(203) 727-7318

Douglas Lemon
Pacific Northwest Labs
P.O. Box 999
Richland, WA 99352
(509) 375-2306

Alexander Lempicki
ALEM Associates/Radiation
Monitoring Devices
303A Commonwealth Avenue
Boston, MA 02115
(617) 353-9581

S. R. Levine
NASA Lewis Research Center
21000 Brookpart Road
Cleveland, OH 44135
(216) 433-3276

A. V. Levy
Lawerence Berkley Lab
University of California
One Cyclotron Road
Berkley, CA 94720
(415) 486-5822

John Lewellen
NE-46/FORS
U.S. Dept. of Energy
Washington, DC 20585
(301) 903-2899

Patrick Lin
Chemat Technology, Inc.
19365 Business Center Drive
Suite 8
Northridge, CA 91324
(818) 727-9786

L. J. Lindberg
Garrett Turbine Engine Co.
111 South 34th Street
P.O. Box 5217
Phoenix, AZ 85010
(602) 231-4002

J. Lipkin
Sandia National Laboratories
Livermore, CA 94550
(415) 422-2417

C. T. Liu, Mtl. Ceram. Div.
ORNL
P.O. Box 2008
Bldg. 4500-S, 115, Rm. S280
Oak Ridge, TN 37831
(615) 574-5516

K. C. Liu
ORNL
P.O. Box 2008
Bldg. 4500-S, MS 155
Oak Ridge, TN 37831
(615) 574-5116

Earl L. Long, Jr.
ORNL, Metals & Ceramics Div.
P.O. Box 2008
Bldg. 4515, 069, Room 229
Oak Ridge, TN 37831
(615) 574-5127

Richard W. Longsderff
Thermacore, Inc.
780 Eden Road
Lancaster, PA 17601
(717) 569-6551

Michael Lopez
U.S. Dept. of Energy
San Francisco Oper. Office
1333 Broadway
Oakland, CA 94612
(415) 273-4264

R. O. Loutfy
Mat. & Electro. Research Corp.
7960 South Kolb Road
Tucson, AZ 85706
(602) 574-1980

T. C. Lowe
Divison 8316
Sandia National Laboratories
Livermore, CA 94550
(415) 422-3187

C. D. Lundin
307 Dougherty Eng. Bldg.
University of Tennessee
Knoxville, TN 37996
(615) 974-5310

MAJ Ross E. Lushbough
DP-225.2/FORS
U.S. Dept. of Energy
Washington, DC 20585
(301) 903-3912

William C. Luth
ER-15
U.S. Dept. of Energy
Washington, DC 20585
(301) 903-5822

E. A. Maestas
West Valley Project Office
U.S. Dept. of Energy
P.O. Box 191
West Valley, NY 14171-0191
(716) 942-4314

Richard Mah
Los Alamos National Lab
P.O. Box 1663
Los Alamos, NM 87545
(505) 607-3238

Mokhtas S. Maklad
EOTEC Corporation
420 Frontage Road
West Haven, CT 06516
(203) 934-7961

Frederick M. Mako
FM Technologies
10529-B Braddock Road
Fairfax, VA 22032
(703) 425-5111

A. C. Makrides
EIC Laboratories, Inc.
111 Downey Street
Norwood, MA 02062
(617) 769-9450

Subhas G. Malghan
NIST
A-258/223
Gaithersburg, MD 20899
(301) 975-6101

Mark K. Malmros
MKM Research/Ohmicron
P.O. Box I
Washington Crossing, PA 18977
(609) 737-9050

Matthew Marrocco
Maxdem, Inc.
140 East Arrow Highway
San Dimas, CA 91773
(909) 394-0644

R. G. Martin
Analysis Consultants
21831 Zuni Drive
El Toro, CA 92630
(714) 380-1204

H. Maru
Energy Research Corporation
3 Great Pasture Road
Danbury, CT 06810
(412) 578-2700

K. Masubuchi
Lab for Manuf. and Prod.
MIT
Cambridge, MA 02139
(617) 255-6820

Ronald D. Matthews
Dept. of Mechanical Engineering
The University of Texas at Austin
Austin, TX 78712
(512) 471-3108

W. A. May, Jr.
LANL
Los Alamos, NM 87545
(505) 667-6362

Jacob Maya
GTE Products Corp
Silvania Lighting Center
Danvers, MA 01923
(617) 777-1900

Douglas McAllister
BIODE, Inc.
2 Oakwood Road
Cape Elizabeth, ME 04107
(207) 883-1492

James W. McCauley, Dean
New York State College of Ceramics
Alfred University
Alfred, NY 14802
(607) 871-2411

Robert W. McClung
ORNL
P.O. Box 2008
Bldg. 4500-S, 151, Rm. D63
Oak Ridge, TN 37831-6088
(615) 574-4466

