DOE/SC-0011

ENERGY MATERIALS COORDINATING COMMITTEE (EMaCC)

Fiscal Year 1998

July 31, 1999

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

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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 chairpersons are:

Electrochemical Technologies - Richard Kelly, ER-132, (301) 903-6051
Metals - Sara Dillich, EE-22, (202) 586-7925
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 1998-1999. The dates, themes and speakers are as follows:

Thursday, November 12, 1998, 10am - 11:10am, Room E-301/GTN

The first EMaCC meeting of FY 1999 emphasized nuclear power oriented research. John Herczeg(NE-50) spoke on the Nuclear Energy Research Initiative, which received $19 million in the FY 1999 budget and an outside guest speaker, Mike McNeill (Nuclear Regulatory Commission and a former EMaCC Chair), spoke on irradiation assisted stress corrosion cracking.

Thursday, January 14, 1999, 10am-11:10am, Room 4-410/GTN

Arnold Gritzke (EM-52) described the Environmental Management Science Program (EMSP) and presented a general overview of the materials science projects being funded by the EMSP. His overview included the number of projects, PI names and affiliations and a brief description of research being performed. Mention was made of the recently issued solicitation for the Environmental Management Science Program: Research Related to Subsurface Contamination/Vadose Zone Issues.

Further details may be found at: http://www.er.doe.gov/production/grants/fr99_06.html or at: http://www.er.doe.gov/production/grants/lab99_06.html for national laboratories.

Our second speaker was Goray Mukhergee, AAAS Executive Branch Fellow from Detroit Edison, who spoke on the need for and increased efficiencies afforded by better process control and instrumentation in the power generation process.

Thursday, March 11, 1999, 10:00am-11:15am; Room GH-019/FORS

Bill Riley of the Albany Research Center (ARC) presented, "An Overview of the Albany Research Center's Capabilities and Expertise in Materials Research." ARC is one of 5 Office of Fossil Energy field offices and is located in Albany, Oregon. Bill described ARC's broad suite of capabilities and expertise in materials research. Its researchers address fundamental mechanisms and processes; and they can melt, cast and fabricate up to 1 ton of materials; completely characterize their chemical and physical properties, and deal with the waste and byproducts of materials processes. During the past 55 years, they have established recognized expertise and capabilities in wear and corrosion, melting and casting, and in materials development. Albany has been a part of the Office of Fossil Energy since 1996 and has or is establishing working relationships with OIT, OTT, the national labs, and others. Bill concluded by saying that Albany's researchers provide analyses and solutions to industrial problems which bridge the gap between laboratory studies and "real world" applications.

Our second presentation was by Charles Sorrell who described the Advanced Industrials Materials Program and the Metals Processing Laboratory User Center at Oak Ridge National Laboratory. Details on the Metals Processing Center User Program can be found at: http://www.ms.ornl.gov/emfacility/mplus/mplus.htm

The May meeting was postponed until July.

Thursday, July 15, 1999, Forrestal Building. Topic: Defense Programs Materials Activities

Thursday, September 16, 1999. Topic: to be determined

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 1998 and describes the materials research programs of various offices and divisions within the Department.

The EMaCC Chair for FY 1998 was Dr. JoAnn Milliken. The compilation of this report was performed by Dr. Charles Sorrell, EMaCC Executive Secretary for FY 1999, with the assistance of FM Technologies, Inc.

Dr. Tim Fitzsimmons
Office of Energy Research
EMaCC Chair, FY 1999

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 Process Systems	Sara Dillich, EE-22	202/586-7925
	Toni Maréchaux, EE-22	202/586-8501
	Brian Volintine, EE-22	202/586-1739
Industrial Crosscut Technologies	Charlie Sorrell, EE-23	202/586-1514
	Debbie Haught, EE-23	202/586-2211
	Pat Hoffman, EE-23	202/586-6074
Transportation Technologies		
Automotive Propulsion System Materials	Patrick Davis, EE-32	202/586-8061
Automotive Lightweight Vehicle Materials	Joseph Carpenter, EE-32	202/586-1022
Advanced Battery Systems	Ray Sutula, EE-32	202/586-8064
Fuel Cell Systems	JoAnn Milliken, EE-32	202/586-2480
Heavy Vehicle Propulsion System Materials	Sidney Diamond, EE-34	202/586-8032
High Strength Weight Reduction Materials	Sidney Diamond, EE-34	202/586-8032
High Temperature Materials Laboratory	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

Table 1. Membership List

ORGANIZATION	REPRESENTATIVE	PHONE NO.
ENERGY RESEARCH		
Basic Energy Sciences		
Materials Sciences	Pat Dehmer, ER-10	301/903-3081
	Iran L. Thomas, ER-13	301/903-3427
Metal and Ceramic Sciences	Robert J. Gottschall, ER-131	301/903-3428
	Alan Dragoo, ER-131	301/903-3428
	Yok Chen, ER-131	301/903-3428
	Helen Kerch, ER-131	301/903-3428
	Tim Fitzsimmons, ER-131	301/903-9830
Solid State Physics and Materials Chemistry	W. Oosterhuis, ER-132	301/903-3426
	Jerry Smith, ER-132	301/903-3426
	Richard Kelly, 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	Nick Woodward, ER-15	301/903-5822
Computational and Technology Research		
Advanced Energy Projects and Laboratory Technology Research	Walter M. Polansky, ER-32	301/903-5995
	Ted Vojnovich, ER-32	301/903-7484
	David Koegel, ER-32	301/903-3159
Laboratory Operations and Environment, Safety and Health		
Environment, Safety and Health	Ted Tomczak, SC-83	301/903-6916
Fusion Energy		
Fusion Technologies	F. W. (Bill) Wiffen, ER-52	301/903-4963
Office of Biological and Environmental Research		
Medical Sciences Division	Larry James, ER-73	301/903-7481
ENVIRONMENTAL RESTORATION AND WASTE MANAGEMENT		
Waste Operations		
Waste Management Projects	Doug Tonkay, EM-34	301/903-7212
Science and Technology		
Research and Development	Chet Miller, EM-34	202/586-3952

ORGANIZATION	REPRESENTATIVE	PHONE NO.
NUCLEAR ENERGY, SCIENCE AND TECHNOLOGY		
Disposition Technologies	William Van Dyke, NE-40 Beverly Cook, NE-40	301/903-4201 301/903-4021
Space and Defense Power Systems	William Barnett, NE-50 John Dowicki, NE-50	301/903-3097 301/903-7729
Naval Reactors	David I. Curtis, NE-60 Tom Kennedy, NE-60	703/603-5561 703/603-1754
Reactor Programs	John Warren, NE-80 Bob Lange, NE-80	301/903-6491 301/903-2915
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 1998 budget summary for DOE Materials Activities is presented on pages 7 and 8. The distribution of these funds between DOE laboratories, private industry, academia and other organizations is presented in tabular form on page 9.

Following the budget summary is a set of detailed program descriptions for the FY 1998 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 1998 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 1998 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 1998
OFFICE OF BUILDING TECHNOLOGY, STATE AND COMMUNITY PROGRAMS	$ 950,000
Office of Building Systems	950,000
OFFICE OF INDUSTRIAL TECHNOLOGIES	$34,458,818
Office of Industrial Strategies	10,413,250
Aluminum Vision Team	6,930,000
Forest Products Vision Team	184,250
Steel Vision Team	470,000
Glass Vision Team	900,000
Metal Casting Vision Team	1,929,000
Office of Crosscut Technologies	24,045,568
Advanced Turbine System (ATS) Program	6,690,000
Continuous Fiber Ceramic Composites (CFCC) Program	8,400,000
Advanced Industrial Materials (AIM) Program	4,990,000
Financial Assistance Program	3,965,568
OFFICE OF TRANSPORTATION TECHNOLOGIES	$26,736,000
Transportation Materials Technology	22,237,000
Automotive Materials Technology	18,889,000
Propulsion Materials	3,639,000
Lightweight Vehicle Materials	15,250,000
Electric Drive Vehicle Technologies	3,348,000
Advanced Battery Materials	2,948,000
Fuel Cell Materials	400,000
Heavy Vehicle Propulsion System Materials	4,499,000
OFFICE OF POWER TECHNOLOGIES	$59,462,600
Office of Solar Energy Conversion	26,290,000
Photovoltaic Technology Division	26,290,000
Office of Geothermal Technologies	672,600
Office of Energy Management	$32,500,000
Advanced Utility Concepts Division	$32,500,000
High Temperature Superconductivity for Electric Systems	$32,500,000

FY 1998 BUDGET SUMMARY FOR DOE MATERIALS ACTIVITIES (continued)

OFFICE OF ENERGY RESEARCH	$494,475,355
Office of Basic Energy Sciences	404,553,700
Division of Materials Sciences	392,475,000
Division of Chemical Sciences	5,333,000
Division of Engineering and Geosciences	6,745,700
Engineering Sciences Research	3,458,800
Geosciences Research	3,286,900
Office of Advanced Scientific Computing Research	78,736,655
Division of Technology Research	78,736,655
Laboratory Technology Research Program	6,182,000
Advanced Energy Projects Program	3,377,000
Small Business Innovation Research Program	65,576,205
Small Business Technology Transfer Research Program	3,597,450
Office of Fusion Energy Sciences	11,189,000
OFFICE OF ENVIRONMENTAL MANAGEMENT	$ 7,991,663
OFFICE OF NUCLEAR ENERGY, SCIENCE AND TECHNOLOGY	$ 70,117,000
Office of Space and Defense Power Systems	3,617,000
Space and National Security Programs	3,617,000
Office of Naval Reactors	66,500,000[1]
OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT	$23,848,000
OFFICE OF DEFENSE PROGRAMS	$67,591,200
The Weapons Research, Development and Test Program	
Sandia National Laboratories	16,886,200
Los Alamos National Laboratory	33,300,000
Lawrence Livermore National Laboratory	17,405,000
OFFICE OF FOSSIL ENERGY	$ 8,771,000
Office of Advanced Research	8,771,000
Fossil Energy AR&TD Materials Program	5,031,000
Advanced Metallurgical Processes Program	3,740,000
TOTAL	$794,401,636

[1]This excludes $48.5 million for the cost of irradiation testing in the Advanced Test Reactor (ATR).

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	$950,000	$0	$0	$0	$950,000
Office of Industrial Technologies	$9,974,700	$19,908,513	$4,035,167	$540,438	$34,458,818
Office of Transportation Technologies	$18,026,000	$6,649,000	$1,761,000	$300,000	$26,736,000
Office of Power Technologies	$43,387,600	$10,150,000	$2,925,000	$3,000,000	$59,462,600
Office of Energy Research	$377,131,000	$69,306,655	$47,316,900	$720,800	$494,475,355
Office of Environmental Management	$5,309,823	$300,000	$2,157,840	$224,000	$7,991,663
Office of Nuclear Energy, Science and Technology	$68,940,000	$0	$1,177,000	$0	$70,117,000
Office of Civilian Radioactive Waste Management	$23,848,000	$0	$0	$0	$23,848,000
Office of Defense Programs	$67,591,200	$0	$0	$0	$67,591,200
Office of Fossil Energy	$7,494,000	$665,000	$599,000	$13,000	$8,771,000
Totals	$622,652,323	$106,979,168	$59,971,907	$4,798,238	$794,401,636

Table 2. Distribution of Funds by Office

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 1998
OFFICE OF BUILDING TECHNOLOGY, STATE AND COMMUNITY PROGRAMS	$ 950,000
Office of Building Systems	950,000
OFFICE OF INDUSTRIAL TECHNOLOGIES	$34,458,818
Office of Industrial Strategies	10,413,250
Aluminum Vision Team	6,930,000
Forest Products Vision Team	184,250
Steel Vision Team	470,000
Glass Vision Team	900,000
Metal Casting Vision Team	1,929,000
Office of Crosscut Technologies	24,045,568
Advanced Turbine System (ATS) Program	6,690,000
Continuous Fiber Ceramic Composites (CFCC) Program	8,400,000
Advanced Industrial Materials (AIM) Program	4,990,000
Financial Assistance Program	3,965,568
OFFICE OF TRANSPORTATION TECHNOLOGIES	$26,736,000
Transportation Materials Technology	26,736,000
Automotive Materials Technology	18,889,000
Propulsion Materials	3,639,000
Lightweight Vehicle Materials	15,250,000
Electric Drive Vehicle Technologies	3,348,000
Advanced Battery Materials	2,948,000
Fuel Cell Materials	400,000
Heavy Vehicle Propulsion System Materials	4,499,000
OFFICE OF POWER TECHNOLOGIES	$59,462,600
Office of Solar Energy Conversion	26,290,000
Photovoltaic Technology Division	26,290,000
Office of Geothermal Technologies	672,600
Office of Energy Management	32,500,000
Advanced Utility Concepts Division	32,500,000
High Temperature Superconductivity for Electric Systems	32,500,000

OFFICE OF BUILDING TECHNOLOGY, STATE AND COMMUNITY PROGRAMS

	FY 1998
Office of Building Technology, State and Community Programs - Grand Total	$950,000
Office of Building Systems	$950,000
Materials Properties, Behavior, Characterization or Testing	$950,000
Evacuated Panel Superinsulation	230,000
Non-HCFC Closed-Cell Foam Insulation	260,000
Existing Materials Performance	100,000
Radiative Heat Transfer in Attic Insulation	180,000
Hygrothermal Property Measurements	180,000

OFFICE OF BUILDING TECHNOLOGY, STATE AND COMMUNITY PROGRAMS

OFFICE OF BUILDING SYSTEMS

The goal of this Office is to reduce energy use of new buildings by 50 percent by 2010, achieve further reductions in energy use through retrofit of existing buildings and reduce annual energy use by 2 quads by 2010 and 5 quads by 2020. 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 Buildings 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 and standardize 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. **EVACUATED PANEL SUPERINSULATION**
   $230,000
   DOE Contact: Arun Vohra, (202) 586-2193
   ORNL Contact: Therese Stoval, (423) 574-0329

This project is for the development of an advanced technology super insulation concept. A filler layer of powder, fiber or foam 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

2. **NON-HCFC CLOSED-CELL FOAM INSULATION**
   $260,000
   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. Long-term tests are being conducted to determine thermal properties and aging characteristics. Models are being developed for aging processes, including the effects of facing materials.

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

3. **EXISTING MATERIALS PERFORMANCE**
   $100,000
   DOE Contact: Arun Vohra, (202) 586-2193
   ORNL Contact: Therese Stovall, (423) 574-0329

This project is for the development of accurate and reproducible data for use by the building materials community, improved test procedures to determine the thermal properties of existing, as well as advanced, insulations, interacting with the building materials research community, manufacturers, trade associations, professional societies, compliance groups and local government, and making and disseminating recommendations on appropriate usage of thermal insulation to conserve energy.

Keywords: Insulation, Buildings

4. **RADIATIVE HEAT TRANSFER IN ATTIC INSULATION**
   $180,000
   DOE Contact: Arun Vohra, (202) 586-2193
   ORNL Contact: Ken Wilkes, (423) 574-5931

This project is for the evaluation of the effect of the radiative environment on the thermal performance of attic insulation. The project is focusing on the effect of penetration of radiation from a hot roof into the top layers of attic insulation. Exploratory experiments are being conducted using small-scale heat flow meter apparatuses. Models are being applied and/or developed to analyze the effects of coupled radiation and conduction. If the exploratory studies show that the effects are significant, further experiments would be conducted in a large-scale attic test module and standardized methods for accounting for the effects would be developed.

Keywords: Fibrous Insulation, Attics, Radiation, Models

5. **HYGROTHERMAL PROPERTY MEASUREMENTS**
$180,000
DOE Contact: Arun Vohra, (202) 586-2193
ORNL Contact: Ken Wilkes, (423) 574-5931

A laboratory is being established for measurements of material properties related to the hygrothermal behavior of buildings materials. Properties that will be measured include sorption and suction isotherms, vapor permeance, liquid diffusivitiy, air permeability, specific heat, and thermal conductivity. Where applicable, the properties will be measured as functions of moisture content and temperature. The laboratory will support other research on measurements and modeling of coupled heat, air, and mixture transfer in building envelopes.

Keywords: Hygrothermal, Moisture, Building Materials, Heat-Air-Moisture, Properties

OFFICE OF INDUSTRIAL TECHNOLOGIES

	FY 1998
Office of Industrial Technologies - Grand Total	$34,458,818
Office of Industrial Strategies	$10,413,250
Aluminum Vision Team	$ 6,930,000
Device or Component Fabrication, Behavior or Testing	$ 2,249,000
Inline Sensors for Electrolytic Aluminum Cells	145,000
Innovative Vertical Floatation Melter (VFM)	330,000
High-efficiency, High-capacity, Low-NO_x Aluminum Melting Using Oxygen-enhanced Combustion	231,000
Technology for Converting Spent Potliner (SPL) to Useful Glass Fiber Products	526,000
Inert Metal Anode Life in Low Temperature Aluminum Reduction Process	725,000
Advanced Anodes and Cathodes Utilized in Energy Efficient Aluminum Production Cells	292,000
Materials Properties, Behavior, Characterization or Testing	$ 920,000
Molten Aluminum Explosion Prevention	100,000
Aluminum Pilot Cell	615,000
Semi Solid Aluminum Alloys	205,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 3,761,000
Recycling Aluminum Salt Cake	800,000
Processing and Recycling of Aluminum Wastes	490,000
Wettable Ceramic-based Drained Cathode Technology for Aluminum Electrolysis Cells	972,000
Aluminum Spray Forming	1,000,000
Potlining Additives	224,000
Improved Grain Refinement Process for Aluminum	275,000
Forest Products Vision Team	$ 184,250
Materials Properties, Behavior, Characterization, or Testing	$ 184,250
Corrosivity Monitoring of Kraft Recovery Boilers	184,250
Corrosion in Kraft Digesters: Characterization of Degradation and Evaluation of Corrosion Control Methods	0
Steel Vision Team	$ 470,000
Device or Component Fabrication, Behavior or Testing	$ 470,000
Intermetallic Alloy Development Related to the Steel Industry	470,000

OFFICE OF INDUSTRIAL TECHNOLOGIES (continued)

	FY 1998
Office of Industrial Strategies (continued)	
Glass Vision Team	$ 900,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 277,000
Chemical Vapor Deposition Ceramic Synthesis	$ 277,000
Materials Properties, Behavior, Characterization or Testing	$ 623,000
Development of Improved Refractories	305,000
Synthesis and Design of $MoSi_2$ Intermetallic Materials	318,000
Metal Casting Vision Team	$ 1,929,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 140,000
In-stream Inoculation for Aluminum Alloy Casting Processes	140,000
Materials Properties, Behavior, Characterization, or Testing	$ 1,789,000
Clean Cast Steel: 1) Machinability of Cast Steel; 2) Accelerated Transfer of Clean Steel Technology	209,000
Clean Cast Steel: 1) Flow of Steel in Gating Systems; 2) Control Ladle Temperature	160,000
Thin Section Steel Castings	124,000
Clean Metal Processing (Aluminum)	343,000
Advanced Lost Foam Casting Technology	222,000
Mechanical Properties Structure Correlation for Commercial Specification of Cast Particulate Metal Matrix Components	119,000
Mechanical Properties of Squeeze and Semi-solid Cast A356	127,000
Ferrite Measurements in Duplex Stainless Steel Castings	37,000
Technology for the Production of Clean, Thin Wall, Machinable Gray and Ductile Iron Castings	213,000
Enhancements in Magnesium Die Casting Die Life and Impact Properties	127,000
Influence of Coatings on Magnesium	108,000
Office of Crosscut Technologies	$24,045,568
Advanced Turbine System (ATS) Program	$ 6,690,000
Materials Properties, Behavior, Characterization or Testing	$490,000
Long-term Testing of Ceramic Components for Stationary Gas Turbines	490,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 2,000,000
ATS Thermal Barrier Coatings	2,000,000
Device or Component Fabrication, Behavior or Testing	$ 4,200,000
Ceramic Components for Stationary Gas Turbines in Cogeneration Service	3,900,000
Air Cooled Ceramic Vanes for Gas Turbines	300,000

OFFICE OF INDUSTRIAL TECHNOLOGIES (continued)