J. I. McCool
SKF Industries, Inc.
1100 First Avenue
King of Prussia, PA 19406
(215) 265-1900

Scott B. McCray
Bend Research, Inc.
64550 Research Road
Bend, OR 97701-8599
(503) 382-4100

D. McCright
LLNL
University of California
Livermore, CA 94550
(213) 423-7051

Roger J. McDonald
Brookhaven National Laboratory
Bldg. 475
Upton, NY 11973
(515) 282-4197

Patrick N. McDonnell
Spire Corporation
One Patriots Park
Bedford, MA 01730-2396
(617) 275-6000

H. K. McDowell
LANL
Los Alamos, NM 87545
(505) 667-4686

David L. McElroy
ORNL
P.O. Box 2008
Bldg. 4508, 092, Rm. 239
Oak Ridge, TN 37831-6088
(615) 574-5976

A. J. McEvily
Metallurgy Dept., U-136
University of Connecticut
Storas, CT 06268
(203) 486-2941

T. D. McGee
Mat. Science & Engineering
110 Engineering Annex
Iowa State University
Ames, IA 50011
(515) 294-9619

R. R. McGuire
Lawrence Livermore Nat. Lab
University of California
P.O. Box 808
Livermore, CA 94550
(415) 422-7792

Carl McHargue
University of Tennessee
Materials & Eng. Dept.
434 Doughtery Eng. Bldg.
Knoxville, TN 37996-2200
(615) 974-8013

M. J. McMonigle
EE-234/FORS
U.S. Dept. of Energy
Washington, DC 20585
(202) 586-2082

Arthur S. Mehner
NE-53/FORS
U.S. Dept. of Energy
Washington, DC 20585
(301) 903-4474

G. H. Meier
848 Benevum Hall
University of Pittsburgh
Pittsburgh, PA 15261
(412) 624-5316

J. E. Mendel
Pacific Northwest Lab.
P.O. Box 999
Richland, WA 99352
(509) 375-2905

P. D. Metz
Brookhaven National Lab.
Upton, NY 11973
(516) 282-3123

A. Meyer
International Fuel Cells
P.O. Box 739
195 Governors Hwy.
South Windsor, CT 06074
(203) 727-2214

B. E. Mills
Sandia National Laboratories
Livermore, CA 94550
(415) 422-3230

M. V. Mitchell
AiResearch Casting Co.
19800 Van Ness
Torrance, CA 90509
(213) 618-7411

Andrew Morrison
M/S 238-343
Flat Plate Solar Array Project
Jet Propulsion Laboratory
Pasadena, CA 91109
(213) 354-7200

Craig Mortenson
BPA/FORS
U.S. Dept. of Energy
Washington, DC 20585
(202) 586-5656

J. Moteff
University of Cincinnati
Department of Material Science
Metallurgical Engineering
498 Rhodes Hall
Cincinnati, OH 45221-0012
(513) 475-3096

Leszek R. Motowidlo
IGC Advanced Superconductors
1875 Thomaston Avenue
Waterbury, CT 06704
(203) 753-5215

Arnulf Muan
Pennsylvania State University
EMS Experiment Station
415 Walker Bldg.
University Park, PA 16802
(814) 865-7659

L. Marty Murphy
NREL
1617 Cole Blvd
Golden, CO 80401
(303) 231-1050

J. Narayan
Materials Science & Eng.
North Carolina State Univ.
Box 7916
Raleigh, NC 27695-7916
(919) 515-7874

J. E. Nasise
LANL
Los Alamos, NM 87545
(505) 667-1459

Michael Nastasi
Los Alamos National Lab
Los Alamos, NM 87545
(505) 667-7007

K. Natesan
Argonne National Lab.
Materials Science Division
9700 South Cass
Argonne, IL 60439
(312) 972-5068

M. Naylor
Cummins Engine Co., Inc.
Box 3005
Mail Code 50183
Columbus, IN 47202-3005
(812) 377-5000

Fred Nichols
Argonne National Laboratory
9700 South Cass
Argonne, IL 60439
(312) 972-8292

M. C. Nichols
Sandia National Laboratories
Livermore, CA 94550
(415) 422-2906

P. J. Nigrey
Division 1150
Sandia National Laboratories
Albuquerque, NM 87185
(505) 844-8985

F. B. Nimick, Division G313
Sandia National Laboratory
P.O. Box 5800
Albuquerque, NM 87185
(505) 844-6696

D. A. Nissen
Sandia National Laboratories
Livermore, CA 94550
(415) 422-2767

R. Gerald Nix
NREL
1617 Cole Blvd
Golden, CO 80401
(303) 231-1757

T. A. Nolan
ORNL
P.O. Box 2008
Bldg. 4515, MS 064
Oak Ridge, TN 37831
(615) 574-0811

Paul C. Nordine
Containerless Research, Inc.
910 University Place
Evanston, IL 60201-3149
(708) 467-2678