	FY 1998
Office of Crosscut Technologies (continued)	
Continuous Fiber Ceramic Composites (CFCC) Program	$ 8,400,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 6,400,000
CFCC Program - Industry Tasks	6,400,000
Materials Properties, Behavior, Characterization or Testing	$ 2,000,000
Continuous Fiber Ceramic Composites (CFCC) Supporting Technologies	2,000,000
Advanced Industrial Materials (AIM) Program	$ 4,990,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 3,085,000
Intermetallic Alloy Development and Technology Transfer of Intermetallic Alloys	450,000
Development of Advanced Intermetallic Alloys	220,000
Synthesis and Design of $MoSi_2$ Intermetallic Materials	100,000
Composites and Coatings Through Reactive Metal Infiltration	440,000
Conducting Polymers: Synthesis and Industrial Applications	250,000
Membrane Systems for Efficient Separation of Light Gases	300,000
Plasma Processing—Advanced Materials for Corrosion and Erosion Resistance	275,000
Uniform Droplet Processing	600,000
Advanced Materials/Processes	450,000
Materials Properties, Behavior, Characterization or Testing	$ 1,300,000
Materials for Recovery Boilers	900,000
Metals Processing Laboratory User (Mplus) Facility	400,000
Materials Structure and Composition	$ 170,000
Metallic and Intermetallic Bonded Ceramic Composites	170,000
Device or Component Fabrication, Behavior or Testing	$ 435,000
Microwave Joining of SiC	45,000
Selective Inorganic Thin Films	350,000
High Temperature Particle Filtration Technology	40,000

OFFICE OF INDUSTRIAL TECHNOLOGIES (continued)

	FY 1998
Office of Crosscut Technologies (continued)	
Financial Assistance Program	$3,965,568
Inventions and Innovations	$2,061,458
Device or Component Fabrication, Behavior or Testing	$ 972,722
Inner Solar Roof System	36,407
Aerocylinder	99,925
Environmental Tensometer	99,223
Energy Efficient, Electric Rotary Furnace for Glass Molding (Repressing) Precision Optical Blanks	99,999
Method for Producing Glass Fiber	97,971
Thermal Heat and Diffusion Treatment of Bulk Powders	99,983
Density Separation in Complex-mode Vibration Fluidized Beds	98,000
Molten Film High-intensity Paper Dryer	99,657
Laser Ultrasonic Furnace Tube Coke Monitor	98,670
Apparatus and Method for Filtering Molten Metal	99,999
Self-dressing Resistance Welding Electrode	42,888
Materials Properties, Behavior, Characterization or Testing	$ 397,807
Tribopolymerization as an Anti-wear Mechanism	99,743
Nickel-based Superalloy with Improved Weldability and Oxidation Resistance	99,174
Foamed Recyclables	98,900
High R-value, Environmentally Safe Rigid Foams Blown with Fluoroiodocarbons (FICS)	99,990
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 399,590
Improved Radiant Burner Material	99,950
High Throughput Manufacturing of High Efficiency Solar Cells	99,761
Composite Electrodes for Advanced Electrochemical Applications	99,975
Process to Recover Acid and Metal Salts from Pickling Liquors	99,904
Materials Structure and Composition	$ 291,339
A Low Platinum Loading, Hydrophilic Fuel Cell Electrode for Use with a Proton Exchange Membrane	99,999
Combined Battery and Structure for Heightened Energy Storage	91,392
Electric Utility Energy Storage Device	99,948

OFFICE OF INDUSTRIAL TECHNOLOGIES (continued)

	FY 1998
Office of Crosscut Technologies (continued)	
Financial Assistance Program (continued)	
National Industrial Competitiveness Through Energy, Environment and Economics (NICE^3)	$1,904,110
Device or Component Fabrication, Behavior or Testing	
Rapid Heat Treatment of Cast Aluminum Components	414,710
Chlorine Reduction in Aluminum Processing	425,000
Demonstrate the Microsmooth[tm] Wheel Finishing Process on Aluminum Wheels	400,000
Lightweight Steel Dispensing Containers	425,000
Process to Recover and Reuse Sulfur Dioxide in Metalcasting Operations	239,400

OFFICE OF INDUSTRIAL TECHNOLOGIES

The mission of the Office of Industrial Technologies (OIT) is to support the development and deployment of advanced energy efficiency, renewable energy and pollution prevention technologies for industrial applications. OIT's R&D portfolio is driven by needs of the Industries of the Future: agriculture, chemicals, forest products, steel, aluminum, metalcasting, mining, petroleum and glass. These industries account for over half of all manufacturing energy use and account for 75 to 90 percent of most manufacturing wastes. For more information on Industries of the Future, see the Office of Industrial Technologies Web site at www.oit.doe.gov.

The Industries of the Future strategy uses industry-developed visions and technology roadmaps to outline the technology that will be needed in order to reach their goals. Through this process, government-funded research is brought to a sharp focus to benefit U.S. industry. OIT's R&D portfolio includes process R&D directly related to specific industries of the future and crosscutting R&D which is applicable to multiple industries. Technology Access programs assist in delivering state-of-the-art and emerging technologies to industry customers.

OFFICE OF INDUSTRIAL STRATEGIES

The Industries of the Future mechanism cost-shares with industry and other organizations technology development identified in industry-wide developed visions and roadmaps. These technologies, specific to industry processes, are chosen based on their ultimate impact on energy and waste reduction, high priority and high risk to meet roadmap targets, widespread industry applicability and pre-competitive nature. Materials research addresses the need for industrial processes to run at increased temperatures with longer service lives, reduced downtime, and lower capital costs.

ALUMINUM VISION TEAM - The DOE Aluminum Team leader is Sara Dillich, (202) 586-7925

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

6. **INLINE SENSORS FOR ELECTROLYTIC ALUMINUM CELLS**
$145,000
DOE Contact: Sara Dillich, (202) 586-7925
ORNL Contact: Jack Young, (423) 5744922

Through an existing Cooperative Research and Development Agreement (CRADA) with industrial partners, Oak Ridge National Laboratory (ORNL), will develop a sensor for use in both conventional and advanced inert anode aluminum production cells. Fiber optic probes and laser-based Raman spectra analytical techniques are being investigated to measure soluble alumina in cryolite. Sensors for measurement of bath ratio and bath temperature will be investigated in future stages of the project. Dynamic process and thermal modeling will be developed in concert with these sensors to enable utility power load leveling through thermal cycling of the production cells without loss of productivity. A Raman cell for laboratory use has been designed and fabricated. Identifying a material that can endure cryolite melts is another barrier to developing a reliable sensor. Thus, research to date has focused on the development of coating materials for a silica probe, and three coating materials (CVD diamond, hot-pressed PBN and TBN) that appear to survive in cryolite melts during preliminary testing have been identified. Investigations are continuing into probe tip fabrication and coating, immersion tests in molten salts, and Raman characterization of cryolite.

Keywords: Sensor, Raman Probe, Fiber Optic Probe, Cryolite, Alumina

7. **INNOVATIVE VERTICAL FLOATATION MELTER (VFM)**
$330,000
DOE Contact: Ramesh Jain, (202) 586-2381

The Energy Research Company, O'Brien & Gere Engineers, Inc., and Stein, Atkinson Stordy Ltd. are project partners for the development of VFM. This technology represents a significantly cleaner and more efficient alternative for processing aluminum scrap. In the new process, the scrap is first dried and de-coated in a rotary kiln dryer that completely removes organics such as oil, paint, and plastics. The heat content of the organics volatizing from the scrap will supply supplementary heat to the de-coater. The dried and de-coated scrap is then melted in the opposed flow VFM, where particles of varying sizes and surface areas are kept in suspension at different levels of the melter, designed with varying velocities to achieve the desired drag forces. The scrap pieces reach an equilibrium in which the scrap weight equals the gas drag force, and the scrap is suspended for 15 to 30 seconds, allowing sufficient residence time for it to melt. The melting particles experience changes in their aerodynamic shape until they reach the liquid state and fall into a molten metal bath. This process also has applications in the glass and steel industries. In the first phase of the project, the VFM process was designed based on experimental measurements, calculations, and issues determined from industry partners. The efficiency of the VFM is estimated to be 57 percent, rising to 75 percent when integrated with IDEX™. In the second phase, a pilot-scale VFM was designed and constructed. Tests on this system are being conducted at a facility of the Energy Research Company in Syracuse, NY.

Keywords: Floatation Melter, Aluminum Scrap

8. **HIGH-EFFICIENCY, HIGH-CAPACITY, LOW-NO_x ALUMINUM MELTING USING OXYGEN-ENHANCED COMBUSTION**
   $231,000
   DOE Contact: Ramesh Jain, (202) 586-2381

Air Products & Chemicals, Inc. along with Argonne National Laboratory, Roth Brothers, and Brigham Young University will develop and demonstrate a novel, high-efficiency, high-capacity, low-NO_x, combustion system integrated with an innovative low-cost, on-site vacuum-swing- absorption (VSA) oxygen generation. This integrated burner/oxygen supply system will offer enhanced productivity, high-energy efficiency, low operating costs, and low NO_x emissions.

This two-year project, which began in September 1997, will be conducted in two phases. The first phase includes the design and construction of a low-NO_x burner at the optimum 35-50 percent combined total oxidizer stream using both the product and the exhaust streams from the VSA. These have been designed and installed on a furnace at Wabash Alloys. The second phase includes the integration of the VSA to meet the average demand through proprietary storage, versus the current, less efficient practice of sizing to meet peak demand. VSA design and construction are complete. The VSA system is on-line at Wabash. Final optimization and performance characterization for the burners and VSA system will be completed in early 1999. The successful demonstration of this project will provide the U.S. aluminum industry with a cost-effective, energy-efficient, environmentally friendly modification for current melting furnaces. Its goal is to increase aluminum melting productivity up to 30 percent with low pollutants emission, accompanied by no increase in melting cost or need for large capital expenditures.

Keywords: Aluminum Melting, Combustion, Burner

9. **TECHNOLOGY FOR CONVERTING SPENT POTLINER (SPL) TO USEFUL GLASS FIBER PRODUCTS**
   $526,000
   DOE Contact: Sara Dillich, (202) 586-7925

Vortec Corporation, assisted by Alumax Primary Aluminum Corp., Hoogovens Technical Services, Inc., and the New York State College of Ceramics at Alfred University, will perform a pilot-scale experimental testing project to evaluate the feasibility of converting SPL (spent potliner) from aluminum smelting plants to commercial quality glass fiber and aluminum fluoride products using Vortec's Cyclone Melting System (CMS™) technology. The project, initiated in September 1997, will be performed during a 20-month period and will include the following activities:

- Design, fabrication, and installation of pilot-scale glass fiberizing and flue gas filtration and analysis equipment into Vortec's existing pilot-scale CMS™ testing facility
- Pilot-scale SPL vitrification test to produce glass fibers
- Testing and analysis of the fibers from the pilot-scale test with respect to commercial quality specifications
- Testing and analysis of fibers with respect to human health considerations
- Sampling and analysis of flue gas from the pilot-scale CMSJ during testing
- Preliminary design of a commercial-scale air pollution system for aluminum fluoride production.

Keywords: Potliner, Aluminum Smelting, Glass Fiber, Aluminum Fluoride

10. **INERT METAL ANODE LIFE IN LOW TEMPERATURE ALUMINUM REDUCTION PROCESS**
    $725,000
    DOE Contact: Sara Dillich, (202) 586-7925

Northwest Aluminum Technologies and Brooks Rand, Ltd. are project partners for the development of this technology. A carbon-free aluminum reduction process is being developed as a modification to the Hall-Héroult process for primary aluminum production. The process uses a non-consumable metal alloy anode, a wetted cathode, and an electrolytic bath, which is kept saturated with alumina at the relatively low temperature of 750°C by means of free alumina particles suspended in the bath. In conducting the research, two primary tasks are involved. First, laboratory scale cells will be operated to firmly establish the viability of the fundamental concepts required for a successful commercial process. Second, a pilot scale 5000-ampere cell will be designed, constructed and operated. This task will address engineering aspects associated with scaling, such as liner fabrication, electrode configuration and design, and bath composition adjustments. This technology, once developed, will produce primary aluminum metal with lower energy intensity, lower cost, and lower environmental degradation than the conventional process.

Keywords: Aluminum Reduction, Inert Metal Anode, Smelting, Alumina Crucible Cell, Voltage

11. **ADVANCED ANODES AND CATHODES UTILIZED IN ENERGY EFFICIENT ALUMINUM PRODUCTION CELLS**
    $292,000
    DOE Contact: Sara Dillich, (202) 586-7925

With the recently developed advanced materials used for anodes and cathodes, it may be possible to significantly reduce the anode-cathode distance and, thus, reduce the energy required for aluminum smelting. Annually, over four million tons of aluminum are produced by smelting by the U.S. aluminum industry at 63,000 Btu/lb. Through this project, the Alcoa Technical Center will demonstrate advanced materials for inert anodes and wetted cathodes and an optimum design and process for smelting aluminum by designing, constructing, and operating advanced bench scale and pilot-scale aluminum production cells. The objective is to assess the long-term chemical stability of oxygen producing ceramic metallic anodes and stable aluminum wetted cathodes for energy efficient electrolytic production of aluminum. The project will also describe how the anode and cathode materials are produced cost effectively, and will define the optimum operating parameters for the production cell.

Keywords: Aluminum Production Cell, Inert Anode, Wetted Cathode, Electrolytic Production

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

12. **MOLTEN ALUMINUM EXPLOSION PREVENTION**
    $100,000
    DOE Contact: Ramesh Jain, (202) 586-2381
    ORNL Contact: Rusi P. Taleyarkhan, (423) 5764735

The goal of this project is to improve industry's understanding of the conditions that trigger aluminum-water explosions and the reasons and extent to which certain coatings prevent those explosions. Project partners (ORNL, The Aluminum Association, Alcoa) will achieve this goal through developing a basic under-standing of entrapment of heat transfer over submerged coated and uncoated surfaces. Oak Ridge National Laboratory has designed and developed the Steam Explosion Triggering Studies (SETS) facility, an experimental test site where the fundamental issues of explosions will be investigated with emphasis on triggering events. Solid tungsten, an element that has thermophysical properties similar to those of liquid aluminum, is used during the experiments to allow the apparatus to be instrumented and the phenomena associated with the breakdown of steam film and triggering investigated without the hazards associated with experiments performed with large amounts of liquid aluminum. ORNL has produced significant data to assess suppression capability for various coatings with full curing times. However, the impact of shorter curing times as well as the study of impact of bare spots are issues that need resolution. Further collection of data for selected coatings with different degrees of curing, together with the effects of the introduction of non-condensable gasses, remain the subjects of Phase II.

Keywords: Explosions, Molten Aluminum, Water

13. **ALUMINUM PILOT CELL**
    $615,000
    DOE Contact: Sara Dillich, (202) 586-7925

The Department of Energy, Office of Industrial Technologies is currently sponsoring a project with the Aluminum Company of America (Alcoa) to demonstrate, through pilot cell tests, viability of an advanced retrofit technology for alumina reduction based on inert, cermet anodes and wettable TiB_2-G cathodes. Phase I of the Alcoa project developed a retrofit commercial cell conceptual design and assessed its economic and environmental impact. Phase II is conducting tests in a pilot-scale cell and an evaluation of lower cost/higher quality fabrication of inert anodes. The objectives of Phase II are to construct, operate, and autopsy two pilot-scale cells; the first based on best available technology and the second optimized as a result of the knowledge gained from the first. These tests will also feature Bayer process improvements, and advanced cell design and control systems. Anodes will be fabricated by isostatic pressing and sintering of metal and oxide powders. Innovative fabrication methods for anode-collector bar assembly are also being investigated.

Keywords: Alumina Reduction, Aluminum Production, Inert Anode, Wettable Cathodes

14. **SEMI SOLID ALUMINUM ALLOYS**
$205,000
DOE Contact: Sara Dillich, (202) 586-7925

Semi-solid material processing offers distinct advantages over other near-net-shape manufacturing processes. In this process, cast parts are produced from a slurry kept at a temperature between the solidus and the liquidus isotherms. This process produces complex parts with better quality when compared to parts made by similar processes. It also allows net-shape forming, reducing further machining operations. The process combines the advantages of both liquid metal casting and solid metal forging. The purpose of this project is to achieve a better understanding of the fundamental issues concerning the constitutive behavior of semi-solid materials and their behavior during processing, so that the applicability of semi-solid forming can be extended to various aluminum alloy systems. Worcester Polytechnic Institute (WPI) will be using numerical simulations to predict die filling and, ultimately, die design optimization. A Herschel-Bulkley fluid model, modified to account for the two-phase nature and time-dependent rheological behavior of SSM slurries, will be used with specially developed computational codes for semi-solid fluid flow and die filling to produce simulations for the filling of two-dimensional and three-dimensional cavities under various processing conditions. Issues related to die design and temperature control will also be addressed using numerical simulations. The Massachusetts Institute of Technology work will concentrate on obtaining fundamental rheological data needed for the WPI modeling and simulation activity. MIT will determine effects of semi-solid slurry structure on flow behavior and flow separation at high shear rates representative of actual forming processes. The work at Oak Ridge National Laboratory will concentrate on characterizing the thermophysical properties of semi-solid aluminum alloys and the development of new optimally designed alloys.

Keywords: Semi-solid Forming, Aluminum Alloys, Net-shape Forming

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

15. **RECYCLING ALUMINUM SALT CAKE**
$800,000
DOE Contact: Sara Dillich, (202) 586-7925
ANL Contact: John Hryn, (630) 252-5894

Salt cake recovery is the most energy and cost intensive unit operation in the recovery of salt cake constituents. In this project, Argonne National Laboratory (ANL) is developing a salt recovery process based on electrodialysis (ED). Laboratory scale experiments and economic analysis has indicated that, for conditions consistent with salt cake recycling, the ED technology is more cost-effective for salt recovery than alternative technologies (e.g., evaporation with vapor recompression). Increasing the market value of non-metallic product (NMP) is critical for cost-effective salt cake recycling. Impurities constitute about 10 percent of NMP and lower its market value. Research investigated hydrometallurgical processes to purify NMP, since higher NMP purity results in higher market value for refractory aggregate and other potential alumina markets. Technical and economic analysis indicated the electrodialysis process to be most promising. Pilot-scale work indicated fiber insulation materials can be made cost-effectively using NMP as a starting material. A new potential use for NMP (i.e. as alternative alumina units for the blast furnace in ironmaking) has been identified. Process flow sheet and engineering design for pilot scale testing of the electrodialysis process have been completed.

Keywords: Aluminum, Salt Cake, Recycling, Electrodialysis

16. **PROCESSING AND RECYCLING OF ALUMINUM WASTES**
$490,000
DOE Contact: Sara Dillich, (202) 586-7925

This project at Michigan Technological University focuses on the development of a technology to divert the salt cake into valuable feedstock materials for the manufacturing of concrete products such as lightweight masonry, foamed concrete, and mine backfill grouts. By using the unique properties inherent in the aluminum salt cake, this by-product can function as a foaming (air entraining) agent, and fine aggregate for use in concrete. The technology is expected to benefit the aluminum, concrete, mining and construction industries. The aluminum industry will be able to increase its recovery of aluminum metal while reducing energy consumption. Technology development objectives include:

- Process by-product waste streams from several aluminum smelters and optimize the processing required to convert wastes into products suitable for use as concrete additives.
- Develop and demonstrate the processing required to effectively utilized the processed by-products developed for the production of mine backfill grouts.

- Develop and demonstrate the processing required for lightweight aggregate/masonry block production utilizing the processed by-products developed.
- Document the environmental acceptability of the smelting by-products used as concrete additives and assess the environmental acceptability of the low-density concrete products made using these additives.

Keywords: Salt Cake, Recycling, Feedstock, Waste Streams, Concrete Additives

17. **WETTABLE CERAMIC-BASED DRAINED CATHODE TECHNOLOGY FOR ALUMINUM ELECTROLYSIS CELLS**
$972,000
DOE Contact: Sara Dillich, (202) 586-7925

Reynolds Metals Company, Kaiser Mead, and Advanced Refractory Technologies (ART) will collaborate to develop and evaluate ceramic-based materials, technology, and the necessary engineering packages to retrofit existing reduction cells as a means to improve the performance of the Hall Héroult cell. ART will produce TiB_2-based tiles or coatings that will be used as the "drained" lining in two 70 kA prebake cells. The durability of the candidate materials and the performance of the drained cathode design will be evaluated during a one-month test using 12 kA pilot reduction cells. This four-year project, initiated in September 1997, will include the following activities:

- Development and evaluation of candidate TiB_2 carbon materials (tiles and coating)
- Development and evaluation of proprietary carbon materials
- Development of the drained cathode design
- Evaluation of the best candidate materials and the drained cathode design in the 12 kA pilot cell
- Design and construction of a 70 kA prebake cell retrofitted with a drained cathode using TiB_2-based and or the proprietary materials
- Startup and operation of two 70 kA prebake cells retrofitted with a drained cathode and TiB_2 and or the proprietary materials

Keywords: Cathode, Aluminum Production, Titanium Diboride

18. **ALUMINUM SPRAY FORMING**
$1,000,000
DOE Contact: Sara Dillich, (202) 586-7925

This project, conducted by the Aluminum Company of America (Alcoa), will translate current bench-scale spray forming technologies into a cost-effective process for the replacement of the energy-intensive ingot casting method. A unique linear spray nozzle system has been designed which has the potential for achieving the desired production rates of 1500 to 3000 lb./hr/in in a single pass operation. Other processing targets include ±2 percent profile flatness, less than 1-inch edge trimming; surface porosity of less than 4 percent not interconnected, and overspray less than 5 percent. Thermomechanical processing studies, microstructural characterization of deposits, and mathematical and numerical modeling are in progress. Investigations are focusing on as-sprayed microstructure and thermomechanical properties of automotive alloy 6111. An Advanced Development Unit, capable of operating in both an experimental and a semi-production mode, is being designed and constructed to investigate the commercial viability of the spray forming process to produce aluminum sheet. The unit will be used to determine costs as well as processing and safety procedures for steady state operations.

Keywords: Aluminum, Spray Forming, Sheet

19. **POTLINING ADDITIVES**
$224,000
DOE Contact: Sara Dillich, (202) 586-7925

This project is designed to further examine the potential benefits derived from the addition of boron oxide to potlining used in primary aluminum production cells. A relatively inexpensive bulk chemical, boron oxide not only suppresses cyanide formation, but also may inhibit sodium intercalation and, above all, promote, in the presence of some titanium, wetting of cathode carbonaceous material by the metal pad, thus reducing ohmic cell resistance and sludge formation. Improvements in energy consumption, waste disposal and overall economics of the process are projected. Laboratory testing and commercial scale testing will investigate parameters that are important for the commercial application. Tests in industrial cells will complement laboratory testing. Carbonaceous potlining components added with boron oxide will be incorporated in industrial cells in later phases of the program, providing results of the first year are positive. Project partners include: Century Aluminum of West Virginia, Inc., EMEC Consultants, the NSA Division of Southwire Company and SGL Carbon Corporation.

Keywords: Potlining, Smelting, Aluminum Production, Boron Oxide, Aluminum Production Cells

20. **IMPROVED GRAIN REFINEMENT PROCESS FOR ALUMINUM**
$275,000
DOE Contact: Sara Dillich, (202) 586-7925

Almost all aluminum cast in the U.S. is grain refined, and the amount of grain refiner consumed in primary plants averages about two pounds per metric ton. A new method of grain refining aluminum, called the fy-Gem process has been demonstrated in a JDC, Inc. laboratory program to be an effective way to refine aluminum castings. This invention (patent applied for) offers significant cost, energy and environmental benefits, and addresses the important issue of how to produce ingots of higher quality, particularly with respect to boride inclusion. The fy-Gem process addresses the problems and costs associated with the use of titanium and boron in grain refiners and is likely to result in cleaner, higher quality castings. This project focuses on establishing commercial viability and reliability in the cast shop. If the development and demonstration is successful, the project partners expect to introduce the grain refinement method into the market place by 2000. Project partners include: Alcoa, GKS Engineering Services, GRAS, Inc., JDC, Inc., Littlestown Hardware and Foundry, and Touchstone Laboratory.

Keywords: Aluminum Casting, Grain Refinement, Liquid Aluminum Metal, Titanium, Boron, fy-Gem

FOREST PRODUCTS VISION TEAM - The DOE Forest Products team leader is Valri Robinson, (202) 586-0937

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION, OR TESTING

21. **CORROSIVITY MONITORING OF KRAFT RECOVERY BOILERS**
$184,250
DOE Contact: Charles A. Sorrell, (202) 586-1514
IPST Contact: Preet Singh, (404) 894-6641

The focus of this project is to develop an extensive corrosion kinetics database as well as a device to measure conditions which control corrosion in an operating recovery boiler. The benefit of such an approach will allow operators to predict or explain the impact of decisions prior to damaging boiler components. The project will be divided into four phases. Phase I will establish the feasibility of the project concept, Phase II will involve detailed studies on the most promising candidates for corrosion measurements, Phase III consists of small scale experiments conducted in a laboratory furnace to test the efficacy of the measurement system developed in Phase II, and in the final Phase IV, the measurement device and corrosion probes will be installed in a operating boiler for comparison.

Keywords: Recovery Boilers, Corrosion, Pulp and Paper

22. **CORROSION IN KRAFT DIGESTERS: CHARACTERIZATION OF DEGRADATION AND EVALUATION OF CORROSION CONTROL METHODS**
$0
DOE Contact: Ingrid Watson, (202) 586-8119
ORNL Contact: James Kaiser, (423) 475-4453

This project will correlate chemical pulping digester conditions with material performance. Digester conditions will be evaluated using a computational fluid dynamics model of flow within a digester. This flow model will be supplemented with a model for the chemical reactions occurring in the digester. In-situ and laboratory corrosion studies will be used to provide information about the corrosion behavior of conventional materials. An assessment of corrosion control methods and alternative materials will be performed.

Keywords: Digester, Corrosion, Pulp and Paper

STEEL VISION TEAM - DOE Steel Team Leader, Scott Richlen, 202-586-2078

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

23. **INTERMETALLIC ALLOY DEVELOPMENT RELATED TO THE STEEL INDUSTRY**
$470,000
DOE Contact: Charles A. Sorrell, (202) 586-1514
ORNL Contacts: M.L. Santella, (423) 574-4805, V.K. Sikka, (423) 574-5112 and P. Angelini, (423) 574-4565.

The objective of this project is to develop and apply the excellent oxidation and carburization resistance and high temperature strength and fatigue resistance of intermetallic alloys, including nickel aluminide (Ni_3Al) to steel industry related manufacturing applications. Progress in bringing technologies to development and commercialization in FY 1998 focused on transfer rolls used in heat treating (austenitizing) steel plates and slabs. The final design for attaching trunnions to the nickel aluminide rolls was completed; joining is done by a combination of pinning and welding. Technology was developed for joining thick sections of nickel aluminide to dissimilar metals and rolls were successfully tested using both HK and HP steel trunnions. At present, 21 rolls are in service and a complete set of 101 rolls is planned. The original two rolls have been in service for over 5 years and are in excellent condition. In FY 1998, additional applications for nickel aluminide were investigated, including guide rolls for continuous casting of steel, and radiant burners being tested at Timken and Ford. Oak Ridge National Laboratory has licensed Sandusky International for (has centrifugally cast and manufactured the rolls), Alloy Engineering and Casting (has sand-cast trunnians), United Defense (has sand cast trunnians), and the Stoody Company (has manufactured weld wire for joining components of nickel aluminide and iron aluminide).

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

GLASS VISION TEAM - The DOE Glass team leader is Theo Johnson, (202) 586-6937

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

24. **CHEMICAL VAPOR DEPOSITION CERAMIC SYNTHESIS**
$277,000
DOE Contact: Charles A. Sorrell, (202) 586-1514
Sandia National Laboratories - 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. In FY 1998 the CRADA with Libby- Owens-Ford Co. on developing new CVD techniques for depositing coatings on glass was continued. The effort focuses on 1) experimental and modeling of the thermal stability and chemical reactions of CVD precursors used to deposit Indium Tin oxide on float glass, and 2) development of on-line sensors. Experimental and modeling results show that various compounds of indium and organic groups are more stable than previously reported in the literature. However, autocatalytic reactions on hot surfaces can significantly accelerate decomposition. A prototype device was constructed which includes two sensors one being a standard residual gas analyzer and the other being a small novel device developed by NASA for achieving residual gas analyses in a small package.

Keywords: Chemical Vapor Deposition, Gas-Phase Chemistry, Modeling, Fibers, Flat Glass

25. **DEVELOPMENT OF IMPROVED REFRACTORIES**
$305,000
DOE Contact: Charles A. Sorrell, (202) 586-1514
Oak Ridge National Laboratory Contact:
A. A. Wereszczak, (423) 574-7601 and
Peter Angelini, (423) 574-4565

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. The goal of this project is to develop improved refractories and to determine critical mechanical and thermophysical and mechanical properties. The results form this R&D will accelerate the use of oxy-fuel firing throughout the glass industry. In FY 1998, the compression creep and corrosion resistance performance of the conventional silica refractory category was completed. Six silica brands were analyzed. For this type of refractory, concurrent changes in materials properties including phase changes have a larger effect on changes in dimensions than creep mechanisms. 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, Oxi-fuel, High Temperature, Mechanical and Thermophysical, Properties, Corrosion

26. **SYNTHESIS AND DESIGN OF $MoSi_2$ INTERMETALLIC MATERIALS**
$318,000
DOE Contact: Charles A. Sorrell, (202) 586-1514
Los Alamos National Laboratory Contacts:
J. J. Petrovic, (505) 667-0125 and
Richard Castro, (505) 667-5191

The objective of this project is to develop MoSi2-based composites that will combine good room temperature fracture toughness with excellent oxidation resistance and high-temperature strength for industrial applications. Activities in FY 1998 included various major tasks. A CRADA with Johns Manville Corporation on the use of $MoSi_2$ for glass industry applications continued. The kinetics of corrosion of plasma sprayed and extruded $MoSi_2$ materials were investigated in molten alkali borosilicate glass under static and dynamic conditions at 1000C to 1550C for 0.5 to 1510h. A phenomenological model was developed to describe the overall process of corrosion at each of the three locations: above, at, and below the melt line.

Keywords: Composites, Intermetallics, Molydisilicide, Coatings, Fiberglass, Glass

METAL CASTING VISION TEAM - The DOE Metalcasting team leader is Harvey Wong, (202) 586-9235

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

27. **IN-STREAM INNOCULATION FOR ALUMINUM ALLOY CASTING PROCESSES**
    $140,000
    DOE Contact: Debbie Haught, (202) 586-2211
    ORNL Contact: Srinath Viswanathan, (423) 576-9917

The objectives of this project are to develop and evaluate approaches for the in-stream inoculation of melt additive during the casting of aluminum alloys, characterize the microstructure and properties of the resulting alloys, and verify the process in participating foundries. Traditionally, the inoculation of molten aluminum alloys during casting has been conducted through a combination of additions in the form of ingot, temperature compensation of the melt immediately after addition, furnace stirring, and residence time to allow for spatial uniformity. Temperature increases and fluctuations usually increase melt losses, reduce furnace life, and consume energy. The time involved in this approach adversely affects productivity. Also, stirring is labor intensive, and also increases melt losses and reduces furnace life.

Keywords: Metalcasting, Inoculation, Aluminum Alloys

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION, OR TESTING

28. **CLEAN CAST STEEL: 1) MACHINABILITY OF CAST STEEL; 2) ACCELERATED TRANSFER OF CLEAN STEEL TECHNOLOGY**
    $209,000
    DOE Contact: Ehr Ping HuangFu, (202) 586-1493
    University of Alabama - Birmingham Contact: Charles Bates, (205) 975-8011

The objective of this project is to improve casting product quality by removing or minimizing oxide defects and allowing the production of higher integrity castings for high speed machining lines. First task of this project is identifying the metallurgical factors influencing machinability of steel to gain an engineering understanding of the mechanism. A series of tests of commercial parts from participating foundries will be performed to evaluate the machinability. Factors to be examined include furnace practice, deoxidation practice, calcium wire injection, and heat treatment. The second task is to provide the steel foundry industry with the technical resources needed to implement clean cast steel technology.

Keywords: Metalcasting, Steel Casting, Machinability

29. **CLEAN CAST STEEL: 1) FLOW OF STEEL IN GATING SYSTEMS; 2) CONTROL LADLE TEMPERATURE**
    $160,000
    DOE Contact: Ehr Ping HuangFu, (202) 586-8501
    University of Alabama - Birmingham Contact: Charles Bates, (205) 975-8011

This project will focus on procedures for improving casting product quality by removing or minimizing oxide defects and allowing the production of higher integrity castings. This project consists of two technical tasks. The first involves computer simulations of metal pouring, flow through runners and flow into mold cavities. The model will be used to examine metal flow and especially the effects of velocity on casting quality. The other task will focus on evaluating methods of homogenizing metal temperature in the ladle treatments, and induction stirring will be examined.

Keywords: Metalcasting, Steel Casting, Gating, Ladle Temperature

30. **THIN SECTION STEEL CASTINGS**
    $124,000
    DOE Contact: Ehr Ping HuangFu, (202) 586-1493
    Pennsylvania State University Contact: Robert C. Voigt, (814) 863-7290

The objective of this project is to develop a fundamental understanding of the key technologies needed to develop lighter weight, thinner section steel castings. The focus will be directed toward an understanding of technologies and practices that will enhance mold cavity filling. Necessary thin section practices will be identified and/or developed from mold making to melting and pouring. As a result of this cooperative industry/university research program, a comprehensive science and practice-based understanding of thinner wall steel casting will be developed.

Keywords: Metalcasting, Steel Casting, Thin Section

31. **CLEAN METAL PROCESSING (ALUMINUM)**
$343,000
DOE Contact: Ehr Ping HuangFu, (202) 586-1493
Worcester Polytechnic Institute Contact:
Diran Apelian, (508) 831-5992

The objective of this project is to develop a technology of clean metal processing that is capable of consistently providing a metal cleanliness level fit for a particular application. The emphasis is on non-ferrous metals, particularly aluminum casting alloys. The project will investigate and prescribe methods for melt containment avoidance. Methods to control process atmosphere using inert and reactive gases to reduce hydrogen absorption will be investigated. Alloying elements and cover media that may substantially reduce melt oxidation will also be considered. In addition, barrier coatings that interfere with in situ carbide formation will be researched.

Keywords: Metalcasting, Clean Metal, Aluminum

32. **ADVANCED LOST FOAM CASTING TECHNOLOGY**
$222,000
DOE Contact: Ehr Ping HuangFu, (202) 586-1493
University of Alabama - Birmingham Contact:
Charles Bates, (205) 975-8011

The objective of this project is to advance the state of the art in Lost Foam Casting technology. It is being carried out at the Lost Foam Technology Center at the University of Alabama at Birmingham. The project provides a means for designers, manufacturers, and purchasers/users of cast metal parts to harvest the benefits of the lost foam process, and furnishes project participants the best available technology. The current research focus is on the general technical areas of casting dimensional precision and freedom from casting defects in aluminum and cast iron. Tasks include foam pyrolysis defects, coating technology, pattern materials and production, computational modeling, casting distortion, and technology transfer.

Keywords: Metalcasting, Lost Foam Casting

33. **MECHANICAL PROPERTIES STRUCTURE CORRELATION FOR COMMERCIAL SPECIFICATION OF CAST PARTICULATE METAL MATRIX COMPONENTS**
$119,000
DOE Contact: Ehr Ping HuangFu, (202) 586-1493
University of Wisconsin - Milwaukee Contact:
Pradeep Rohadgi, (414) 229-4987

The objective of this project is to evaluate mechanical testing and structural characterization procedures for commercially available particulate metal matrix composites, particularly for aluminum alloy – silicon carbide particle composites. This research will provide quantitative data generated cooperatively by material suppliers, casting producers, and casting users, to establish industry procedures for mechanical testing and structural characterization. Another objective is to analyze the variability in properties as a function of casting procedures and microstructural parameters of the composite and to prescribe processing techniques to minimize the variability in properties to achieve the targeted handbook properties.

Keywords: Metalcasting, Metal Matrix Composite, Mechanical Testing

34. **MECHANICAL PROPERTIES OF SQUEEZE AND SEMI-SOLID CAST A356**
$127,000
DOE Contact: Ehr Ping HuangFu, (202) 586-1493
Case Western Reserve University Contact:
Robert Aikin, (216) 368-4221

Squeeze casting and semi-solid casting are both emerging processes that cast molten metal in a steel die under high pressure. Both processes produce pore free castings with very low defect inclusion contents. For alloys such as aluminum, the processes generate the highest mechanical properties attainable in a cast product. Currently, the lack of a reliable mechanical property database is slowing the introduction of components produced by these high-pressure processes. The objective of this project is to develop a mechanical property database for A356 castings produced by the processes of squeeze casting and semi-solid casting.

Keywords: Metalcasting, Aluminum, Squeeze Casting, Semi-solid Casting

35. **FERRITE MEASUREMENTS IN DUPLEX STAINLESS STEEL CASTINGS**
$37,000
DOE Contact: Ehr Ping HuangFu, (202) 586-1493
University of Tennessee Contact: Carl Lundin, (423) 974-5310

Duplex stainless steel castings are receiving greater attention since the use of wrought duplex components is on the increase. The duplex stainless steels are now often considered for severe service because of their unique properties with regard to corrosion resistance (especially pitting resistance), strength and toughness. Unfortunately, a standardized method does not currently exist for calibrating instruments for the direct assessment or measurement of the ferrite-austenite phase relationships. The objective of this project is to develop calibration standards that will be applicable to duplex stainless steel castings and which will cover the full spectrum of the traditional duplexes and the newly-introduced super duplex , which contains special alloy additions for enhanced properties.

Keywords: Metalcasting, Calibration, Duplex Stainless Steel

36. **TECHNOLOGY FOR THE PRODUCTION OF CLEAN, THIN WALL, MACHINABLE GRAY AND DUCTILE IRON CASTINGS**
$213,000
DOE Contact: Ehr Ping HuangFu, (202) 586-1493
University of Alabama - Birmingham Contact: Charles Bates, (205) 975-8011

The primary focus of this project is to determine how the machinability of gray and ductile iron castings can be improved to support the development of thin walled gray and ductile iron castings for use in the ground transportation industry. Excessive microcarbides have been found in prior research to be a dominant factor degrading machinability of iron castings. One of the major emphases is to determine how the occurrence of microcarbides can be controlled by normal foundry processing changes.

Keywords: Metalcasting, Gray Iron, Cast Iron, Inclusions, Machinability

37. **ENHANCEMENTS IN MAGNESIUM DIE CASTING DIE LIFE AND IMPACT PROPERTIES**
$127,000
DOE Contact: Ehr Ping HuangFu, (202) 586-1493
Case Western Reserve University Contact: Jack Wallace, (216) 368-4222

This project builds on the success at Case Western Reserve University on improving the life of dies for aluminum die castings. The objective is to improve the toughness of cast magnesium alloy products as well as to evaluate the effects these alloys have on the thermal fatigue life of steel dies used in making the castings. Jointly, these improvements are expected to accelerate the penetration of magnesium components into the automotive and commercial markets. The scope of work includes the alloy selection, the processing conditions, and the life of dies and tools that are employed.

Keywords: Metalcasting, Die Casting Dies, Die Casting Die Life, Magnesium, Impact Properties

38. **INFLUENCE OF COATINGS ON MAGNESIUM**
$108,000
DOE Contact: Ehr Ping HuangFu, (202) 586-1493
Ohio State University Contact: Carroll Mobley, (614) 292-5770

Die cast magnesium alloys are finding increased utilization in reducing the weight and improving the fuel efficiency of vehicles. These magnesium castings are intended for engineering or load bearing applications. A major need exists to establish a reliable database for mechanical properties of die cast magnesium alloys of various section thicknesses. This project aims to explore and characterize the influence of the type of alloy, section thickness, and a number of surface coating systems on the mechanical properties of the cast magnesium alloys. Results of this study are intended for design engineers, particularly in the automotive industry, where major growth in the usage of magnesium-based castings will yield significant energy savings.

Keywords: Metalcasting, Die Casting, Coating, Magnesium

OFFICE OF CROSSCUT TECHNOLOGIES

The Office of Crosscut Technologies funds cost-shared research with industry and other organizations on technology development beneficial to and of high priority for many industries. Power generation equipment, combustion equipment, advanced materials, and sensors and controls are being pursued. The three planning units that fund materials research include the Advanced Turbine Systems (ATS) Program, Continuous Fiber Ceramic Composites (CFCC) Program and the Advanced Industrial Materials (AIM) Program.

ADVANCED TURBINE SYSTEM (ATS) PROGRAM

The Advanced Turbine Systems (ATS) Program will develop and demonstrate the next generation of gas turbines for both utility and industrial applications, including cogeneration and combined heat and power. The goals of the ATS program are to improve the efficiency (15 percent increase) and environmental performance (80 percent reduction in emissions) of gas turbines while reducing the cost of electricity by 10 percent. The DOE program manager is Patricia Hoffman, (202) 586-6074.

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

39. **LONG-TERM TESTING OF CERAMIC COMPONENTS FOR STATIONARY GAS TURBINES**
    $490,000
    DOE Contact: Pat Hoffman, (202) 586-6074
    ORNL Contact: Matt Ferber, (423) 576-0818

Compared to aircraft turbines, the service life requirements for land-based Advanced Turbine Systems (ATS) significantly affect the objectives of respective materials development programs. Land-based turbines generally operate under longer maintenance intervals and endure a high percentage of time under full-load conditions. In addition to cyclic fatigue, creep damage becomes the major consideration for both metallic and ceramic systems. This program characterizes the long-term properties of advanced materials systems under the ATS materials/manufacturing program.