P. C. Odegard
Divison 8216
Sandia National Laboratories
Livermore, CA 94550
(415) 422-2789

G. R. Odette
Dept. of Chem. & Nuclear Eng.
University of California
Santa Barbara, CA 93106
(805) 961-3525

Thomas Ohlemiller
Center for Bldg. Technology
National Institute of Standards
and Technology
Gaithersburg, MD 20899
(301) 921-3771

Ben Oliver
Materials Science & Eng.
421 Dougherty Hall
Knoxville, TN 37996
(615) 974-5326

Randall B. Olsen
Chronos Research Labs, Inc.
3025 Via de Caballo
Olivenhaim, CA 92024
(619) 756-1447

Mark J. O'Neill
ENTECH, Inc.
P.O. Box 612246
DFW Airport, TX 75261
(214) 456-0900

G. C. Osbourn
Division 1130
Sandia National Laboratories
Albuquerque, NM 87185
(505) 844-8850

Roland Otto
Lawrence Berkeley Lab.
Bldg 73, 106A
Berkeley, CA 94720
(415) 486-5289

V. Oversby
LLNL
University of California
Livermore, CA 94550
(213) 423-2228

G. M. Ozeryansky
IGC Superconductors, Inc.
1875 Thomaston Avenue
Waterbury, CT 06704
(203) 753-5215

Richard H. Pantell
Electrical Engineering Dept.
Stanford University
Stanford, CA 94305
(415) 723-2564

E. R. Parker
456 Hearst
Univ. of Ca., Berkeley
Berkeley, CA 24720
(415) 642-0863

Bill Parks
EE-221/FORS
U.S. Dept. of Energy
Washington, DC 20585
(202) 586-2093

D. O. Patten
Norton Company
High Performance Ceramics
Goddard Road
Northboro, MA 01532
(617) 393-5963

H. C. Peebles
Divsion 1831
Sandia National Laboratories
Albuquerque, NM 87185
(505) 844-1647

David Pellish
EE-231/FORS
U.S. Dept. of Energy
Washington, DC 20585
(202) 586-6436

Ahmad Pesaran
NREL
1617 Cole Blvd.
Golden, CO 80401
(303) 231-7636

Randy Petri
IGT
3424 S. Stale St.
Chicago, IL 60616
(312) 567-3985

John Petrovic
Chemistry-Mat. Science Div.
Los Alamos National Laboratory
Los Alamos, NM 87545
(505) 667-5452

S. T. Picraux
Division 1110
Sandia National Laboratories
Albuquerque, NM 87185
(505) 844-7681

R. D. Pierce
Argonne National Laboratories
Chemical Tech Division
Bldg. 205, Room W-125
Argonne, IL 60439
(312) 972-4450

Melvin A. Piestrup
Adelphi Technology
13800 Skyline Blvd.
Woodside, CA 94062
(415) 851-0633

James E. Plank
Charles Evans and Associates
301 Chesapeake Drive
Redwood City, CA 94063
(415) 369-4567

L. E. Pope
Division 1834
Sandia National Laboratories
Albuquerque, NM 87185
(505) 844-5041

Joseph Prahl
Case Western Reserve Univ.
Cleveland, OH 44106
(216) 368-2000

Mark A. Prelas
Nuclear Engineering Program
University of Missouri
Columbia, MO 65211
(314) 882-3550

Donald Priesty
ER-542/FORS
U.S. Dept. of Energy
Washington, DC 20585
(301) 903-3421

G. T. Privon
ORNL
P.O. Box 2009
Building 9102-2, Rm. 209
Oak Ridge, TN 37831
(615) 574-1013

Peter Pronko
Universal Energy Systems
4401 Dayton-Xenia Road
Dayton, OH 45432
(513) 426-6900

Michael Pulscak
EE-352/FORS
U.S. Dept. of Energy
Washington, DC 20585
(202) 586-1726

Herbert Pummes
Altex Corporation
P.O. Box 10084
Chicago, IL 60610
(312) 372-3440

R. Quinn
Division 1846
Sandia National Labs
Albuquerque, NM 87185
(505) 844-1933

Herschel Rabitz
Dept. of Chemistry
Princeton University
Princeton, NJ 08544-1009
(609) 258-3917

P. B. Rand
Division 1813
Sandia National Labs
Albuquerque, NM 87185
(505) 844-7953

Robert Rapp
Dept. of Metal. Eng.
Ohio State University
Columbus, OH 43210
(614) 422-2491

Bhakta B. Rath, Assoc. Dir. Res.
Naval Research Laboratory
Mat. Science & Component Tech.
Building 43, Room 212 - Code 6000
Washington, DC 20375-5000
(202) 767-3566

Rod Ray
Bend Research, Inc.
64550 Research Road
Bend, OR 97701-8599
(503) 382-4100

Richard Razgaitis
Battelle-Columbus Labs
505 King Avenue
Columbus, OH 43201
(614) 424-4212