Keywords: Structural Ceramics, Creep Damage, Gas Turbines, Silicon Nitride

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

40. **ATS THERMAL BARRIER COATINGS**
    $2,000,000
    DOE Contact: Pat Hoffman, (202) 586-6074
    ORNL Contact: Mike Karnitz, (423) 576-5150
    Pratt & Whitney Contact: Mladen Trubelja, (860) 565-0249
    Siemens Westinghouse Contact: Steve Sabol, (407) 281-5136

ORNL, Pratt & Whitney Aircraft Company, and Siemens Westinghouse Power Corporation are developing, characterizing, and testing thermal barrier coatings for use on critical hot section components of gas turbines. Thermal barrier coatings (TBCs) allow surface temperatures to increase without compromising the structural properties of the underlying alloy. This results in considerable improvements in the durability of hot-section turbine components as well as increases in gas turbine efficacy. TBCs typically consist of a ceramic thermal-insulating layer, deposited onto the substrate with an intervening metallic layer (bond coat) which imparts oxidation protection to the substrate and provides a surface to which the ceramic layer can adhere. The goal of this project is to: (1) develop dependable TBCs that will enable increased turbine rotor inlet temperatures, while maintaining airfoil substrate temperatures at levels to meet advanced turbine systems (ATS) life goals; (2) model and verify lifetime predictions of TBCs; and (3) determine failure mechanisms and repair techniques.

Keywords: Gas Turbines, Thermal Barrier Coatings

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

41. **CERAMIC COMPONENTS FOR STATIONARY GAS TURBINES IN COGENERATION SERVICE**
    $3,900,000
    DOE Contact: Pat Hoffman, (202) 586-6074
    Solar Contact: Jeff Price, (619) 544-5538

The performance of stationary gas turbines is limited by the temperature and strength capabilities of the metallic structural materials in the engine hot section. To realize the benefits of higher temperature, uncooled ceramics with superior high temperature strength and durability with lower emissions signature will be substituted for metallic parts in the engine hot section. The ceramic parts comprise the first stage silicon nitride blades, first stage silicon nitride nozzles and silicon carbide-based ceramic composite combustor liners. This project will design and test these components for a stationary 4.0

Mw gas turbine for cogeneration service. Ceramic composite combustor liners have been run in field tests for more than 4,000 cumulative hours; silicon nitride blades have been field-tested for more than 1,200 hours.

Keywords: Structural Ceramics, Ceramic Composites, Cogeneration, Gas Turbines, Silicon Nitride

42. **AIR COOLED CERAMIC VANES FOR GAS TURBINES**
$300,000
DOE Contact: Pat Hoffman, (202) 586-6074
Pratt and Whitney Contact: Bill Day, (860) 565-0086

Pratt and Whitney and United Technologies Research Center (UTRC) are developing an impingement cooled and vented first stage turbine vane in silicon nitride ceramic. Compared to a gas turbine with air-cooled metal components, low cooling of first stage ceramic vanes helps the ceramic gas turbine realize increased efficiency and power output. First stage ceramic vanes can better withstand the intense gas turbine environment and require substantially less cooling air. Air-cooled ceramic vanes provide higher inlet temperature to the rotor without raising combustor outlet temperature or emissions. Goals for the ceramic vane project include reducing the cooling air required by the first stage vane by approximately 5 percent of total core flow, while limiting surface material temperatures of the silicon nitride vanes to a level allowing extended operational intervals in field use. The project partners plan to evaluate the ceramic vanes in a sector rig cascade test under temperature, temperature distribution, and pressure conditions similar to those encountered in actual engine operation.

Keywords: Gas Turbines, Ceramic Vanes, Silicon Nitride

CONTINUOUS FIBER CERAMIC COMPOSITES (CFCC) PROGRAM

The Continuous Fiber Ceramic Composites (CFCC) Program operates as a collaborative effort between industry, national laboratories, universities and the government to develop advanced ceramic composite materials to a point at which the industry will assume full risk of further development. There are currently five industrial teams developing more than 15 industrial applications for continuous fiber ceramic composite materials. The National Laboratories, along with universities, are developing supporting technologies (e.g. material design, processing methods, manufacturing techniques) and conducting performance evaluations. The DOE program managers are Merrill Smith, (202) 586-3646 and Debbie Haught, (202) 586-2211.

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

43. **CFCC PROGRAM - INDUSTRY TASKS**
$6,400,000
DOE Contact: Merrill 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 such as gas turbine components, heat exchangers, and hot gas filters. 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. Industrial participants include AlliedSignal Composites, Dow Corning, General Electric, McDermott Technologies, and Textron.

Keywords: Ceramic Composites, Continuous Fiber

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

44. **CONTINUOUS FIBER CERAMIC COMPOSITES (CFCC) SUPPORTING TECHNOLOGIES**
$2,000,000
DOE Contact: Debbie Haught, (202) 586-2211
ORNL Contact: Mike 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, Material Characterization, Test Methods

ADVANCED INDUSTRIAL MATERIALS (AIM) 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 effort and of crosscutting industries including carbon products, forging, heat treating, and welding. Efforts in FY 1998 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

45. INTERMETALLIC ALLOY DEVELOPMENT AND TECHNOLOGY TRANSFER OF INTERMETALLIC ALLOYS

$450,000
DOE Contact: Charles A. Sorrell, (202) 586-1514
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 applications. Progress in bringing technologies to development and commercialization in FY 1998 included: (1) identified IC-438 as a higher strength Ni_3Al base alloy castable composition for higher temperature service than IC-221M; and determined thermophysical and thermomechanical properties; (2) weld microstructure of IC-221LA (weld metal) in IC-221M was identified; and thermal aging of IC-221M after 5000h service at 900C was determined, and (3) preliminary deformation maps for nickel aluminide were developed for workability of cast or powder metallurgy materials to sheet, bar and wire, and (4) three additional licensees have been added, Alcon Industries, Inc (casting); Stoody and Polymet Corporation (welding wire).

Keywords: Nickel Aluminides, Processing, Steel, Metalcasting, Heat Treating, Welding, Chemical, Properties

46. DEVELOPMENT OF ADVANCED INTERMETALLIC ALLOYS

$220,000
DOE Contact: Charles A. Sorrell, (202) 586-1514
ORNL Contact: P. J. Maziasz, (423) 574-5082, M. L. Santella, (423) 574-4805 and V. K. Sikka, (423) 574-5112 and C. T. Liu, (423) 574-4459
Univ. of Cincinnati Contacts: A. Jordan and O. N. C. Uwakweh, (513) 556-3108

The objectives of this project are to develop advanced intermetallic alloys including FeAl and Ni_3Si. The FeAl effort is focused on alloys with improved weldability and mechanical and corrosion properties for use in structural applications; and the development of weldable FeAl alloys for use in weld-overlay cladding applications. The Ni_3Si effort focuses on alloy composition, welding and processing. Developments made in FY 1998 include: (1) interactions continued with DuPont and Dow with evaluation of specimens in various commercial chemical environments, (2) the melting of two 500lb heats and casting into heavy wall tubes was performed, (3) evaluated FeAl for use in salt bath heat treating processing at a steel plant, (4) developed weld overlay technologies for FeAl on various substrates, (5) mechanical properties of cast FeAl were determined, and (6) various compositions of Ni_3Si were prepared and welding tests were successful on various alloys.

Keywords: Iron Aluminides, Nickel Aluminides, Coatings, Claddings, Thermophysical Properties, Casting, Thermomechanical Properties, Chemical Industry, Steel Industry, Welding, Alloys

47. SYNTHESIS AND DESIGN OF $MoSi_2$ INTERMETALLIC MATERIALS

$100,000
DOE Contact: Charles A. Sorrell, (202) 586-1514
Los Alamos National Laboratory Contacts: J. J. Petrovic, (505) 667-0125 and Richard Castro, (505) 667-5191

Th objective of this effort is to develop structural silicide-based materials with optimum combinations of high temperature strength/creep resistance, low temperature fracture toughness, and high temperature oxidation resistance. In FY 1998, testing of suite of materials in a gas radiant tube furnace facility was performed (339h; at temperature between 1000°C and 1100°C depending on location). Specimens were placed on both the outside and on the inside of the radiant tubes to evaluate the materials behavior in endothermic and combustion environments. Most materials performed very well. Additional efforts focused on the use of molybdenum disilicide for corrosion resistant sight tubes and temperature measurement systems for glass related applications.

Keywords: Composites, Intermetallics, Molydisilicides, Coatings, Radiant Tubes

48. **COMPOSITES AND COATINGS THROUGH REACTIVE METAL INFILTRATION**
$440,000
DOE Contact: Charles A. Sorrell, (202) 586-1514
Sandia National Laboratories Contact:
R. E. Loehman, (505) 844-2222 (includes effort on coating technology at Stanford Research Institute)

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 1998 (1) $MoSiO_2$-Al_2O_3 composites were made by reacting Mo, Al, and mullite powders and mechanical property measurements were made, and (2) composites of Al_2O_3-Nb, Al_2O_3-Ni, Al_2O_3-Mo$(SiAl)_2$ were successfully prepared. Discussions are on-going with a refractory supplier and a manufacturer of ceramic-metal composites for potential applications of this technology.

The effort on coating technology at Stanford University focuses on developing a low-cost approach to paint based coatings by combining preceramic polymers and inorganic powder fillers. In FY 1998 efforts related to improving formulations using modified polymers and evaluation of a number of fillers including AL/Al_2O_3, Zn/Al_2O_3 and TiO_2/Al_2O_3.

Keywords: Metal Matrix Composites, Reactive Metal Infiltration, Ceramics, Composites, Inorganic Coatings, Corrosion

49. **CONDUCTING POLYMERS: SYNTHESIS AND INDUSTRIAL APPLICATIONS**
$250,000
DOE Contact: Charles A. Sorrell, (202) 586-1514
Los Alamos National Laboratory 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. In FY 1998, the use of conducting polymers for electrochemical reactors (ECRs) based on polymeric electrolytes was addressed. The objective of this effort is to develop and test electrochemical reactors for the chlor-alkali industry, based on polymer membrane/electrode assemblies and on oxygen or air electrodes. In FY 1998, a new cell configuration was produced which has high performance and stability of a Chlor-alkali ECR with an oxygen cathode. The stable cell performance parameters include operation at 2.2 V at 400A/ft^{2}This is compared to current state-of-the-art ECRs in the chlor alkali industry which operate at 3.2V, and 300-400 A/ft^2.

Keywords: Electrically Conducting Polymers, Gas Separation, Electrochemical Reactors, Cathodes

50. **MEMBRANE SYSTEMS FOR EFFICIENT SEPARATION OF LIGHT GASES**
$ 300,000
DOE Contact: Charles A. Sorrell, (202) 586-1514
Los Alamos National Laboratory: D. J. Devlin, (505) 667-9914

Ethylene and Propylene are two of the largest commodity chemicals in the U.S. and are major building blocks for other chemicals. More energy efficient separation processes are necessary. The main technical objective of this project is the development and precise control of the pore structure of membrane material. Membranes must have specially shaped channels in the 2 to 4 nanometer range. In FY 1997, membranes produced by oblique angle sputter deposition techniques have been tested for a number of systems. Systems consisting of gas mixtures of methane, ethane, propane, nitrogen, and propylene/hydrogen have been evaluated. Good separation with exceptional fluxes have been obtained for tested systems. The effort will continue in FY 1999 as a CRADA with Amoco.

Keywords: Sputtering, Separations, Olefins, Hydrogen, Methane, Membranes

51. **PLASMA PROCESSING—ADVANCED MATERIALS FOR CORROSION AND EROSION RESISTANCE**
$275,000
DOE Contact: Charles A. Sorrell, (202) 586-1514
Los Alamos National Laboratory: M. Trkula

The project focuses on developing coating technologies to obtain erosion, and corrosion resistant, thermo-dynamically stable, and adherent coatings on die materials used to cast aluminum and other metals. Low temperature organometallic chemical vapor deposition combined with immersion ion processing is being developed as the coating technology. In FY 1998, B-C-H, Al/N, and Cr-C-O coatings were produced on stainless steel substrates. The Cr-C-O coating was found to be effective against corrosion of Al on Steel.

Keywords: Plasma, Processing, Corrosion, Erosion, Coatings, Materials

52. **UNIFORM DROPLET PROCESSING**
$600,000
DOE: Contact: Charles A. Sorrell, (202) 586-1514
ORNL Contact: Craig A. Blue, (423) 574-4351, and Vinod Sikka, (423) 574-5123
Massachusetts Institute of Technology Contact: J-H Chun, (617) 253-1759
Northeastern University Contact: T. Ando, (617) 373-3811

The purpose of this project is to adapt the uniform droplet 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 the research include Oak Ridge National Laboratory, Massachusetts Institute of Technology, Northeastern University and powder metal companies. In FY 1998: (1) the medium temperature system (up to 1200°C) was competed and the high temperature unit was started; (2) systems were completed for multi-nozzle spraying; multi-nozzle spraying of Al sheet was successfully performed; conditions were studied for the production of porosity free aluminum strip; and materials were characterized; (3) analytical models were developed to explain the fundamental mechanisms during droplet formation and splashing during sheet formation.

Keywords: Powder, Near Net Shape Forming, Aluminum, Alloys, Steel, Copper, Intermetallic Alloys

53. **ADVANCED MATERIALS/PROCESSES**
$450,000
DOE Contact: Charles A. Sorrell, (202) 586-1514
ORNL Contact: P. Angelini, (423) 574-4459

The goals of this project are to develop new and improved materials. Many metals, intermetallic alloys, refractories and ceramics possess unique properties and have the potential to be developed as new materials for energy related applications. In FY 1998: (1) infra red transient liquid coating technology was developed; it is based on room temperature application of materials followed by infra red heating to enable very rapid and controlled formation of coatings; (2) an invention disclosure was prepared on infra red heating technology, (3) corrosion resistant, weldable and formable Iron-Chromium-Silicon alloys were developed and tests continued in various glass industry applications.

Keywords: Intermetallic, Alloys, Metalcasting, Glass, Alloys, Welding, Corrosion, Infra Red Heating, Coatings

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

54. **MATERIALS FOR RECOVERY BOILERS**
$900,000
DOE Contact: Charles A. Sorrell, (202) 586-1514
ORNL Contact: James R. Keiser, (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) to obtain operating data and failure analyses, (2) determination of residual stresses in new and used composite tubes and microstructural characteristics of tubes, and (3) development of new materials and/or fabrication methods for improvements in boiler efficiency, service life, and safety. In FY 1998, (1) short transient temperature excursions (up to 100°C above operating temperature) were confirmed to occur in boiler floors; (2) residual stresses in tubes have been measured under simulated operating conditions; (3) modeling efforts have identified optimum alloys for use in composite tubes for boiler floor operations; (4) panels fabricated from more optimum alloys for use as boiler tubes were installed in operating boilers and are being monitored and evaluated. Participants include Oak Ridge National Laboratory (ORNL), Institute of Paper Science and Technology (IPST), and the Pulp and Paper Research Institute of Canada (PAPRICAN), 18 pulp and paper companies, and 6 boiler and materials suppliers.

Keywords: Corrosion, Recovery Boilers, Composite Tubes, Pulp and Paper, Alloys, Stresses, Neutron Residual Stress, Measurements, Modeling, Mechanical Properties

55. **METALS PROCESSING LABORATORY USER (MPLUS) FACILITY**
$400,000
DOE Contact: Charles A. Sorrell, (202) 586-1514
Oak Ridge National Laboratory Contact:
G. M. Mackiewicz-Ludtka, (423) 576-4652
and H. W. Hayden, (423) 574-6936

The Metals Processing Laboratory User (MPLUS) Facility was officially designated as a DOE User Facility in February 1996. Its primary focus is related to the Office of Industrial Technologies (OIT) efforts including the "Industries of the Future," national, and cross-cutting programs. The purpose of MPLUS is to assist U.S. industry and academia in improving energy efficiency and enhancing U.S. competitiveness. MPLUS includes the following user centers: Metals Processing, Metal Joining, Metals Characterization and Metals Process Modeling. As of the end of FY 1998, 107 proposals were received from 60 different companies and universities representing states across the U.S.A. Projects crosscut all of the seven industries in the Industries of the Future effort; other crosscutting industries including forging, heat treating, and welding; and national programs.

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

MATERIALS STRUCTURE AND COMPOSITION

56. **METALLIC AND INTERMETALLIC BONDED CERAMIC COMPOSITES**
$170,000
DOE Contact: Charles A. Sorrell, (202) 586-1514
ORNL Contacts: P. F. Becher, (423) 574-5197,
and T. N. Tiegs, (423) 574-5173
Southern Illinois University: R. Koc,
(618) 453-7005.

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. This 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 1998 properties database was developed for the new materials and specimens were tested in a number of environments.

The effort on ceramic powder processing has the objective of developing new synthesis methods using carbothermic reduction of carbon coated precursors for producing high purity, submicron metal carbide, metal nitride and metal boride systems. During FY 1998 the formation of TiC was investigated from carbon-coated precursors (kinetics of reaction) and the materials used to understand the sintering behavior of resultant TiC powder with Nickel. TiC powder was also supplied to ORNL for additional testing and evaluation.

Keywords: Ceramics, Composites, Nickel Aluminide, Powder, Carbides, Borides

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

57. **MICROWAVE JOINING OF SiC**
$45,000
DOE Contact: Charles A. Sorrell, (202) 586-1514
FM Technologies, Inc. Contact: R. Silberglitt,
(703) 425-5111

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 1998 the effort included a detailed investigation of SiC produced from several different commercially available polymer precursors in order to assess their relative usefulness as filler materials of microwave joining. A study of the shrinkage during pyrolysis and annealing of SiC particulate loaded polymer was completed relative to microwave joining technology. Tubes were successfully joined with the use of microwave technology. The tubes were then tested to failure at 1050°C at the Oak Ridge National Laboratory. All failures occurred at the tubes or collars and no failures were observed at joints.

Keywords: Microwave Processing, Microwave Joining, SiC, Tubes, Heat Exchangers

58. **SELECTIVE INORGANIC THIN FILMS**
$350,000
DOE Contact: Charles A. Sorrell, (202) 586-1514
Sandia National Laboratories contact:
T. M. Nenoff, (505) 844-0340

The purpose of this research is to develop a new class of inorganic zeolite based 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 zeolithic phases from sol-gel derived amorphous coatings, using porous filters and gas membranes as supports for these films. In FY 1998. the CRADA with Amoco was continued. Modeling was performed for predicting separations through inorganic crystalline pores. Membranes were synthesized, with the variables studied including composition, crystallite size, extent of coverage, supports, and "caulking" media. Defect-free composite films have been successfully produced and tested.

Keywords: Coatings, Sol-Gel Processing, Membranes, Separations, Zeolite

59. **HIGH TEMPERATURE PARTICLE FILTRATION TECHNOLOGY**
    $40,000 (project also includes additional effort from the CFCC program)
    DOE Contact: Charles A. Sorrell, (202) 586-1514
    Oak Ridge National Laboratory Contact:
    T. M. Besmann, (423) 574-6852

The objective of this project is to develop high temperature materials for high temperature filtration needs. High temperature filters are critical in many chemical and other industrial processes. The effort includes bench-scale testing and analyses of compatibility of materials in various environments up to over 1000C. The current focus is on filtration technology for the dimethyldichlorosilane process. In FY 1998, the CRADA with Dow Corning continued. The filter media evaluated included carbon, silicon carbide, oxide ceramics, and metal alloys. After exposure specimens were characterized and mechanical properties testing performed.

Keywords: High Temperature, Filtration, Chemicals, Compatibility, Corrosion, Composites, Ceramics, Metals

FINANCIAL ASSISTANCE PROGRAM

The goal of the Financial Assistance Program is to support the IOF effort by providing critical financial assistance to: (1) speed the development of new energy efficient inventions, and (2) leverage industry and other resources to demonstrate, and promote the benefits of energy savings, pollution prevention and cost savings possible through the adoption of clean, energy-efficient industrial technologies. OIT provides grants and assistance to independent inventors and small businesses with promising new ideas through its inventions and innovation (I&I) Program. OIT also provides grants to help fund technology demonstrations through its National Industrial Competitiveness through Energy, Environment and Economics (NICE^3) Program.

INVENTIONS AND INNOVATIONS - DOE Contact Sandy Glatt, (202) 586-3897

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

60. **INNER SOLAR ROOF SYSTEM**
    $36,407
    DOE Contact: Rolf Butters, (202) 586-0984
    Inner Solar Roof Systems, Inc. Contact:
    Joseph Allegro, (561) 997-8479

The purpose of this project is to develop an unglazed solar collector used to replace the roof, intended for residential installation. Solar roof panels will be designed, built and tested with a monitoring system on a test roof. Additional testing will be performed by Sandia National Laboratory.