Brian Rennex
Natl. Institute of Standards
and Technology
Center of Bldg. Technology
Gaithersburg, MD 20899
(301) 921-3195

W. G. Reuter
Materials Technology Div.
Idaho National Eng. Lab
Idaho Falls, ID 83415
(205) 526-0111

William Richards
EE-121/FORS
U.S. Dept. of Energy
Washington, DC 20585
(202) 586-5410

S. Richlen
EE-221/FORS
U.S. Dept. of Energy
Washington, DC 20585
(202) 586-2078

R. O. Ritchie
456 Hearst
University of Cal., Berkeley
Berkeley, CA 24720
(415) 642-0863

P. L. Rittenhouse
ORNL
P.O. Box 2008
Bldg. 45005, 138, Rm. A158
Oak Ridge, TN 37831
(615) 574-5103

H. F. Rizzo
Lawrence Livermore Nat. Lab
University of California
P.O. Box 808
Livermore, CA 94550
(415) 422-6369

R. B. Roberto
ORNL
Solid State Division
P.O. Box 2008
Oak Ridge, TN 37831-6030
(423) 574-6151

D. I. Roberts
GA Technologies
P.O. Box 81608
San Diego, CA 92138
(619) 455-2560

S. L. Robinson
Division 8314
Sandia National Laboratories
Livermore, CA 94550
(415) 422-2209

A. D. Romig
Division 1832
Sandia National Laboratories
Albuquerque, NM 87185
(505) 844-8358

Timothy L. Rose
EIC Laboratories, Inc.
111 Downing Street
Norwood, MA 02062
(617) 764-9450

R. S. Rosen
LLNL
University of California
P.O. Box 808
Livermore, CA 94550
(415) 422-9559

John H. Rosenfeld
Thermacore, Inc.
780 Eden Road
Lancaster, PA 17601
(717) 569-6551

P. N. Ross
Mat. & Metal. Research Div.
Lawrence Berkeley Labs
University of Berkeley
Berkeley, CA 94720
(415) 486-4000

Giulio A. Rossi
Norton Company
Goddard Road
Northboro, MA 01532-1545
(617) 393-5829

Walter Rossiter
Center for Bldg. Technology
National Institute of Standards
and Technology
Gaithersburg, MD 20899
(301) 921-3109

Arthur Rowcliffe, Met/Ceram Div.
ORNL
P.O. Box 2008
Bldg. 5500, 376, Rm. A111
Oak Ridge, TN 37831
(615) 576-4864

M. Rubin
Lawrence Berkeley Laboratory
University of California
Berkeley, CA 94720
(415) 486-7124

E. Russell
LLNL
University of California
Livermore, CA 94550
(213) 423-6398

C. O. Ruud
159 MRL
University Park, PA 16802
(814) 863-2843

John Ryan
EE-422/FORS
U.S. Dept. of Energy
Washington, DC 20585
(202) 586-9130

J. R. Sadoway
MIT
77 Massachussetts Avenue
Cambridge, MA 02139
(617) 253-3300

Djordjiji R. Sain
Nuclear Con. Services, Inc.
P.O. Box 29151
Columbus, OH 43229
(614) 846-5710

Robert Salat
Vactronic Laboratory Equipment, Inc.
160 Wilbur Place
Bohemia, NY 11716
(516) 567-0520

Peter H. Salmon-Cox
Dir. of Office Ind. Processes
EE-23/FORS
U.S. Dept. of Energy
Washington, DC 20585
(202) 586-2380

F. Salzano
Brookhaven National Laboratory
Upton, NY 11973
(516) 282-4458

R. J. Salzbrenner
Division 1832
Sandia National Laboratories
Albuquerque, NM 87185
(505) 844-5041

Anthony F. Sammells
Eltron Research, Inc.
2830 Wilderness Place, Suite E
Boulder, CO 80301-5455
(303) 440-8008

Eileen E. Sammells
Eltron Research, Inc.
2830 Wilderness Place, Suite E
Boulder, CO 80301-5455
(303) 440-8008

Stuart Samuelson
Deltronic Crystal Industries, Inc.
60 Harding Avenue
Dover, NJ 07801
(201) 361-2222

J. Sankar
Dept of Mechanical Engineering
North Carolina A&T University
Greensboro, NC 27411
(919) 379-7620

Mike L. Santella
ORNL
P.O. Box 2008
Oak Ridge, TN 37831-6088
(615) 574-4805

Srinivasan Sarangapani
ICET, Inc.
916 Pleasant Street
Unit 12
Norwood, MA 02062
(617) 679-6064

V. K. Sarin
GTE
40 Sylvan Road
Waltham, MA 02254
(617) 890-8460

Suri A. Sastri
Surmet Corporation
33 B Street
Burlington, MA 01803
(617) 272-3250

C. M. Scheuerman
NASA Lewis Research Center
21000 Brookpark Road, MS 49-1
Cleveland, OH 44135
(216) 433-3205

Y. Schienle
Garrett Turbine Engine Co.
111 South 34th Street
P.O. Box 5217
Phoenix, AZ 85034
(602) 231-4666

Paul Schissel
NREL
1617 Cole Blvd.
Golden, CO 80401
(303) 231-1226

Jerome J. Schmidt
Jet Process Corporation
25 Science Park
New Haven, CT 06511
(203) 786-5130

S. J. Schneider
National Institute of Standards
and Technology
Gaithersburg, MD 20899
(301) 921-2901

G. D. Schnittgrund
Rockwell International
Rocketdyne Division
6633 Canoga Avenue
Canoga Park, CA 91304
(818) 710-5972

W. K. Schubert
Division 1815, SNL
Albuquerque, NM 87185
(505) 846-2466

Erland M. Schulson
33 Haskins Road
Hanover, NH 03755
(603) 646-2888

Robert B. Schulz
EE-34/FORS
U.S. Dept. of Energy
Washington, DC 20585
(202) 586-8051

James Schwarz
Dept. Chem. Eng/Mat Science
Syracuse University
320 Hinds Hall
Syracuse, NY 13244
(315) 423-4575

Peter Scofield
EE-421/FORS
U.S. Dept. of Energy
Washington, DC 20585
(202) 586-9193

James L. Scott
Metals and Ceramics Div.
ORNL
P.O. Box 2008, Bldg. 4508
Oak Ridge, TN 37831-6091
(615) 624-4834

Timothy C. Scott
Chemical Technology Division
Oak Ridge National Laboratory
P.O. Box 2008
Oak Ridge, TN 37831
(615) 574-5962

R. E. Setchell
Division 1130
Sandia National Labs
Albuquerque, NM 87185
(505) 844-5459

J. A. Seydel
Materials Science Division
Idaho National Eng. Lab
Idaho Falls, ID 84315
(208) 526-0111

D. J. Sharp
Division 1831
Sandia National Laboratories
Albuquerque, NM 87185
(505) 844-8604

B. J. Shaw
Westinghouse R&D Center
1310 Beulah Road
Pittsburgh, PA 15235
(412) 256-1201

Suzanne C. Shea
Praxis Engineers, Inc.
852 North Hillview Drive
Milpitas, CA 95035
(408) 945-4282

D. E. Shelor
RW-3/FORS
U.S. Dept. of Energy
Washington, DC 20585
(202) 586-9433

V. K. Sikka
ORNL
P.O. Box 2008
Bldg. 4508, 083, Rm. 129
Oak Ridge, TN 37831
(615) 574-5112

Richard Silberglitt
FM Technologies, Inc.
Patriot Square
10529-B Braddock Road
Fairfax, VA 22032
(703) 425-5111

T. B. Simpson
FE-34/FORS
U.S. Dept. of Energy
Washington, DC 20585
(301) 903-3913

J. P. Singh
Argonne National Labs
9700 South Cass
Argonne, IL 60439
(312) 972-5068

Maurice J. Sinnott
Chemical and Metall. Eng.
University of Michigan
H Dow Building
Ann Arbor, MI 48109-2136
(313) 764-4314

Piran Sioshamsi
Spire Corporation
Patriots Park
Bedford, MA 02173
(617) 275-6000

Kurt D. Sisson
EE-222/FORS
U.S. Dept. of Energy
Washington, DC 20585
(202) 586-6750

Hal Sliney
NASA Lewis Research Center
21000 Brookpark Road
MS 23-2
Cleveland, OH 44135
(216) 433-6055

Jerry Smith
ER-132/GTN
U.S. Dept. of Energy
Washington, DC 20545
(301) 903-3426

M. F. Smith
Division 1834
Sandia National Laboratories
Albuquerque, NM 87185
(505) 846-4270

Paul Smith
Materials Dept.
Univ. of CA, Santa Barbara
Santa Barbara, CA 93103
(805) 893-8104

Peter L. Smith
Newton Optical Technologies
167 Valentine Street
Newton, MA 02165
(617) 495-4984

J. E. Smugeresky
Division 8312
Sandia National Laboratories
Livermore, CA 94550
(415) 422-2910

N. R. Sorensen
Division 1841
Sandia National Laboratories
Albuquerque, NM 87185
(505) 844-1097

Charles A. Sorrell
AIM Program
EE-232/FORS
U.S. Dept. of Energy
Washington, DC 20585
(202) 586-1514

R. F. Sperlein
U.S. Dept. of Energy
P.O. Box 10940
Pittsburgh, PA 15236
(312) 972-5985

Bernard F. Spielvogel
Boron Biologicals, Inc.
533 Pylon Drive
Raleigh, NC 27606
(919) 832-2044

J. R. Springarn
Division 8312, SNL
Livermore, CA 94550
(415) 422-3307

William Sproul
Borg-Warner Company
1200 South Wolf Road
Des Plaines, IL 60018
(312) 827-3131