Keywords: Residential, Solar, Roof

61. **AEROCYLINDER**
    $99,925
    DOE Contact: Ramesh Jain, (202) 586-2381
    Aeroproducts International, Ltd, Corp. Contact:
    Kenneth L. Smedberg, (773) 734-3064

The technology uses airspring bellows combined into assemblies for use on machines such as punch presses, in place of conventional air cylinders, to control motion and large masses. The air springs act as counter balances and press cushions and eliminate alignment problems associated with conventional air cylinders. The project work includes building and testing several cylinders in a controlled environment, as well as field performance testing.

Keywords: Air Cylinder, Metal Stamping, Punch Press

62. **ENVIRONMENTAL TENSOMETER**
    $99,223
    DOE Contact: Ramesh Jain, (202) 586-2381
    Contact: Richard E. Tressler, (814) 466-3168

The invention is a system for high temperature testing of the tensile strength and related physical properties of single filament refractory fibers under varying atmospheric conditions. The system integrates a furnace, testing unit, gas handling system, vacuum system and PC based software. Work will focus on refining the design of the environmental tensometer, and building and testing a second-generation prototype of the device. The unit will then be tested in a laboratory setting.

Keywords: Filament Refractory Fiber

63. **ENERGY EFFICIENT, ELECTRIC ROTARY FURNACE FOR GLASS MOLDING (REPRESSING) PRECISION OPTICAL BLANKS**
    $99,999
    DOE Contact: Rolf Butters, (202) 586-0984
    Advanced Glass Industries Contact: Tony Marino, (716) 458-8040

The invention is an electrically heated rotary furnace for glass molding (i.e., repressing) to produce precision optical blanks. The proposed oven design can automate and optimize the production heat cycle for each of over a thousand types of glass, thereby converting from a highly labor intensive process to an automated flexible manufacturing operation which greatly increases production capacity. The project work will focus on reducing output quality variations; improving temperature control and reducing variances; increasing production capacities; and maximizing energy efficiency.

Keywords: Glass, Rotary Furnace

64. **METHOD FOR PRODUCING GLASS FIBER**
    $97,971
    DOE Contact: Rolf Butters, (202) 586-0984
    Glass Fiber Technologies Contact: Warren (Wendell) Drummond, (352) 377-4429

This is a system for producing glass fiber for glass insulation and composite materials, where glass fiber is used as a reinforcing member. This new system can reduce energy consumption per ton of glass fiber produced by 40 percent. Project work will develop and demonstrate a pilot-scale melter to produce consistent diameter textile fiberglass.

Keywords: Glass Fiber, Insulation, Composite, Fiberglass

65. **THERMAL HEAT AND DIFFUSION TREATMENT OF BULK POWDERS**
    $99,983
    DOE Contact: Rolf Butters, (202) 586-0984
    Kemp Development Corporation (KDC) Contact: Willard E. Kemp, (281) 492-6767

The technology is a process and hardware design to treat powdered metals during production for making parts. This system significantly increases energy efficiency and productivity for the domestic powder metal industry by about 70 percent. The hardware consists of a rotating kiln that holds a batch of powdered metals under vacuum while annealing and/or carrying out gas phase reactions necessary to nitride, aluminize, carburize etc., metal powder particles. The project aim is to build and demonstrate the technical and economic suitability of a mechanically fluidized powder treatment machine, which produces high-quality products through thermo-chemical treatments of industrial powders. A machine will be designed, constructed and tested with a wide range of metal and cermet powder treatments. Sufficient treatments will be demonstrated to prove technical and economic capability of the machine and method. Other treatments not currently possible by existing means will also be investigated.

Keywords: Metal Powder, Ceramic Powder, Vacuum, Anneal, Aluminize, Carburize

66. **DENSITY SEPARATION IN COMPLEX-MODE VIBRATION FLUIDIZED BEDS**
    $98,000
    DOE Contact: David Crouch, (202) 586-4844
    Incisive Engineering, Inc. Contact: Arthur P. Fraas, (423) 525-4095

A new generic process of solids-solids separation using complex-mode mechanical vibrations to fluidize and effect separation of components of streams of crushed solids that consist of particles of different densities and sizes. Normal linear mechanical vibrations do not produce fluidization and a satisfactory separation of materials of different sizes. Project work will focus on developing a complex-mode separations machine for coal and mineral separations.

Keywords: Solids Separation, Fluidized Bed

67. **MOLTEN FILM HIGH-INTENSITY PAPER DRYER**
    $99,657
    DOE Contact: David Crouch, (202) 586-4844
    Harvest Technology Contact: David Walter Warren, (818) 767-3157

The technology is a system for high-intensity drying of paper utilizing surface-applied molten films composed of low melting point eutectic alloys. The project work will build and test a heat-integrated molten fluid dryer, which will allow continuous steady-state operation of the dryer over extended time periods. Extended dryer test runs will be conducted at varying speeds, paper grades, and molten bath temperatures. Test result data will be analyzed to determine overall operational and scale-up performance.

Keywords: Paper Drying

68. **LASER ULTRASONIC FURNACE TUBE COKE MONITOR**
    $98,670
    DOE Contact: David Crouch, (202) 586-4844
    Contact: David Walter Warren, Harvest Energy Technology, Inc., (818) 767-3157

The technology is a laser-based instrument for measuring the thickness of coke deposits in a tubular industrial furnace while the furnace is in use. The real-time measurement data on coke deposition can then be integrated with control and simulation software for optimization of furnace variables. Project work will demonstrate the performance and practical use of a laser ultrasonic probe for measuring the thickness of coke deposits located within the high-temperature tubes of a thermal cracking furnace.

Keywords: Sensor, Coke, Thermal Cracking Furnace, Laser Ultrasonic

69. **APPARATUS AND METHOD FOR FILTERING MOLTEN METAL**
    $99,999
    DOE Contact: David Crouch, (202) 586-4844
    Contact: Jay R. Hitchings, (610) 269-4513

The invention is an automated means of filtering slag, dross, and other non-metallic impurities from molten metals, through the use of refractory filter cloth, in the process of casting metal parts on injection molding metal casting machines. A filtering cloth is automatically advanced to a clean portion between each injection shot of the molding or casting machine. The project work will focus on developing and testing a large and small working prototype units. These units will then be tested at an appropriate commercial foundries.

Keywords: Metal Casting, Filter

70. **SELF-DRESSING RESISTANCE WELDING ELECTRODE**
    $42,888
    DOE Contact: Lisa Tunstall-German, (202) 586-2487
    Lektro Corp. Contact: Bryan Prucher, (248) 644-1233

The technology is a spot-welding electrode cap designed to operate at lower average temperature and to maintain a constant contact area during extended operation, thus minimizing weld energy requirements. The project will produce an electrode from a unique metal matrix composite material that employs a ceramic substrate as the load bearing element and a metal matrix as the conduit for the electric current flow. The model will be verified, performance tested, and evaluated.

Keywords: Welding Electrode

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

71. **TRIBOPOLYMERIZATION AS AN ANTI-WEAR MECHANISM**
    $99,743
    DOE Contact: David Crouch, (202) 586-4844
    Virginia Polytechnic Institute & State University Contact: Michael J. Furey, (540) 231-7193

The technology is a process for improving lubricity and reducing wear in high temperature ceramic engines and similar applications. A carrier liquid containing a low concentration of selectively polymerized monomers is used. These monomers form adhering lubricating films that are regenerated as they wear. An advanced testing platform will be designed and constructed to simulate ceramic engine operating conditions. This platform will be used to test various tribopolymerization formulae. Samples that perform favorably will then undergo further analysis.

Keywords: Ceramic Lubrication, Polymerized Monomers

72. **NICKEL-BASED SUPERALLOY WITH IMPROVED WELDABILITY AND OXIDATION RESISTANCE**
    $99,174
    DOE Contact: David Crouch, (202) 586-4844
    Pennsylvania State University Contact: Eric Whitney, (814) 865-3916

The invention is a new composition of nickel-based superalloys with the addition of up to 50 atomic percent palladium. This material should permit the welding of superalloy components, such as jet engine rotor tips (and other parts exposed to very high temperatures) so that damage from high temperature erosion and corrosion can be repaired. Project work will focus on defining the compositional range of an alloy that is suitable for evaluation and qualification by a commercial enterprise. The following alloy properties will be determined: weldability, oxidation resistance, creep strength, resistance to thermo-mechanical fatigue, microstructure stability, and cost.

Keywords: Welding, Superalloy, Nickel, Palladium

73. **FOAMED RECYCLABLES**
$98,900
DOE Contact: Lisa Tunstall-German, (202) 586-2487
Kaiser Ceramic Composites Contact: Wade H. Brown, (510) 562-2456 x251

This process produces low cost, lightweight, foamed structures using polymers and filling agents such as fly ash or bauxite residue (red mud). This technology can reduce waste disposal problems associated with fly ash and bauxite residue. This also has the potential to create new products at lower cost, especially for the home building industry. Work includes the design and development of a production line for foamed and solid recyclables; testing of foamed and solid recyclables; and the development of specialized products.

Keywords: Fly Ash, Bauxite, Foam

74. **HIGH R-VALUE, ENVIRONMENTALLY SAFE RIGID FOAMS BLOWN WITH FLUOROIODOCARBONS (FICs)**
$99,990
DOE Contact: David Crouch, (202) 586-4844
Environmental Technology & Education Center Contact: Jon Nimitz, (505) 345-2707

The invention consists of using fluoroiodocarbons (fluorine, iodine and carbon - FICs) as blowing agents for the manufacture of such foam insulation materials as polyurethane, polyisocyanurate and polystyrene. This foam is used for insulating refrigerators and water heaters and as building insulation. The FICs would replace now-banned CFC-11 and the current interim use of HCFC blowing agents. The overall goal is to make rigid insulating foams with performance and environmental properties superior to foams blown with CFC-11 or CFC-12. Sample foams will be produced and tested. Properties of these foams will be determined by appropriate ASTM testing procedures. An improved synthesis of the preferred FIC blowing agent will then be designed and tested in the laboratory.

Keywords: Foam, Refrigerant, Fluoroiodocarbons, Fluorine, Iodine and Carbon, FIC, CFC-11, CFC-12, HCFC, Polyurethane, Polyisocyanurate, Polystyrene

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

75. **IMPROVED RADIANT BURNER MATERIAL**
$99,950
DOE Contact: Rolf Butters, (202) 586-0984
Superkinetic, Inc. Contact: John V. Milewski, (505) 856-6259

The technology is a manufacturing process for producing single crystal ceramic fibers, specifically single crystal sapphire fibers for use in radiant burners. The process is based on vapor-deposition and produces single crystal fibers. The higher-purity, single-crystal fibers from this process have significant advantages over polycrystalline fibers. The project work focuses on constructing a single crystal fiber growth facility sized to meet the radiant burner prototype needs and growing highly perfect single-crystals. A furnace and control assembly will be designed and built. Fibers of sufficient quantity and quality will be grown for felt formation. A test apparatus to simulate burner operating conditions will be constructed. A prototype burner using the felt material will be constructed and tested under a variety of conditions.

Keywords: Ceramic Fibers, Single Crystal

76. **HIGH THROUGHPUT MANUFACTURING OF HIGH EFFICIENCY SOLAR CELLS**
$99,761
DOE Contact: Rolf Butters, (202) 586-0984
AVA Technologies Contact: Kurt L. Barth, (970) 491-8411

This technology is a continuous vacuum chemical vapor deposition (CVD) process designed to replace conventional batch CVD processes for manufacturing high efficiency cadmium telluride (CdTe) solar cells. The process is amenable to automation. Project work will develop a manufacturing prototype unit that will continuously produce one 10 percent efficient 3x3-inch CdTe solar cell per minute. Pre-production prototype processes will be optimized. Process robustness will be studied by producing and testing the process stability and efficiency of several lots of 200 consecutive cells.

Keywords: Solar Cell Fabrication, Cadmium Telluride, CdTe, Automation

77. **COMPOSITE ELECTRODES FOR ADVANCED ELECTROCHEMICAL APPLICATIONS**
$99,975
DOE Contact: David Crouch, (202) 586-4844
North Coast Crystals Contact: Chris Kovach, (216) 231-5524

A process to reduce thermal expansion stresses between CVD deposited diamond thin films on copper. The technology would enable using copper electrodes with a stable inert coating in electrochemical applications. The project work will develop a proof-of-principal composite electrode using titanium substrates. This includes sample preparation, coating analysis, coating preparation, and electrode testing.

Keywords: Composite, Electrode, Electrochemical

78. **PROCESS TO RECOVER ACID AND METAL SALTS FROM PICKLING LIQUORS**
$99,904
DOE Contact: David Crouch, (202) 586-4844
Green Technology Group Contact: Douglas R. Olsen, (914) 855-0331

An innovative process for recycling waste pickling liquor from sulfuric acid-based baths in the iron and steel processing industries with several economic and environmental advantages and benefits over competing processes will be pursued. This project focuses on conducting two pilot tests at different metals processing facilities using this process. The process will be tested with copper metal and sulfuric acid, and with iron and steel and hydrochloric acid.

Keywords: Acid Recovery, Iron, Steel, Galvanize, Sulfuric Acid, Hydrochloric Acid

MATERIALS STRUCTURE AND COMPOSITION

79. **A LOW PLATINUM LOADING, HYDROPHILIC FUEL CELL ELECTRODE FOR USE WITH A PROTON EXCHANGE MEMBRANE**
$99,999
DOE Contact: Rolf Butters, (202) 586-0984
Contact: George Marchetti, (630) 759-0800

This technology demonstrates a new design approach for Proton Exchange Membrane (PEM) fuel cells. This electrode provides more efficient hydration with good water control, which gives better hydronium ion migration rates and thus more power density. The project aim is to build an engineering prototype of a fuel cell battery using low platinum loading, hydrophilic graphite electrodes with a proton exchange membrane and demonstrating on-site power delivery capabilities.

Keywords: Fuel Cell, , Hydrophilic Proton Exchange Membrane (PEM)

80. **COMBINED BATTERY AND STRUCTURE FOR HEIGHTENED ENERGY STORAGE**
$91,392
DOE Contact: David Crouch, (202) 586-4844
Boundless Corp. Contact: Philip C. Lyman, (303) 415-9029

The invention is a nickel-metal-hydride (NiMH) structural battery system for electric vehicles, portable electronic devices, etc. The batteries are assembled in the form of lightweight honeycomb structural panels. The battery panels can form integral structural members of the device. An initial application of this technology will be for portable electronics. A prototype structural battery for equipment needing long-lasting, lightweight battery power will be built.

Keywords: Structural Battery, Nickel Metal Hydride (NIMH), Electric Vehicle

81. **ELECTRIC UTILITY ENERGY STORAGE DEVICE**
$99,948
DOE Contact: Rolf Butters, (202) 586-0984
ZBB Technologies, Inc. Contact: Philip A. Eidler, (414) 228-2436

The invention is a design of a modular flow-through zinc/bromine battery. Its purpose is to allow load-leveling by electric utility companies. The project involves designing, building and testing an 80 kWh energy storage module based on the zinc/bromine battery technology. The self-contained module will hold two bromine reservoirs and a compartment for the battery stacks. The module will be an integral part of the battery system and include sensors, level detectors, pumps, motors, and a cooling system. These components will all be incorporated in the design to simplify final module fabrication.

Keywords: Battery, Zinc Bromide, Utility, Load Leveling

NATIONAL INDUSTRIAL COMPETITIVENESS THROUGH ENERGY, ENVIRONMENT AND ECONOMICS (NICE[3]) - DOE Contact Lisa Barnett, (202) 586-2212

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

82. **RAPID HEAT TREATMENT OF CAST ALUMINUM COMPONENTS**
$414,710
DOE Contact: Lisa Barnett, (202) 586-2212
Technomics Contact: Steve Krause, (612) 475-1752

The project conducted by the Minnesota Office of Environmental Assistance and Technomics Inc. of Plymouth, MN will demonstrate and commercialize an automated, in-line continuous processing fluidized bed system for heat-treating cast aluminum components. Technomics will build and operate a full-scale facility for demonstrating to manufacturers, with their own cast aluminum components, an automated in-line heat treating and quenching system. This system uses fluidized bed technology that reduces the time required to achieve specifications by 80-90 percent. The process also reduces nitrous oxide and CO_2 process air emissions, energy use, and water and ground pollution from sand casting by 80-90 percent. Unlike current convection and vacuum furnaces, the system uses closed-loop air circulation, pulse-fired burners, and direct heating of the energy transfer medium to reduce energy use by rapidly heating individual components to molecular structure alteration temperatures.

Keywords: Aluminum, Heat Treating, Fluidized Bed

83. **CHLORINE REDUCTION IN ALUMINUM PROCESSING**
$425,000
DOE Contact: Lisa Barnett, (202) 586-2212
Reynolds Contact: Shirley Painter, (804) 281-2655

The Virginia Department of Environmental Quality (VDEQ) and Reynolds Metals Co will demonstrate an emission monitoring system that is integrated with an in-line process that efficiently introduces chlorine into the fluxing process. In the course of producing aluminum by electrolytic reduction, impurities such as calcium, lithium, and sodium can cause problems during processing, and are detrimental to various aluminum alloy properties. Chlorine fluxing is a standard procedure for eliminating impurities. The U.S. EPA is currently developing regulations to limit the amount of chloride emissions from aluminum furnace operations where fluxing typically occurs. This project will demonstrate the use of stack emission monitoring to provide closed-loop control of chlorine in order to decrease the amount of excess chlorine used without harming metal quality. Since the use of chlorine will be reduced by 73 percent in the fluxing process, the energy required to manufacture chlorine will also be reduced.

Keywords: Aluminum, Chlorine Fluxing, Emission Monitoring

84. **DEMONSTRATE THE MICROSMOOTH™ WHEEL FINISHING PROCESS ON ALUMINUM WHEELS**
$400,000
DOE Contact: Lisa Barnett, (202) 586-2212
Metal Arts Contact: Stanley J. Dahle, (716) 342-2980

The New York State Energy and Research Development Authority (NYSERDA) and Metal Arts Company, Inc. of Rochester, NY, and their partner, The Aluminum Company of America (ALCOA) of Cleveland, OH, will demonstrate and commercialize a new aluminum wheel finishing process. This objective is to demonstrate the use of an innovative electroless nickel-plating process, using Microsmooth™, a streamlined replacement for conventional process nickel/chrome plating in the finished products segment of the aluminum industry. Using Microsmooth™ in chrome-plating forged aluminum wheels results in a superior product and substantially reduces energy and chemical (zinc, copper, cyanide, caustic etch, and nitric acid) usage, thus providing environmental, economic, and worker health benefits. Approximately 11 million chrome-plated aluminum wheels are manufactured every year in the U.S. The Microsmooth™ process is expected to save 71 percent of the waste produced, 33 percent of the electricity consumed, and 59 percent of the natural gas currently consumed by the wheel plating industry

Keywords: Aluminum Wheel, Electroless Nickel Plating, Chrome-Plating

85. **LIGHTWEIGHT STEEL DISPENSING CONTAINERS**
$425,000
DOE Contact: Lisa Barnett, (202) 586-2212
DCC Contact: George B. Diamond, (908) 832-7882

The Pennsylvania Department of Environmental Protection (DEP) and Dispensing Containers Corporation (DCC) will demonstrate and commercialize innovative lightweight steel dispensing containers. Approximately 3 ounces of steel are consumed in the production of a steel dispensing container, with about

3 billion cans produced annually in the U.S. and 9 billion produced worldwide. Steel dispensing cans are used for a variety of end-products including hair spray, shave cream, and cheese. DCC has developed a thin-walled dispensing container of equivalent strength that utilizes an average of 1.7 ounces of steel, representing a metal reduction of approximately 40 percent in the container body. DCC has also developed a lightweight dome (top) which, when used with the DCC container body, brings the average total metal reduction per container to approximately 43.5 percent. DCC's technology relies on the can's internal pressure, rather than wall thickness, to retain the rigidity of the container. As a result of the lower steel requirements, DCC's technology is expected to result in significant energy and waste savings.

Keywords: Steel Cans, Dispensing Containers

86. **PROCESS TO RECOVER AND REUSE SULFUR DIOXIDE IN METALCASTING OPERATIONS**
$239,400
DOE Contact: Lisa Barnett, (202) 586-2212
Adsorption Research Contact: Kent Knabel, (614) 798-9090

The Ohio Department of Development and Adsorption Research, Inc. of Dublin, will demonstrate and commercialize a sulfur dioxide recovery and reuse system for the metal casting industry. Sulfur dioxide is used as a catalyst in forming cold box molds and cores. With existing technology, SO_2 is used once and then discarded by purging the mold with dry air or nitrogen. That effluent is then scrubbed (at about 98 percent efficiency) with a caustic solution, which is then flushed into a sewer or delivered to a waste treatment facility. The new process recovers 99.5 percent of the sulfur dioxide and 99.8 percent of the carrier gas so that both can be reused without scrubber treatment. The process will be applied to sulfur-producing industrial operations such as lead and copper smelting, food preservation, and power generation. It is based on existing pressure swing adsorption technology requiring no regenerant, and therefore produces no waste stream. The principal operating costs are associated with the power consumed in evacuating the adsorbent vessels during blowdown and in maintaining low pressure during purge. Employing this process will eliminate the need for a caustic scrubber, as well as the related effluent.

Keywords: Metalcasting, Sulfur Dioxide, Pressure Swing Adsorption, Cold Box Molds, Cores

OFFICE OF TRANSPORTATION TECHNOLOGIES

	FY 1998
Office of Transportation Technologies - Grand Total	$26,736,000
Transportation Materials Technology	$26,736,000
Automotive Materials Technology	$18,889,000
Propulsion Materials	$ 3,689,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$975,000
Gelcasting: Scale-up and Commercialization	350,000
Material Support for Nonthermal Plasma Development	100,000
Optimization of Silicon Nitride Ceramics	0
Development of Silicon Nitride Ceramic Materials with Elongated Grain Microstructures Exhibiting High Fracture Toughness	525,000
Materials Properties, Behavior, Characterization or Testing	$940,000
Characterization and Life Prediction of Ceramic Recuperator Materials	40,000
Component Verification	275,000
High Frequency Fatigue of Structural Ceramics and Components	210,000
Stress Rupture and Creep of Structural Ceramics	70,000
Bolt-Load Retention and Creep of Magnesium Alloys	170,000
Characterization and Metrology of CIDI Fuel Injector Holes	25,000
Life Prediction Methodology	0
Environmental Effects in Toughened Ceramics	0
NDE of Silicon Nitride and Coatings	150,000
Technology Transfer and Management Coordination	$490,000
Technical Project Management	490,000
Device or Component Fabrication, Behavior or Testing	$1,234,000
Corrosion-Resistant Coatings for Si_3N_4	145,000
Rapid Surface Modification of Aluminum Engine Block Bores by a High-Density Infrared Process	150,000
Lead-Free Solders for Automotive Electronics	50,000
Mechanical Reliability Assessment of Electronic Ceramics and Electronic Ceramic Components	100,000
Carbon Fiber/CVI Bipolar Plate	200,000
Carbon Foam Thermal Management Materials for Electronic Packaging	235,000
Functionally Graded Material for Packaging/Thermal Management	200,000
Microwave Regenerated Diesel Exhaust Particulate Filter	54,000
Thermal Management in Automotive Integrated Power Modules	100,000

OFFICE OF TRANSPORTATION TECHNOLOGIES (continued)

	FY 1998
Transportation Materials Technology (continued)	
Automotive Materials Technology (continued)	
Lightweight Vehicle Materials	$15,250,000
Device or Component Fabrication, Behavior or Testing	$15,250,000
Low-Cost High Performance Wrought Aluminum Components for Automotive Applications	3,280,000
Low-Cost High Performance Cast Light Metals for Automotive Applications	1,775,000
Advanced Materials and Processes for Automotive Applications	1,860,000
Automotive-Related Graduate Fellowships	100,000
Materials and Processes for Propulsion System Applications	400,000
Technology Assessment and Evaluation	475,000
Reinforced Composite Materials—Joining, Durability, and Enabling Technologies	2,900,000
USAMP Cooperative Agreement	1,275,000
Carbon Fiber Based Composite Materials Technology	1,750,000
Development of Low-Cost Lightweight Metals and Alloys	635,000
Recycling	550,000
Structural Reliability of Lightweight Glazing Alternatives	250,000
Electric Drive Vehicle Technologies	$3,348,000
Advanced Battery Materials	$2,948,000
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
Development of Novel Electrolytes for Rechargeable Lithium Cells	100,000
Materials Properties, Behavior, Characterization or Testing	$1,704,000
Carbon Electrochemistry	250,000
Fabrication & Testing of Carbon Electrodes as Lithium Intercalation Anodes	75,000
Reactivity and Safety Aspects of Carbonaceous Anodes in Lithium Batteries	140,000
Battery Materials: Structure and Characterization	140,000
Composite Polymer Electrolytes for Use in Lithium and Lithium-Ion Batteries	100,000
Polymer Electrolyte for Ambient Temperature Traction Batteries: Conductivity Optimization	99,000
Analysis and Simulation of Electrochemical Systems	255,000
Corrosion of Current Collectors in Rechargeable Lithium Batteries	200,000
Electrode Surface Layers	200,000
Microstructural Modeling of Highly Porous NiMH Battery Substrates	145,000
Electrode Surface Layers	100,000

OFFICE OF TRANSPORTATION TECHNOLOGIES (continued)

	FY 1998
Transportation Materials Technology (continued)	
Electric Drive Vehicle Technologies (continued)	
Advanced Battery Materials (continued)	
Device or Component Fabrication, Behavior or Testing	$361,000
Development of a Thin-Film Rechargeable Lithium Battery for Electric Vehicles	71,000
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	200,000
Fuel Cell Materials	$400,000
Materials Properties, Behavior, Characterization or Testing	$400,000
Electrode Kinetics and Electrocatalysis	300,000
Poisoning of Fuel Cell Electrocatalyst Surfaces: NMR Spectroscopic Studies	100,000
Heavy Vehicle Propulsion System Materials	$4,499,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	2,409,000
Cost-Effective Smart Materials for Diesel Engine Applications	400,000
Cost-Effective Sintering	144,000
Low Cost, High Toughness Ceramics	350,000
Intermetallic-Bonded Cermets	60,000
Characterization/Testing of Low CTE Materials	100,000
Insulating Structural Ceramics for High Efficiency, Low Emission Engines	0
Thick Thermal Barrier Coatings (TTBCs) for Low Emissions, High Efficiency Diesel Engine Components	0
Materials for Low Emissions, High Efficiency Diesel Engine Components	605,000
Materials for Low Emissions, High Efficiency Diesel Engine Components	750,000
High Strength Materials for Diesel Engine Fuel Injectors	0
Materials Properties, Behavior, Characterization or Testing	$1,020,000
Diesel Exhaust Catalyst Characterization	200,000
Life Prediction Verification	200,000
High Temperature Tensile Testing	0
Computed Tomography	120,000
On-Machine Inspection	0
International Exchange Agreement (IEA)	200,000
Standard Reference Materials	200,000
Mechanical Property Standardization	100,000

OFFICE OF TRANSPORTATION TECHNOLOGIES (continued)

	FY 1998
Transportation Materials Technology (continued)	
Heavy Vehicle Propulsion System Materials (continued)	
Technology Transfer and Management Coordination	$565,000
Technical Project Management	565,000
Device or Component Fabrication, Behavior or Testing	$505,000
Durability of Diesel Engine Component Materials	200,000
Advanced Machining/Manufacturing	225,000
Laser-Based NDE Methods	80,000

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. **Transportation Materials Technologies R&D** is conducted by the Office of Advanced Automotive Technologies (OAAT) and the Office of Heavy Vehicle Technologies (OHVT) to address critical needs of automobiles and heavy vehicles, respectively. These 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, the bulk of the materials R&D is carried out through the **Transportation Materials Technologies** program, with additional specialty materials R&D in the **Advanced Battery Program** and in the **Transportation Fuel Cell Program.** The **Transportation Materials Technologies** program develops: (a) ***Automotive Propulsion 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 power train are critical to attaining the challenging performance standards for advanced automotive vehicles. The DOE contacts are Patrick Davis, (202) 586-8061, for automotive propulsion materials and Joseph Carpenter, (202) 586-1022, for automotive lightweight vehicle materials. For advanced battery materials R&D, the DOE contact is Ray Sutula, (202) 586-8064; for fuel cell materials R&D, the DOE contact is JoAnn Milliken, (202) 586-2480.

Within OHVT, the **Transportation Materials Technologies** 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 emission, 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 contact is Sidney Diamond, (202) 586-8032.

To support mainly propulsion system materials R&D, 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 Sidney Diamond, (202) 586-8032.

TRANSPORTATION MATERIALS TECHNOLOGY

AUTOMOTIVE MATERIALS TECHNOLOGY

PROPULSION MATERIALS

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

87. **GELCASTING: SCALE-UP AND COMMERCIALIZATION**
$350,000
DOE Contact: P. Davis, (202) 586-8061
ORNL Contact: D. P. Stinton, (423) 574-4556
ORNL Contact: S. D. Nunn, (423) 576-1668

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; improve the gelcasting chemical system to enhance control of processing parameters and molded-part characteristics; improve gelcasting compositions and machining methods to produce high-precision components with features which are machined in the green ceramic body; evaluate new mold materials, new mold-surface-preparation techniques, and mold-release agents which enhance separation of the part from the mold to yield high-quality surface finish.

Keywords: Silicon Nitride, Ceramics, Gelcasting, Forming

88. **MATERIAL SUPPORT FOR NONTHERMAL PLASMA DEVELOPMENT**
$100,000
DOE Contact: P. Davis, (202) 586-8061
ORNL Contact: D. P. Stinton, (423) 574-4556
ORNL Contact: S. D. Nunn, (423) 576-1668

The purpose of this work is to provide ceramic material support to Pacific Northwest National Laboratory (PNNL) for development and fabrication of new component designs for use in nonthermal plasma reactors for the treatment of diesel exhaust gases, and to fabricate components for testing at PNNL.

Keywords: Diesel, Fabrication, Gelcasting

89. **OPTIMIZATION OF SILICON NITRIDE CERAMICS**
$0
DOE Contact: P. Davis, (202) 586-8061
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 develop low-cost silicon nitride ceramics with properties meeting DOE's goal for high-temperature structural applications. The results of this investigation will eventually be transferred to industry for production. An L18 ($2^1 \times 3^6$) experimental design is being used in the investigation to study the effect of additives and processing conditions to obtain silicon nitride ceramics with optimum properties.

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

90. **DEVELOPMENT OF SILICON NITRIDE CERAMIC MATERIALS WITH ELONGATED GRAIN MICROSTRUCTURES EXHIBITING HIGH FRACTURE TOUGHNESS**
$525,000
DOE Contact: P. Davis, (202) 586-8061
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 demonstrate the reproducibility of gelcast and slipcast AS800 properties in a production environment, characterize and improve AS800 fabrication process to improve strength and oxidation resistance, and demonstrate the ability to gelcast and densify thick sections required for lower-cost integral gas turbine rotors.

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

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

91. **CHARACTERIZATION AND LIFE PREDICTION OF CERAMIC RECUPERATOR MATERIALS**
$40,000
DOE Contact: P. Davis, (202) 586-8061
ORNL Contact: D. P. Stinton, (423) 574-4556
Teledyne Ryan Contact: S. F. Duffy, (330) 678-7328

This purpose of this effort is to characterize the thermomechanical response, and define and help establish (in conjunction with design engineers at

Teledyne Ryan) the requisite material database, as well as perform life-prediction estimates for Teledyne Ryan's ceramic recuperator.

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

92. **COMPONENT VERIFICATION**
$275,000
DOE Contact: P. Davis, (202) 586-8061
ORNL Contact: D. P. Stinton, (423) 574-4556
ORNL Contact: H.-T. Lin, (423) 576-8857

The objectives of this effort are to evaluate and document the long-term mechanical properties of ceramics from complex-shaped components (e.g., blades, nozzles, vanes, and rotors) at elevated temperatures, and to generate a mechanical-properties database for recuperator thin sheet ceramic matrix composites developed by Du Pont Lanxide Composites (DLC) Inc. The database will be used for the finite element analysis of life prediction of the recuperator components employed in the Hybrid Electric Vehicle Engines.

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

93. **HIGH FREQUENCY FATIGUE OF STRUCTURAL CERAMICS AND COMPONENTS**
$210,000
DOE Contact: P. Davis, (202) 586-8061
ORNL Contact: D. P. Stinton, (423) 574-4556
ORNL Contact: K. C. Liu, (423) 574-5116

The objective of this task was to develop the baseline information on high-cyclic-fatigue (HCF) behavior of structural ceramics at elevated temperatures and high frequencies (> 1000 Hz), and establish reliable HCF life-prediction methods for components under conditions typical of HCF in turbine and automotive propulsion systems, with a special aim toward understanding the effects of high mean stress (simulating high centrifugal force in rotating components) on HCF behavior.

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

94. **STRESS RUPTURE AND CREEP OF STRUCTURAL CERAMICS**
$70,000
DOE Contact: P. Davis, (202) 586-8061
ORNL Contact: D. P. Stinton, (423) 574-4556
ORNL Contact: K. C. Liu, (423) 574-5116

The objective of this task was to develop the baseline information on 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, and to develop material-behavior models to facilitate design analysis of components for improved reliability.

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

95. **BOLT-LOAD RETENTION AND CREEP OF MAGNESIUM ALLOYS**
$170,000
DOE Contact: P. Davis, (202) 586-8061
ORNL Contact: D. P. Stinton, (423) 574-4556
ORNL Contact: K. C. Liu, (423) 574-5116

The purpose of this work was to develop a creep database and a material model for a candidate magnesium alloy for predicting bolt-load retention characteristics and evaluating the predictability by comparison with experimental data obtained from bolt-load retention tests.

Keywords: Alloys, Creep, Modeling

96. **CHARACTERIZATION AND METROLOGY OF CIDI FUEL INJECTOR HOLES**
$25,000
DOE Contact: P. Davis, (202) 586-8061
ORNL Contact: D. P. Stinton, (423) 574-4556
ORNL Contact: K. C. Liu, (423) 574-5116

The purpose of this work was to develop a robust technique to measure the size and characterize the shape of CIDI fuel injector holes, using an optical method based on the principle of Fraunhofer-Fresnel (F-F) diffraction.

Keywords: Characterization, Measurements

97. **LIFE PREDICTION METHODOLOGY**
$0
DOE Contact: P. Davis, (202) 586-8061
ORNL Contact: C. R. Brinkman, (423) 574-5106
AlliedSignal Engines Contact: B. Schenk, (602) 231-4130

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

98. **ENVIRONMENTAL EFFECTS IN TOUGHENED CERAMICS**
$0
DOE Contact: P. Davis, (202) 586-8061
ORNL Contact: D. P. Stinton, (423) 574-4556
University of Dayton Contact: N. L. Hecht, (513) 229-4341

The objectives of this task are to evaluate high-temperature fatigue behavior, develop life-prediction analysis, and measure the thermal-mechanical properties of as-sintered versus machined specimens of the latest-vintage Si_3N_4 ceramics. Additional goals include a better understanding of the degradation mechanisms affecting heat engine materials and extension of the database for these candidate ceramic materials. A final objective is a better understanding of the effects of different machining methods on the mechanical behavior of these candidate ceramics. Currently, the latest- vintage AS-800, SN-281, and SN-282 are being evaluated.

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

99. **NDE OF SILICON NITRIDE AND COATINGS**
$150,000
DOE Contact: P. Davis, (202) 586-8061
ORNL Contact: D. P. Stinton, (423) 574-4556
ORNL Contact: W. A. Simpson, Jr., (423) 574-4421

The objective of this program was to develop nondestructive evaluation techniques capable of detecting critical flaws in structural ceramic components.

Keywords: NDE, Structural Ceramics, Ultrasonics

TECHNOLOGY TRANSFER AND MANAGEMENT COORDINATION

100. **TECHNICAL PROJECT MANAGEMENT**
$490,000
DOE Contact: P. Davis, (202) 586-8061
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, Alloys, Carbon, Coordination, Metals, Management, Structural Ceramics

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

101. **CORROSION-RESISTANT COATINGS FOR Si_3N_4**
$145,000
DOE Contact: P. Davis, (202) 586-8061
ORNL Contact: D. P. Stinton, (423) 574-4556
ORNL Contact: J. A. Haynes, (423) 576-2894

The objectives of this research program are to develop a coating system to increase the durability of Si_3N_4 ceramic components in hostile combustion environments (e.g., hot corrosion and active oxidation), and to assess coating manufacturability issues that will lead to component demonstration and commercialization.

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

102. **RAPID SURFACE MODIFICATION OF ALUMINUM ENGINE BLOCK BORES BY A HIGH-DENSITY INFRARED PROCESS**
$150,000
DOE Contact: P. Davis, (202) 586-8061
ORNL Contact: D. P. Stinton, (423) 574-4556
ORNL Contact: C. Blue, (423) 574-5112

An innovative process that uses a high-intensity IR heat source to fuse a wear-enhancing additive into a surface in a matter of seconds is being developed to produce uniform, wear-resistant coatings for aluminum engine block cylinder bores. Treating the cylinder internal bores to enhance wear resistance and lower friction is intended to eliminate the need for heavy cast iron cylinder liners.

Keywords: Cost Reduction, Wear

103. **LEAD-FREE SOLDERS FOR AUTOMOTIVE ELECTRONICS**
$50,000
DOE Contact: P. Davis, (202) 586-8061
ORNL Contact: D. P. Stinton, (423) 574-4556
ORNL Contact: M. L. Santella, (423) 574-4805

The objective of this task is to evaluate the feasibility of using automated-ball-indentation (ABI) testing to measure the tensile properties and strain-rate sensitivity of selected solder joints. This will be done by ABI testing solder alloys and comparing these data to those from conventional testing. Alloying and mechanical-property studies are also being done to support the development of high-temperature solders.

Keywords: Electronics, Joining/Welding, Testing

104. **MECHANICAL RELIABILITY ASSESSMENT OF ELECTRONIC CERAMICS AND ELECTRONIC CERAMIC COMPONENTS**
$100,000
DOE Contact: P. Davis, (202) 586-8061
ORNL Contact: D. P. Stinton, (423) 574-4556
ORNL Contact: A. A. Wereszczak, (423) 574-7601

The objectives of this task are to provide expertise and characterization facilities for the assessment and prediction of mechanical reliability of electronic ceramics (ECs) and electronic ceramic components (ECCs), and to utilize life-prediction algorithms to increase service reliability of ECs and ECCs.

Keywords: Components, Electronics, Failure Analysis, Failure Testing, Life Prediction, Mechanical Properties

105. **CARBON FIBER/CVI BIPOLAR PLATE**
$200,000
DOE Contact: P. Davis, (202) 586-8061
ORNL Contact: D. P. Stinton, (423) 574-4556
ORNL Contact: T. M. Besmann, (423) 574-6852

The purpose of this work is to develop a slurry molded carbon fiber material with a carbon chemical-vapor-infiltrated (CVI) sealed surface as a bipolar plate. In addition, information will be obtained from potential manufacturers with regard to the manufacturability of such components.

Keywords: Carbon Products, Fuel Cells, Manufacturing

106. **CARBON FOAM THERMAL MANAGEMENT MATERIALS FOR ELECTRONIC PACKAGING**
$235,000
DOE Contact: P. Davis, (202) 586-8061
ORNL Contact: D. P. Stinton, (423) 574-4556
ORNL Contact: J. W. Klett, (423) 574-5220

The purpose of this work is to develop thermal-management materials for electronic packaging utilizing the high-thermal-conductivity carbon foam. This will consist of primarily two methods for cooling: (1) porous-media heat exchangers for substrates, and (2) high-thermal- conductivity heat sinks.

Keywords: Carbon Products, Electronics, Heat Transfer

107. **FUNCTIONALLY GRADED MATERIAL FOR PACKAGING/THERMAL MANAGEMENT**
$200,000
DOE Contact: P. Davis, (202) 586-8061
ORNL Contact: D. P. Stinton, (423) 574-4556
ORNL Contact: A. J. Moorhead, (423) 574-4667

The purpose of this work was to develop a graded transition material that minimizes thermal fatigue in multichip power modules by having a low coefficient of thermal expansion on one surface (near that of silicon devices) and a high coefficient of expansion on the other (near that of an aluminum heat sink). The material must also have a high thermal conductivity. The technical approach is to fabricate AlN preforms that are graded in porosity levels through the thickness and which are subsequently infiltrated with molten aluminum.

Keywords: Aluminum, Electronics, Fabrication, Thermal Fatigue

108. **MICROWAVE REGENERATED DIESEL EXHAUST PARTICULATE FILTER**
$54,000
DOE Contact: P. Davis, (202) 586-8061
ORNL Contact: D. P. Stinton, (423) 574-4556
Industrial Ceramic Solutions Contact: R. Nixdorf, (423) 482-7552

The objective of this effort is to define the heating efficiency of the Microwave Regenerated Particulate Trap when exposed to various air velocities during the regeneration cycle. This will be determined by a mass balance of heat energy in and out of the filter.