Mark B. Spitzer
Spire Corporation
Patriots Park
Bedford, MA 01730
(617) 275-6000

Gregory C. Stangle
School of Cer. Eng.
2 Pine Street
Alfred University
Alfred, NY 14802
(607) 871-2798

T. L. Starr
Georgia Tech Res. Inst.
Georgia Inst. of Technology
Atlanta, GA 30332
(404) 894-3678

Carl A. Stearns
NASA Lewis Research Center
MS 106-1
21000 Brookpark Road
Cleveland, OH 44135
(216) 433-5504

Wayne S. Steffier
Hyper-Therm, Inc.
18411 Gothard Street
Units B & C
Huntington Beach, CA 92648
(714) 375-4085

Charles Stein
Thermal Electric Devices, Inc.
1009 Bradbury Drive, Southeast
Albuquerque, NM 87106
(505) 272-7505

Joseph R. Stephens
NASA Lewis Research Center
21000 Brookpark Road
Cleveland, OH 44135
(216) 433-3195

Helmut F. Stern
Arcanum Corporation
P.O. Box 1482
Ann Arbor, MI 48106
(313) 665-4421

George Stickford
Battelle-Columbus Labs
505 King Avenue
Columbus, OH 43201
(614) 424-4810

Thomas J. Stiner
AstroPower, Inc.
Solar Park
Newark, DE 19716
(302) 366-0400

Robert J. Stinner
ISM Technologies, Inc.
9965 Carroll Canyon Road
San Diego, CA 92131
(619) 530-2332

D. P. Stinton
ORNL
P.O. Box 2008
Bldg. 4515, 063, Rm. 111
Oak Ridge, TN 37831
(615) 574-4556

Thomas G. Stoebe
Chairman, Mat. Sci. & Eng.
University of Washington
Roberts Hall, FB-10
Seattle, WA 98195
(206) 543-2600

Norman Stoloff
Materials Engineering Dept.
Rensselaer Polytechnic Inst.
Troy, NY 12181
(518) 266-6436

Paul D. Stone
The Dow Chemical Company
1776 Eye Street, NW, #575
Washington, DC 20006

J. E. Stoneking
Dept. of Eng. Science & Mech.
310 Perkins Hall
Knoxville, TN 37996
(615) 974-2171

G. Stoner
University of Virginia
Charlottesville, VA 22901
(804) 924-3277

Roger S. Storm
Carborundum
Government Programs
P.O. Box 832
Niagara Falls, NY 14302
(716) 278-2000

Edwin E. Strain
Garrett Corporation
111 S. 34th Street
P.O. Box 5217, MS 301-2N
Phoenix, AZ 85010
(602) 231-2797

Reinhold N. W. Strnot
KJS Associates
1616 Hillrose Place
Fairborn, OH 45324
(513) 879-0114

Thomas N. Strom
NASA Lewis Research Center
21000 Brookpark Road, MS 77-6
Cleveland, OH 44135
(216) 433-3408

David Sutter
ER-224/FORS
U.S. Dept. of Energy
Washington, DC 20585
(301) 903-5228

Patrick Sutton
EE-151/FORS
U.S. Dept. of Energy
Washington, DC 20585
(202) 586-8012

Jeffrey J. Swab
U.S. Army Materials Tech. Lab
405 Arsenal Street
Watertown, MA 02172
(617) 923-5410

Richard Swanson
SunPower Corporation
435 Indio Way
Sunnyvale, CA 94086
(408) 991-0900

Arthur D. Sweet
Goremotive Industries, Inc.
20944 Sherman Way
Suite 206
Canoga Park, CA 91303
(818) 884-0015

R. W. Swindeman
ORNL
P.O. Box 2008
Bldg. 4500-S, 155, Rm. 0040
Oak Ridge, TN 37831
(615) 574-5108

W. Tabakoff
Dept. of Aerospace Eng.
M/L 70
University of Cincinnati
Cincinnati, OH 45221
(513) 475-2849

L. E. Tanner
LLNL
University of California
P.O. Box 808
Livermore, CA 94550
(415) 423-2653

H. L. Tardy
Sandia National Laboratories
Org. 6213
P.O. Box 5800
Albuquerque, NM 87185-5800
(505) 846-6548

Michael Teresinski
ER-13/GTN
U.S. Dept. of Energy
Washington, DC 20545
(301) 903-5155

Giuliana Tesoro
Plastics Institute of America
Stevens Institutes of Tech.
Castle Point Station
Hoboken, NJ 07030
(201) 420-5552

C. A. Thomas
U.S. Dept. of Energy
P.O. Box 10940
Pittsburgh, PA 15236
(312) 972-5731

Iran L. Thomas
ER-10/GTN
U.S. Dept. of Energy
Washington, DC 20545
(301) 903-3426