Keywords: Automotive Applications, Microwave Processing

109. **THERMAL MANAGEMENT IN AUTOMOTIVE INTEGRATED POWER MODULES**
$100,000
DOE Contact: P. Davis, (202) 586-8061
ORNL Contact: D. P. Stinton, (423) 574-4556
Sandia National Laboratories Contact: D. A. Benson, (505) 844-1187

The objectives of this effort were to develop new technology concepts for automotive electronics thermal management, support PNGV team members in characterization of thermal requirements for specific applications, and to develop detailed thermal models for typical electronic applications to optimize performance and assess reliability.

Keywords: Automotive Applications, Electronics, Modeling

LIGHTWEIGHT VEHICLE MATERIALS

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

110. **LOW-COST HIGH PERFORMANCE WROUGHT ALUMINUM COMPONENTS FOR AUTOMOTIVE APPLICATIONS**
$3,280,000
DOE Contact: Joseph Carpenter, (202) 586-1022
ORNL Contact: Phil Sklad, (423) 574-5069
PNNL Contact: Mark Smith, (509) 376-2847
Laboratory Partners: ORNL, LANL, INEEL, PNNL
Industry Partners: Alcoa, University of Michigan, Michigan Technological University (MTI), University of Stuttgart (IFU), Erie Press Systems, Imageware, AutoDie International, Advanced Technology Associates, Reynolds Metals Company, American Society of Mechanical Engineers (ASME), Commonwealth Aluminum, ARCO Aluminum, Century Aluminum

The objectives of this effort are: to evaluate and improve aluminum forming processes for automotive applications; to develop and implement low-cost continuous casting technologies for production of high-quality aluminum sheet; to develop a non-heat treatable aluminum alloy sheet product for automotive applications, such as exterior body panels or structural components; the development of numerical-based analysis tools that can be used to develop and optimize the forming process and predict distortions of multi-element structures (NATT),and to develop and optimize tailored blank fabrication and forming for high-volume, low-cost automotive panels and structures (NATT).

Keywords: Aluminum, Sheet Forming, Extrusion, Tailor Welded Blanks, Automotive

111. **LOW-COST HIGH PERFORMANCE CAST LIGHT METALS FOR AUTOMOTIVE APPLICATIONS**
$1,775,000
DOE Contact: Joseph Carpenter, (202) 586-1022
ORNL Contact: Phil Sklad, (423) 574-5069
PNNL Contact: Ed Courtright, (509) 375-6926
Laboratory Partners: LLNL, ORNL, SNL, INEEL, PNNL, ANL
Industry Partners: USAMP (Ford, GM, Chrysler), LEP (Ford, GM, Chrysler), Thixomat

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 low-cost method for producing prototype tools for lightweight metals in metal mold processes such as die casting, injection molding, and stamping; to reduce the lead time for production of prototype tools; to improve the energy efficiency and cost effectiveness of large-scale automotive aluminum die castings by extending die life and reducing die wear (NATT); to develop magnesium die casting alloys with improved high temperature properties, and to demonstrate semi-solid molding methods for the production of high-temperature creep-resistant alloys (NATT).

Keywords: Aluminum, Magnesium, Cast Metals, Rapid Prototyping, Automotive, Die Life, Die Wear, Die Castings

112. **ADVANCED MATERIALS AND PROCESSES FOR AUTOMOTIVE APPLICATIONS**
$1,860,000
DOE Contact: Joseph Carpenter, (202) 586-1022
ORNL Contact: Phil Sklad, (423) 574-5069
PNNL Contact: Mark Smith, (509) 376-2847
Laboratory Partners: Ames Laboratory, PNNL, ORNL
University Partners: University of Wisconsin-Milwaukee
Industry Partners: USAMP (Ford, GM, Chrysler), The Electric Power Research Institute (EPRI), Alcoa, MC-21

The objectives of this effort are: to develop low cost powder metallurgy (PM) manufacturing methods for particle reinforced aluminum (PRA) composite components; to advance PRA machining technology and PRA composite design methodologies; to produce and evaluate the use of aluminum "ashalloys"— metal matrix composites that incorporate coal fly ash in the commercial manufacture of cast automotive parts; to develop a new low-cost process for the efficient on-site stir-casting of aluminum metal matrix composites suitable for the production of automotive components (NATT); and to develop a technology to produce thin wall aluminum automotive components having greater than 15 percent ductility using a robust die casting process based on semi-solid molding .

Keywords: Metal Matrix Composites, Powder Metallurgy, Aluminum, Particle Reinforced Aluminum, Semi-Solid Molding

113. **AUTOMOTIVE-RELATED GRADUATE FELLOWSHIPS**
$100,000
DOE Contact: Joseph Carpenter, (202) 586-1022
ORNL Contact: Arvid Pasto, (423) 574-5123

The fellowship program, administered by the High Temperature Materials Laboratory (HTML) of Oak Ridge National Laboratory through Oak Ridge Associated Universities (ORAU), sponsors Master's and Ph.D degree students who are U.S. citizens and are interested in pursuing a career in the area of lightweight materials for automotive applications. Projects must be relevant to interest areas of the Office of Advanced Automotive Technologies (OAAT). The objectives of the program are to provide a mechanism for training researchers in state-of-the-art advanced characterization techniques using instruments at HTML and encourage research in areas of interest to OAAT and DOE.

Keywords: Fellowship, Master's Degree, Ph.D. Degree, Lightweight Materials, Research, Automotive Applications, Characterization Techniques

114. **MATERIALS AND PROCESSES FOR PROPULSION SYSTEM APPLICATIONS**
$400,000
DOE Contact: Joseph Carpenter, (202) 586-1022
ORNL Contact: Phil Sklad, (423) 574-5069
Laboratory Partners: SNL
Industry Partners: USAMP (Ford, GM and Chrysler)

The objective of these efforts are: to develop a multi-physics computational model of the induction heating and hardening process to predict part performance, to develop science-based, closed-loop controllers applicable to a broad range of steels, to use these tools to develop steel components with optimized strength-to-weight ratios.

Keywords: Induction Hardening, Nondestructive Evaluation, Steel

115. **TECHNOLOGY ASSESSMENT AND EVALUATION**
$475,000
DOE Contact: Joseph Carpenter, (202) 586-1022
ORNL Contact: Phil Sklad, (423) 574-5069;
Dave Warren, (423)574-9693, Dick Ziegler, (423) 574-5149
Laboratory Partners: ORNL

The objective of these activities is: to provide assessment of the cost-effectiveness of various technologies; to evaluate the ability of the industrial infrastructure to accommodate emerging technologies; and to provide guidance to program management as to appropriate investments for R&D funding.

Keywords: Cost, Infrastructure

116. **REINFORCED COMPOSITE MATERIALS— JOINING, DURABILITY, AND ENABLING TECHNOLOGIES**
$2,900,000
DOE Contact: Joseph Carpenter, (202)586-1022
ORNL Contact: Dave Warren (423)574-9693
Laboratory Partners: INEEL, LBNL, LLNL, ORNL
Industry Partners: USAMP/Automotive Composites Consortium (ACC), University of Texas-Austin, University of Tennessee, Oak Ridge Institute of Science and Technology, Tennessee State University, Goodrich, Baydur Adhesives, University of Tulsa, University of Michigan, University of Santa Barbara, University of Cincinnati, Wayne State University, Stanford University, University of Nottingham, Michigan Materials and Processing Institute, Budd Company, Dow

The objective of this effort is to develop critical enabling technologies necessary for the implementation of advanced structural composite materials. In cooperation with the ACC Energy Management working group, develop material and component models for composite materials in high energy impacts for prediction of passenger safety and optimization of component designs. Develop long term durability test methodologies, durability driven design guidelines, adhesive test methods, non-destructive inspection techniques and material models which can be used in designing automotive components. Specific technology thrust areas include the development of Mode I, Mode II, and Mixed Mode Fracture test methods and computer-based models for adhesively bonded joints. This work includes the characterization of bulk adhesives, sheet composite, and adhesive-adherends pairs using three composite adherend and three adhesives (2 epoxy and 1 urethane). Models are to simulate the fracture behavior of bonded joints under a wide range of mode mixes and define the fracture envelope. Composite research is to lead to the development of 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 NDE technology to evaluate bonded joint integrity of automotive assemblies, such as a body-in-white. Adhesive joint and composite research includes bulk material characterization, fracture, fatigue, creep, and creep fracture. This work also includes the development of NDE methods, advanced curing technologies and structural analysis model. Technology implementation is conducted through Automotive Composites Consortium focal projects. Demonstrate key technologies through focal projects which incorporate advances from various projects into manufacturable, cost effective pre-production prototypes that meet or exceed the requirements of current production assemblies.

Keywords: Polymer, Composites, Joining, Fracture, Durability, Preforming, Automotive, Adhesives, Non-Destructive Inspection

117. **USAMP COOPERATIVE AGREEMENT**
$1,275,000
DOE Contact: Joseph Carpenter, (202) 586-1022
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, Full Field NDT of Adhesive Bonding, ACC Focal Project II and ACC Focal Project III. 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

118. **CARBON FIBER BASED COMPOSITE MATERIALS TECHNOLOGY**
$1,750,000
DOE Contact: Joseph Carpenter, (202)586-1022
ORNL Contact: Dave Warren (423)574-9693
Laboratory Partners: ORNL
Industry Partners: USAMP/Automotive Composites Consortium, Lambda Technologies, AKZO Fortafil Fibers, Amoco

The objective is to conduct materials research to lead to the development of low cost carbon fiber for automotive applications. Research includes investigation of alternate energy deposition methods, and alternate precursors for producing carbon fiber as well as the development of improved thermal processing methods and equipment for fiber manufacture. This work examines the fiber architecture and manufacturing issues associated with carbon fiber usage to take advantage of this material's high strength and modulus while minimizing the effects of its low strain to failure. Candidate resin systems are screened for potential of meeting automotive industry requirements. In cooperation with the ACC Energy Management working group, develop material and component models for composite materials in high energy impacts for prediction of passenger safety and optimization of component designs.

Keywords: Polymer, Composites, Carbon Fiber, Durability, High Energy Impact

119. **DEVELOPMENT OF LOW-COST LIGHTWEIGHT METALS AND ALLOYS**
$635,000
DOE Contact: Joseph Carpenter, (202)586-1022
ORNL Contact: Phil Sklad, (423) 574-5069
PNNL Contact: Russ Jones, (509) 376-4276
Laboratory Partners: PNNL
Industry Partners: Alcoa, EIMEx, LLC/Boston University, Santa Fe Alloys

The objective of this work is to develop technologies for lowering the cost of primary light metals. Technologies which offer potential to produce sufficient quantities of raw materials for automotive use at substantially reduced cost will be investigated. Efforts include: the evaluation of plasma torch for heating molten bath at atmospheric pressure to allow continuous Mg production at reduced cost (NATT); demonstrate the proof-of principle for the direct reduction of Mg from its oxide using an oxygen ion-conductiong membrane electrolytic process (NATT); development of commercial titanium powder production using continuous, molten salt processing (NATT).

Keywords: Primary Metal, Low Cost, Reduction Technologies

120. **RECYCLING**
$550,000
DOE Contact: Joseph Carpenter, (202)586-1022
ORNL Contact: Phil Sklad, (423) 574-5069
ANL Contact: George Fenske, (630) 252-5190
Laboratory Partners: PNNL, ANL, Albany Research Laboratory
Industry Partners: Aluminum Association, Garfield Alloys, Alcoa

The objectives of this effort include: to develop cost competitive technologies for sorting shredded aluminum automotive scrap; to demonstrate color etching technology for separation of wrought aluminum alloys (NATT); to determine optimum processing to achieve virgin die cast properties for magnesium alloys from recycled scrap (NATT); to demonstrate technology for separating cast and wrought aluminum alloys and the separation of zinc from the aluminum recycling stream (NATT); to investigate cost-effective technologies for recycling polymer composites.

Keywords: Recycle, Scrap, Sorting

121. **STRUCTURAL RELIABILITY OF LIGHTWEIGHT GLAZING ALTERNATIVES**
$250,000
DOE Contact: Joseph Carpenter, (202) 586-1022
ORNL Contact: Phil Sklad, (423) 574-5069
PNNL Contact:M. A. Khaleel, (509) 375-2438
Laboratory Partners: PNNL
Industry Partners:Visteon

The objective of this project is to develop numerical modeling and simulation tools to evaluate the structural behavior and reliability of lightweight, thin glazing designs (NATT).

Keywords: Lightweight Materials, Glazing, Modeling, Simulation

ELECTRIC DRIVE VEHICLE TECHNOLOGIES

ADVANCED BATTERY MATERIALS

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

122. **ADVANCED ELECTRODE RESEARCH**
$300,000
DOE Contact: Ray Sutula, (202) 586-8064
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 been developed. Greatly improved utilization of the active material in the range of 80-90 percent for the reaction $2Li + S \Rightarrow Li_2S$ was obtained, corresponding to capacities of 1350-1500 mAh/g sulfur.

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

123. **ELECTROCHEMICAL PROPERTIES OF SOLID-ELECTROLYTES**
$200,000
DOE Contact: Ray Sutula, (202) 586-8064
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. Conductivities as high as 10^{-6} S/cm at 80°C were obtained with two-phase nanocomposite mixtures with no added salt or plasticizers, comparable to, or greater than, that of recently developed, dry, single-ion conducting polymers

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

124. **PREPARATION AND CHARACTERIZATION OF NEW POLYMER ELECTROLYTES**
$210,000
DOE Contact: Ray Sutula, (202) 586-8064
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. The thermal and transport property study on Parel (high-MW PPO)/$LiCF_3SO_3$ was completed.

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

125. **NEW CATHODE MATERIALS**
$73,000
DOE Contact: Ray Sutula, (202) 586-8064
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. The range of structures formed by vanadium oxides was determined, and some structures that may be good models for manganese oxides were identified.

Keywords: Intercalation Electrodes, Rechargeable Batteries

126. **DEVELOPMENT OF NOVEL ELECTROLYTES FOR RECHARGEABLE LITHIUM CELLS**
$100,000
DOE Contact: Ray Sutula, (202) 586-8064
Delaware State University Contact: K. Wheeler, (302) 739-4934

The objective of this project is to investigate alternative electrolytes for rechargeable lithium batteries. Families of chloroaluminate-based ionic liquids were considered. The electrolyte component, 1-ethyl-3-methylimidazolium tetrachloroaluminate, was synthesized using non-aqueous, inert atmosphere techniques.

Keywords: Intercalation Electrodes, Rechargeable Batteries

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

127. **CARBON ELECTROCHEMISTRY**
$250,000
DOE Contact: Ray Sutula, (202) 586-8064
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. An electrochemical cell was fabricated and used for *in situ* ellipsometry studies of the carbon/electrolyte interface in 1 M $LiPF_6$ + ethylene carbonate-dimethyl carbonate. Detectable changes in the ellipsometry parameters (D and Y) were measured at potentials near 1.5 V, where a high cathodic current was observed on a carbon film electrode.

Keywords: Carbon, Li Batteries, Li Intercalation

128. **FABRICATION & TESTING OF CARBON ELECTRODES AS LITHIUM INTERCALATION ANODES**
$75,000
DOE Contact: Ray Sutula, (202) 586-8064
LLNL 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. The Li intercalation capacities of fluid coke and the Santa Maria coke were found to have x-values (in Li_xC_6) of 0.65 and 0.83, respectively. The capacity for Santa Maria coke is among the highest observed for untreated coke materials.

Keywords: Carbon, Li Batteries, Intercalation

129. **REACTIVITY AND SAFETY ASPECTS OF CARBONACEOUS ANODES IN LITHIUM-ION BATTERIES**
$140,000
DOE Contact: Ray Sutula, (202) 586-8064
University of Michigan Contact: Abbas Nazri, (810) 986-0737

The objective of this research is to investigate the chemical, electrochemical and safety aspects of carbon anodes used in Li-ion batteries, and to identify the reaction products that form during charge discharge cycling. Twelve electrolytes and eleven graphitic materials were analyzed to determine the quantity and identity of gaseous species produced during initial charge/discharge cycles. A direct correlation was established between electrochemical capacity and ratio of basal plane area to edge area of graphitic materials.

Keywords: Carbon, Li Batteries, Li Intercalation, Electrolyte Decomposition

130. **BATTERY MATERIALS: STRUCTURE AND CHARACTERIZATION**
$140,000
DOE Contact: Ray Sutula, (202) 586-8064
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 lithium manganese oxides and nickel oxide electrodes. Both *in situ* XRD and XAS studies were used to study mixed cation oxides in rechargeable lithium cells, and the role of both transition metals in mixed cation oxides was elucidated for Ni- and Cu- substituted manganese spinels.

Keywords: Electrodes, Batteries, EXAFS

131. **COMPOSITE POLYMER ELECTROLYTES FOR USE IN LITHIUM AND LITHIUM-ION BATTERIES**
$100,000
DOE Contact: Ray Sutula, (202) 586-8064
North Carolina State University Contact: S. Khan, (919) 515-4519

The goal of this research is to prepare and characterize a new class of composite polymer electrolytes based on a combination of an inorganic (e.g., high-surface-are silica) phase in a polymer matrix. The conductivity of composite electrolytes was found to be independent of silica surface chemistry, and decreased only slightly with silica weight fraction. In all cases the conductivity exceeded 10^{-3} S/cm at room-temperature.

Keywords: Batteries, Electric Vehicles, Polymeric Electrolytes

132. **POLYMER ELECTROLYTE FOR AMBIENT TEMPERATURE TRACTION BATTERIES: MOLECULAR LEVEL MODELING FOR CONDUCTIVITY OPTIMIZATION**
$99,000
DOE Contact: Ray Sutula, (202) 586-8064
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. Ab-initio electronic structure calculations are showing excellent correlation with the few experimental data available on trapping barriers. Experimental analysis of carbonate-based electrolytes demonstrated that the importance of mobility is generally greater than that of ion screening.

Keywords: Batteries, Electric Vehicles, Polymeric Electrolytes

133. **ANALYSIS AND SIMULATION OF ELECTROCHEMICAL SYSTEMS**
$255,000
DOE Contact: Ray Sutula, (202) 586-8064
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. Short-time experiments with intercalation electrodes have been fitted by a mathematical model using computer simulations and yielded reasonably constant fundamental diffusion coefficients of the Stephan-Maxwell transport equations.

Keywords: Electrochemical Phenomena, Galvanostatic Charge/Discharge

134. **CORROSION OF CURRENT COLLECTORS IN RECHARGEABLE LITHIUM BATTERIES**
$200,000
DOE Contact: Ray Sutula, (202) 586-8064
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. Serious corrosion of Al current collectors in Li-polymer batteries during overcharging was identified in three types of cells: (a) Li/V_6O_{13} (composite electrode), (b) Li/TiS_2 (composite electrode), and (c) Li/V_6O_{13} (thin-film electrode).

Keywords: Current Collectors, Advanced Batteries

135. **ELECTRODE SURFACE LAYERS**
$200,000
DOE Contact: Ray Sutula, (202) 586-8064
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. Raman bands at 450 cm^{-1} and at 480 and 560 cm^{-1} were obtained for the reduced and oxidized $Ni(OH)_2$ films, respectively, which are in perfect agreement with the literature data and the previously reported results for thinner films.

Keywords: Ion Implantation, Electrodes, Rechargeable Batteries

136. **MICROSTRUCTURAL MODELING OF HIGHLY POROUS NiMH BATTERY SUBSTRATES**
$145,000
DOE Contact: Ray Sutula, (202) 586-8064
University of Michigan Contact: Ann Marie Sastry, (313) 764-3061

The objective of this research is to develop predictive capability for determining performance of Li-ion negative substrates, comprised of fibrous and particulate carbon, using combined stochastic-mechanical simulation. A novel stochastic network generation technique was developed, with sufficient simulations performed to model the effects of manufacturing parameters upon important descriptors of connectivity.

Keywords: MH/NiOOH Batteries, Modeling, Microstructural Characterization

137. **ELECTRODE SURFACE LAYERS**
$100,000
DOE Contact: Ray Sutula, (202) 586-8064
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 understanding at the molecular level of the reactions that occur at the Li/electrolyte interface to form the solid electrolyte interfacial (SEI) layer. Measurements indicate that Li reacts with water vigorously even at 160 K with LiOH as the majority reaction product in the presence of excess surface water.