D. O. Thompson
Ames Laboratory
Iowa State University
Ames, IA 50011
(515) 294-5320

John K. Tien
Columbia University
1137 S.W. Mudd Building
New York, NY 10027
(212) 280-5192

T. Y. Tien
Mat. and Metal. Eng.
University of Michigan
Ann Arbor, MI 48109
(813) 764-9449

T. N. Tiegs
ORNL
Bldg. 4515, 069, Rm. 230
P.O. Box 2008
Oak Ridge, TN 37831-6088
(615) 574-5173

Jyh-Ming Ting
Applied Sciences, Inc.
141 West Xenia Avenue
P.O. Box 579
Cedarville, OH 45314
(513) 766-2020

R. H. Titran
NASA Lewis Research Center
21000 Brookpark Road, MS 49-1
Cleveland, OH 44135
(216) 433-3198

Zygmunt Tomczuk
Chemical Technology Division
Argonne National Laboratory
9700 South Cass Avenue
Argonne, IL 60439
(708) 252-7294

Micha Tomkiewicz
Physics Department
Brooklyn College of City
University of New York
Brooklyn, NY 11210
(718) 951-5357

John J. Tomlinson
ORNL
Bldg. 9204-1, MS 8045
P.O. Box 2009
Oak Ridge, TN 37831-8045
(615) 574-0768

Timothy Tong
Dept. of Mechanical Eng.
University of Kentucky
Lexington, KY 40506
(606) 257-3236

J. A. VanDenAvyle
Division 1832
Sandia National Laboratories
Albuquerque, NM 87185
(505) 844-1016

D. van Rooyen
Brookhaven National Lab.
Upton, NY 11973
(516) 282-4050

Carl R. Vander Linden
Vander Linden & Associates
AIC Materials Program
5 Brassie Way
Littleton, CO 80123
(303) 794-8309

William VanDyke
NE-33/GTN
U.S. Dept. of Energy
Washington, DC 20545
(301) 903-4201

Richard D. Varjian
Dow Chemical Company, Inc.
Central Research - Catalysis
1776 Building
Midland, MI 49675
(517) 636-6557

Alex Vary
NASA Lewis Research Center
21000 Brookpark Road
Cleveland, OH 44135
(216) 433-6019

Krishna Vedula
Dept. of Metal. & Mat. Science
Case Western Reserve University
10900 Euclid Avenue
Cleveland, OH 44115
(216) 368-4211

Ted Vojnovich
ER-80/FORS
U.S. Dept. of Energy
Washington, DC 20585
(202) 586-2343

Brian G. Volintine
EE-232
5F-059/FORS
U.S. Dept. of Energy
Washington, DC 20585
(202) 586-1739

Robert W. Vukusich
UES, Inc.
4401 Dayton-Xenia Road
Dayton, OH 45432-1894
(513) 426-6900

David Waksman
National Institute of Standards
and Technology
Building 226
Gaithersburg, MD 20899
(301) 921-3114

H. F. Walter
EM-34/GTN
U.S. Dept. of Energy
Washington, DC 20545
(301) 903-7192

J. B. Walter
Materials Technology Div.
Idaho National Eng. Lab
Idaho Falls, ID 83415
(208) 526-2627

John Walter
IntraSpec, Inc.
P.O. Box 4579
Oak Ridge, TN 37831
(615) 483-1859

William K. Warburton
X-ray Instrumentation Associates
1300 Mills Street
Menlo Park, CA 94025-3210
(415) 903-9980

Craig N. Ward
Ultramet
12173 Montague Street
Pacoima, CA 91331
(818) 899-0236

Gary S. Was
Dept. of Nuclear Eng.
University of Michigan
Ann Arbor, MI 48109
(313) 763-4675

Michael R. Wasielewski
Chemistry Division
Argonne National Laboratory
9700 South Cass Avenue
Argonne, IL 60439
(708) 252-3538

Rolf Weil
Dep. of Mat. & Metal. Eng.
Stevens Inst. of Technology
Castle Point Station
Hoboken, NJ 07030
(201) 420-5257

Roy Weinstein
Instit. for Particle Beam Dynamics
University of Houston
Houston, TX 77204-5502
(713) 743-3600

C. D. Weiss
Caterpillar, Inc.
100 N.E. Adams Street
Peoria, IL 61629
(309) 578-8672

Elizabeth G. Weiss
Membrane Technology and Research, Inc.
1360 Willow Road, Suite 103
Menlo Park, CA 94025
(415) 328-2228

Haskell Weiss
LLNL
University of California
P.O. Box 808
Livermore, CA 94550
(415) 422-6268

Joseph F. Wenkus
Areas Corporation
202 Boston Road
North Billerica, MA 01862
(617) 667-3000

James Wert
Dept. of Mat. Science & Eng.
Vanderbilt University
Station B, P.O. Box 1621
Nashville, TN 37235
(615) 322-3583

Stanley Whetstone
ER-23/GTN
U.S. Dept. of Energy
Washington, DC 20545
(301) 903-3613

A. D. White
DELTA M Corporation
525 Warehouse Road
Oakridge, TN 37830
(615) 483-1569

J. B. Whitley
Sandia National Laboratories
Albuquerque, NM 87185
(505) 844-5353

Sheldon M. Wiederhorn
National Institute of Standards
and Technology
Bldg. 223, #A329
Gaithersburg, MD 20899
(301) 975-2000

F. W. Wiffen
ER-543/GTN
U.S. Dept. of Energy
Washington, DC 20545
(301) 903-4963

Daniel E. Wiley
Dir. of Improved Energy Prod.
EE-231/FORS
U.S. Dept. of Energy
Washington, DC 2085
(202) 586-2099

William Wilhelm
Brookhaven National Lab
Solar Technology Group
Building 701
Upton, NY 11973
(516) 282-4708

Frank Wilkins
EE-222/FORS
U.S. Dept. of Energy
Washington, DC 20585
(202) 586-8072

A. D. Wilks
Signal UOP Research Center
50 UOP Plaza
Des Plaines, IL 60016
(312) 492-3179

Robin Williams
ORNL
P.O. Box 2008
Bldg. 4508, 092, Rm. 243
Oak Ridge, TN 37831
(615) 576-2631

A. Wilson
LANL
Los Alamos, NM 87545
(505) 667-6404

Ward O. Winer
Mechanical Eng. Department
Georgia Inst. of Technology
Atlanta, GA 30332
(404) 894-3270

C. E. Witherell
LLNL
University of California
P.O. Box 808
Livermore, CA 94550
(415) 422-8341

J. C. Withers
Mat. & Electro. Res. Corp.
7960 South Kolb Road
Tucson, AZ 85706
(602) 574-1980

D. E. Wittmer
S. Illinois Univ./Carbondale
Dept. of Mech. Eng. & Egy Pro.
Carbondale, IL 62901
(618) 536-2396, ext. 21

T. Wolery
LLNL
University of California
Livermore, CA 94550
(213) 423-5789

Stanley M. Wolf
EM-54/GTN
U.S. Dept. of Energy
Washington, DC 20545
(301) 903-7962

James C. Wood
NASA Lewis Research Center
MS 500-210
21000 Brookpark Road
Cleveland, OH 44135
(216) 433-4000

J. R. Wooten
Rocketdyne
6633 Canoga Avenue
Mail Code BA-26
Canoga Park, CA 91303
(818) 710-5972

I. G. Wright
Battelle-Columbus Labs
505 King Ave
Columbus, OH 43201-2693
(614) 424-4377

John D. Wright
TDA Research, Inc.
12345 West 52nd Avenue
Wheat Ridge, CO 80033
(303) 940-2301

R. N. Wright
Materials Technology Div.
Idaho National Eng. Laboratory
Idaho Falls, ID 83415
FTS 583-2627

Howard Yacobucci
NASA Lewis Research Center
21000 Brookpark Road, MS 77-6
Cleveland, OH 44135
(216) 433-3415

David Yarbrough
Department of Chem. Eng.
Tennessee Tech. University
1155 N. Dixie Ave.
Cookville, TN 38505
(615) 528-3494

H. C. Yeh
Air Research Casting Co.
19800 VanNess Avenue
Torrance, CA 90509
(213) 618-7449

Thomas M. Yonushonis
Cummins Engine Co., Inc.
Box 3005
Mail Code 50183
Columbus, IN 47202-3005
(812) 377-7078

J. Yow
LLNL
University of California
Livermore, CA 94550
(213) 423-3521

Dingan Yu
Supercon, Inc.
830 Boston Turnpike
Shrewsbury, MA 01545
(508) 842-0174

Charlie Yust
ORNL
P.O. Box 2008
Bldg. 4515, 063, Rm. 106
Oak Ridge, TN 37830
(615) 574-4812

Frederica Zangrando
NREL
1617 Cole Blvd.
Golden, CO 80401
(303) 231-1716

F. J. Zanner
Division 1833
Sandia National Laboratories
Albuquerque, NM 87185
(505) 844-7073

C. M. Zeh
METC
P.O. Box 880
Morgantown, WV 26505
(304) 291-4265

B. A. Zeitlin
IGC Adv. Superconductors, Inc.
1875 Thomaston Avenue
Waterbury, CT 06704
(203) 753-5215

R. M. Zimmerman, Division 6313
Sandia National Laboratory
P.O. Box 5800
Albuquerque, NM 87185
(505) 846-0187

Kenneth Zwiebel
NREL
1617 Cole Blvd
Golden, CO 80401
(303) 231-7141

INDEX

A

B

C

D

G

H

I

J

K

L

M

N

O

P

Q

R

S

T

U

V

W

X

Y

Z