Keywords: Spectrographic Analysis, Electrocatalysts, Electrooxidation

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

138. **DEVELOPMENT OF A THIN-FILM RECHARGEABLE LITHIUM BATTERY FOR ELECTRIC VEHICLES**
$71,000
DOE Contact: Ray Sutula, (202) 586-8064
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. $LiMn_2O_4$ sheets near theoretical density ($4.3 g/cm^3$) with 1–5 mm grains have been fabricated using well-milled powders and a small amount of V_2O_5 as a low -temperature sintering aid. Project has been completed.

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

139. **OPTIMIZATION OF METAL HYDRIDE PROPERTIES IN MH/NiOOH CELLS FOR ELECTRIC VEHICLE APPLICATIONS**
$90,000
DOE Contact: Ray Sutula, (202) 586-8064
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 micro-encapsulation of hydrogen storage alloys metal hydride electrodes for MH/NiOOH batteries. The three-step process for electroless plating of Ni, Ni-P, Co and Co-P has been simplified to a one-step process eliminating the costly activation step with palladium and tin chloride.

Keywords: MH/NiOOH Batteries, Hydrogen Storage, $LaNi_4.27Sn^{0.24}$ Alloy, Microencapsulation

140. **PREPARATION OF IMPROVED, LOW COST METAL HYDRIDE ELECTRODES FOR AUTOMOTIVE APPLICATIONS**
$200,000
DOE Contact: Ray Sutula, (202) 586-8064
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 crystal structure of $LaNi_{3.55}Co_{0.75}Mn_{0.4}Al_{0.3}$ and its thermal expansion coefficient were determined from 10 to 300K.

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

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

Research is conducted on the kinetics and mechanisms of the electrode reactions in low temperature polymer electrolyte membrane (PEM) fuel cells. Based on these results new electrocatalysts are being developed using a material-by-design approach. Multimetallic catalysts are synthesized under carefully controlled conditions producing tailor-made surfaces. Surface composition and structure is determined using a combination of surface analytical techniques, Low Energy Electron Diffraction (LEED), Low Energy Ion Scattering (LEIS) and Auger Electron Spectroscopy (AES). It was found that a new Pt75Mo25 alloy electrocatalyst produced the highest level of CC-tolerance (electrooxidation of H_2 in the presence of small amounts of CO) in a PEM fuel cell anode of any material yet investigated. Even more promising multimetallic systems are under development.

Keywords: Spectrographic Analysis, Electrocatalysts, Electrooxidation

142. **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 and platinum alloys constitute the family of electrocatalysts for high-performance PEM fuel cells. However, with CO-containing reformate fuelds, CO 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) resulting from CO in reformate, or the direct CH_3OH electrooxidation on PT-based electrocatalysts by NMR, and to use this information in the identification of improved electrocatalysts. The unwanted coupling of the NMR sample to the coil was eliminated, thereby permitting the acquisition of meaningful NMR spectra of fuel-cell electrode surface species under open-circuit conditions and strongly suggesting the possibility of acquiring spectra under conditions of *in situ* electrode potential control. NMR coupled to electrochemical experiments has resulted in the identification of three adsorbed CO species, the conditions under which they are formed and their electrochemical behavior on Pt/C, Pt-RU/C and Pt-Sn/C. Important differences in the behavior of CO on these electrocatalysts have been identified using the NMR-electrochemical methods we have developed.

Keywords: NMR, Electrooxidation, Fuel Cells

HEAVY VEHICLE PROPULSION SYSTEM MATERIALS

The Office of Transportation Technologies, Office of Heavy Vehicle Technologies (OTT OHVT), recognizes a significant opportunity for reduction in petroleum consumption by dieselization of pickup trucks, vans, and sport utility vehicles. Application of the diesel engine to class 1, 2, and 3 trucks is expected to yield a 35 percent increase in fuel economy per vehicle. The foremost barrier to diesel use in this market is emissions control. Once an engine is made certifiable, subsequent challenges will be in cost; noise, vibration, and harshness (NVH); and performance.

OTT OHVT also has an active program to develop by 2001 the technology for advanced LE-55 diesel engines with 55 percent efficiency and low emissions levels of 2.0 g/bhp-h NO_x and 0.05 g/bhp-h particulates. The goal is also for the LE-55 engine to run on natural gas with an efficiency approaching that of diesel fuel.

The design of advanced components for high-efficiency diesel engines has, in some cases, pushed the performance envelope for materials of construction past the point of reliable operation. Higher mechanical and tribological stresses and higher temperatures of advanced designs limit the engine designer; advanced materials allow the design of components that may operate reliably at higher stresses and temperatures, thus enabling more efficient engine designs. Advanced materials also offer the opportunity to improve the emissions, NVH, and performance of diesel engines for pickup trucks, vans, and sport utility vehicles.

The purpose of the Heavy Vehicle Propulsion System Materials Program is to develop enabling materials technology to support the dieselization of class 1-3 trucks to achieve a 35 percent fuel economy improvement over current gasoline-fueled trucks and to support fuel-flexible LE-55 low-emissions, high-efficiency diesel engines for class 7-8 trucks.

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

143. **COST-EFFECTIVE SMART MATERIALS FOR DIESEL ENGINE APPLICATIONS**
$400,000
DOE Contact: Sidney Diamond, (202) 586-8032
ORNL Contact: D.R. Johnson, (423) 576-6832
ORNL Contact: J.O. Kiggans, Jr., (423) 574-8863

There are two major objectives of this research element. The first is to evaluate the cost- effectiveness and maturity of various "Smart Materials Technologies" under consideration for diesel engine applications, such as fuel injection systems. The second consideration is to develop "Smart Materials" to be incorporated into working actuators and sensors.

Keywords: Cost Effective Ceramics, Sensors, Smart Materials

144. **COST-EFFECTIVE SINTERING**
$144,000
DOE Contact: Sidney Diamond, (202) 586-8032
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, mixed oxides, carbides, and cermets through the development of continuous sintering techniques.

Keywords: Cermets, Cost Effective Ceramics, Oxides, Silicon Nitride, Sintering

145. **LOW COST, HIGH TOUGHNESS CERAMICS**
$350,000
DOE Contact: Sidney Diamond, (202) 586-8032
ORNL Contact: D.R. Johnson, (423) 576-6832
ORNL Contact: T.N. Tiegs, (423) 574-5173

Significant improvements in the reliability of structural ceramics for advanced diesel engine applications could be attained if the critical fracture toughness, (K_{Ic}), were increased without strength degradation. 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. Currently, studies on toughening of ceramics by two methods, microstructure development in oxide-based ceramics and incorporation of ductile intermetallic phases, have been initiated.

Keywords: Composites, Intermetallics, Mullite, Toughened Ceramics

146. **INTERMETALLIC-BONDED CERMETS**
$60,000
DOE Contact: Sidney Diamond, (202) 586-8032
ORNL Contact: D.R. Johnson, (423) 576-6832
ORNL Contact: P.F. Becher, (423) 574-5157

The goal of this task is to develop materials for diesel-engine applications, specifically for fuel-delivery systems and wear components (e.g., valve seats and turbocharger components).

Keywords: Cermets, Composites, Diesel, Intermetallics

147. **CHARACTERIZATION/TESTING OF LOW CTE MATERIALS**
$100,000
DOE Contact: Sidney Diamond, (202) 586-8032
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 $Ba_{1+x}Zr_4P_{6-2x}Si_{2x}O_{24}$ 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

148. **INSULATING STRUCTURAL CERAMICS FOR HIGH EFFICIENCY, LOW EMISSION ENGINES**
$0
DOE Contact: Sidney Diamond, (202) 586-8032
ORNL Contact: D.R. Johnson, (423) 576-6832
Caterpillar Contact: M.C. Long, (309) 578-8672

The overall objective of this 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

149. **THICK THERMAL BARRIER COATINGS (TTBCS) FOR LOW EMISSIONS, HIGH EFFICIENCY DIESEL ENGINE COMPONENTS**
$0
DOE Contact: Sidney Diamond, (202) 586-8032
ORNL Contact: D.R. Johnson, (423) 576-6832
Caterpillar Contact: M. Brad Beardsley, (309) 578-8514

The objective of this program is to develop cost-effective, durable, thick thermal barrier coating (TTBC) systems for use in higher-efficiency and lower-emissions diesel engines.

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

150. **MATERIALS FOR LOW EMISSIONS, HIGH EFFICIENCY DIESEL ENGINE COMPONENTS**
$605,000
DOE Contact: Sidney Diamond, (202) 586-8032
ORNL Contact: D.R. Johnson, (423) 576-6832
Cummins Contact: Paul Becker, (812) 377-4701

The goal of this 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

151. **MATERIALS FOR LOW EMISSIONS, HIGH EFFICIENCY DIESEL ENGINE COMPONENTS**
$750,000
DOE Contact: Sidney Diamond, (202) 586-8032
ORNL Contact: D.R. Johnson, (423) 576-6832
Detroit Diesel Contact: Yuri Kalish, (313) 592-7825

In this program, DDC will investigate the feasibility of using a smart-materials-based actuator in place of a solenoid for fuel injection actuation.

Keywords: Ceramics, Components, Diesel, Engines, Intermetallics, Smart Materials

152. **HIGH STRENGTH MATERIALS FOR DIESEL ENGINE FUEL INJECTORS**
$0
DOE Contact: Sidney Diamond, (202) 586-8032
ORNL Contact: D.R. Johnson, (423) 576-6832
Cummins Contact: Thomas Yonushonis, (812) 377-7078

The objective of this effort is to develop advanced ceramics and cermet materials for diesel fuel injector components. The effort concentrates on developing cost-effective materials systems that have superior strength, fracture toughness, beat-in resistance, scuffing resistance, corrosion resistance, and wear resistance compared to existing material systems.

Keywords: Ceramics, Cermets, Components, Diesel

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

153. **DIESEL EXHAUST CATALYST CHARACTERIZATION**
$200,000
DOE Contact: Sidney Diamond, (202) 586-8032
ORNL Contact: D.R. Johnson, (423) 576-6832
ORNL Contact: L.F. Allard, (423) 574-4981

The purpose of this work is to use analytical and high-resolution transmission electron microscopy (TEM) to characterize the microstructures of emission control catalysts. Emphasis is placed on relating micro-structural changes to performance of diesel NO_x reduction catalysts. The research is focussed on understanding these changes through TEM studies of experimental catalyst materials reacted in an ex situ catalyst reactor system especially constructed to allow appropriate control of the reaction conditions and the transfer of the sample between reactor and microscope.

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

154. **LIFE PREDICTION VERIFICATION**
$200,000
DOE Contact: Sidney Diamond, (202) 586-8032
ORNL Contact: D.R. Johnson, (423) 576-6832
ORNL Contact: A.A. Wereszczak, (423) 574-7601

The first goal of the proposed research program is to generate mechanical-engineering data from ambient to high temperatures for candidate structural ceramics, to characterize failure phenomena in these ceramics and components fabricated from them, and the application and verification of probabilistic life- prediction methods using diesel engine components as test cases. The second goal of this effort is to characterize the evolution and role of damage mechanisms, and changes in the microstructure linked to the ceramic's mechanical performance, at representative engine component service conditions. Lastly, numerical probabilistic models (i.e., life-prediction codes) will be used in conjunction with the generated strength and fatigue data to predict the failure probability and reliability of complex-shaped components, such as a silicon nitride diesel valve, subjected to mechanical loading.

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

155. **HIGH TEMPERATURE TENSILE TESTING**
$0
DOE Contact: Sidney Diamond, (202) 586-8032
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 advanced diesel engine materials 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: Advanced Materials, Creep, Diesel, Fracture, Microscopy, Silicon Nitride, Tensile Testing

156. **COMPUTED TOMOGRAPHY**
$120,000
DOE Contact: Sidney Diamond, (202) 586-8032
ORNL Contact: D.R. Johnson, (423) 576-6832
Argonne National Lab Contact: W.A. Ellingson, (312) 972-5068

The objective of this project was redefined to study 3D X-ray CT densitometry reliability relative to detection of density variations in GS-44 with chopped carbon fibers. GS-44 with chopped carbon fibers is being developed as a material for diesel engine valve guides with reduced wear. Caterpillar Technical Center is a cooperating partner. The nondestructive evaluation approach taken utilized 3D X-ray computed tomographic imaging technology with an emphasis on correlation of image data with destructive analysis. However, since this material is not performing as initially predicted, this work is again being refocussed.

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

157. **ON-MACHINE INSPECTION**
$0
DOE Contact: Sidney Diamond, (202) 586-8032
ORNL Contact: D.R. Johnson, (423) 576-6832
Caterpillar Contact: M.K. Haselkorn, (309) 578-6224

A nondestructive evaluation (NDE) method is needed to quantify the effect of abrasive machining parameters on the performance of a ceramic component. Quantifying this effect will enable the optimization of a machining process for both surface quality and processing time. Elastic optical scattering techniques can identify both surface and near-surface defects in silicon nitride. The overall objective of this program is to determine relationships between the elastic optical scattering results and surface and flexural strength of machined sintered reaction bonded and sintered silicon nitride specimens.

Keywords: Machining, Nondestructive Evaluation, Silicon Nitride, Structural Ceramics

158. **INTERNATIONAL EXCHANGE AGREEMENT (IEA)**
$200,000
DOE Contact: Sidney Diamond, (202) 586-8032
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 9, Thermal Shock, and Subtask 10, Ceramic Powder Characterization.

Keywords: IEA, Powder Characterization

159. **STANDARD REFERENCE MATERIALS**
$200,000
DOE Contact: Sidney Diamond, (202) 586-8032
ORNL Contact: D.R. Johnson, (423) 576-6832
NIST Contact: L.-S. Lum, (301) 975-3674

This objective of this project is to tighten and finalize procedures for the characterization of secondary properties of powders. There are four focus areas relating to the secondary properties: dispersion of powders from slurry preparation, slurry preparation, spray-dried powders, and green body evaluation.

Keywords: IEA, Reference Material, Powder Characterization

160. **MECHANICAL PROPERTY STANDARDIZATION**
$100,000
DOE Contact: Sidney Diamond, (202) 586-8032
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 Propulsion System Materials Program.

Keywords: Mechanical Properties, Test Procedures

TECHNOLOGY TRANSFER AND MANAGEMENT COORDINATION

161. **TECHNICAL PROJECT MANAGEMENT**
$565,000
DOE Contact: Sidney Diamond, (202) 586-8032
ORNL Contact: D.R. Johnson, (423) 576-6832

The objective of this effort is to assess the materials technology needs for high-efficiency diesel engines, formulate technical plans to meet these needs, and prioritize and implement a long-range research and development program.

Keywords: Advanced Heat Engines, Alloys, Cermets, Coordination, Diesel, Intermetallics, Management, Structural Ceramics

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

162. **DURABILITY OF DIESEL ENGINE COMPONENT MATERIALS**
$200,000
DOE Contact: Sidney Diamond, (202) 586-8032
ORNL Contact: D.R. Johnson, (423) 576-6832
ORNL Contact: P.J. Blau, (423) 574-5377

The purpose of this task is to enable the development of more durable, low-friction moving diesel engine parts for heavy vehicle propulsion systems by conducting friction, lubrication, and wear assessments and analyses on advanced materials, surface treatments, and coatings. The scope of materials and coatings is broad and includes any metallic alloy, intermetallic compound, ceramic, or composite material which is likely to be the best-suited for the given application. Parts of current interest include valves, valve guides, and fuel injector plungers. The technical approach is to use bench-scale simulations of the rubbing conditions in diesel engine environments to study the accumulation of surface damage, and to correlate this behavior with the properties and compositions of the surface species.

Keywords: Alloys, Coatings, Composites, Components, Diesel, Intermetallics, Silicon Nitride, Structural Ceramics, Wear

163. **ADVANCED MACHINING/MANUFACTURING**
$225,000
DOE Contact: Sidney Diamond, (202) 586-8032
ORNL Contact: D.R. Johnson, (423) 576-6832
ORNL Contact: S.B. McSpadden, Jr.,
(423) 574-5444

The objective of this effort is to develop and demonstrate optimized grinding processes for the production of difficult-to-machine components for use in diesel engines.

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

164. **LASER-BASED NDE METHODS**
$80,000
DOE Contact: Sidney Diamond, (202) 586-8032
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

OFFICE OF POWER TECHNOLOGIES

	FY 1998
Office of Power Technologies - Grand Total	$59,462,600
Office of Solar Energy Conversion	$26,290,000
Photovoltaic Technology Division	$26,290,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$16,942,000
Amorphous Silicon for Solar Cells	2,080,000
Polycrystalline Thin Film Materials for Solar Cells	13,920,000
Deposition of III-V Semiconductors for High-Efficiency Solar Cells	942,000
Materials Properties, Behavior, Characterization or Testing	$ 5,500,000
Materials and Device Characterization	$ 5,500,000
Device or Component Fabrication, Behavior or Testing	$ 3,848,000
High-Efficiency Crystalline Silicon Solar Cells	3,848,000
Office of Geothermal Technologies	$672,600
Materials Preparation, Synthesis, Deposition, Growth or Forming	$124,400
Thermally Conductive Composites for Heat Exchangers	124,400
Materials Properties, Behavior, Characterization or Testing	$548,200
Advanced High Temperature Geothermal Well Cements	125,000
Elastomer/Metal Bonding	99,400
Advanced Coating Materials	188,800
Thermally Conductive Cementitious Grouts for Geothermal Heat Pumps	135,000
Office of Energy Management	$32,500,000
Advanced Utility Concepts Division	$32,500,000
High Temperature Superconductivity for Electric Systems	$32,500,000
Device or Component Fabrication, Behavior or Testing	$32,500,000
The Superconductivity Partnership Initiative	14,500,000
The 2nd Generation Wire Initiative	8,000,000
Strategic Research	10,000,000

OFFICE OF POWER TECHNOLOGIES

OFFICE OF SOLAR ENERGY CONVERSION

PHOTOVOLTAIC 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

165. **AMORPHOUS SILICON FOR SOLAR CELLS**
$2,080,000
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 (4000 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 photovoltaic modules with cost under \$50/m^2 and with 30-year lifetime. This will allow an entire system lifetime energy cost of under \$0.06/kWh. Achievement of this goal will allow wide competition of silicon-based PV in large-scale distributed power scenarios.

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

166. **POLYCRYSTALLINE THIN FILM MATERIALS FOR SOLAR CELLS**
$13,920,000
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 (4000 cm^2) areas. The films are deposited by chemical and physical vapor deposition, electrodeposition and sputtering. The long term goal of this effort is to develop the technology for 15 percent efficient photovoltaic modules with cost under \$50/m^2 and with 30-year lifetime. This will allow an entire system lifetime energy cost of under \$0.06/kWh. Achievement of this goal will allow these technologies to compete favorably in large-scale distributed power scenarios.

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

167. **DEPOSITION OF III-V SEMICONDUCTORS FOR HIGH-EFFICIENCY SOLAR CELLS**
$942,000
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 is to develop multi-junction GaAs-based cells that will attain 38 percent efficiency under high concentration.

Keywords: Semiconductors, Chemical Vapor Deposition, Solar Cells

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

168. **MATERIALS AND DEVICE CHARACTERIZATION**
$5,500,000
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, Solar Cells

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

169. **HIGH-EFFICIENCY CRYSTALLINE SILICON SOLAR CELLS**
$3,848,000
DOE Contact: Jeffrey Mazer, (202) 586-2455
NREL Contact: John Benner, (303) 384-6496
SNL Contact: Margie Tatro, (505) 844-3154

This project performs applied research upon crystalline silicon devices to improve solar-to-electric conversion efficiency. The project employs new and improved dopant profiles, back-surface fields, and bulk passivation treatments to reduce electron-hole recombination at cell surfaces and in the bulk. Control of point defects in crystalline silicon is being studied by a variety of techniques, and is thoroughly discussed at the annual NREL-sponsored Silicon Devices Conference. Additionally, improved light-trapping surface treatments for thin cells (~50 to 100 microns thick), and improved methods for inexpensive silver-paste contact screen printing are also under development. One of the major goals of this project is to develop a rapid-thermal-processing (RTP)-based, screen-printed-contact, photolithography-free protocol that will yield 18 percent efficient 100 cm^2 cells on multi-crystalline material in a commercial production environment.

Keywords: Semiconductors, Solar Cells, Crystal Silicon

OFFICE OF GEOTHERMAL TECHNOLOGIES (OGT)

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 OGT-sponsored materials research and development.

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

170. **THERMALLY CONDUCTIVE COMPOSITES FOR HEAT EXCHANGERS**
$124,400
DOE Contact: R. LaSala, (202) 586-4198
BNL Contact: M.L. Allan, (516) 344-3060

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 composite material if sufficient heat transfer and anti-fouling properties can be achieved. The work consists of determination 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 antioxidant, SiC fillers and low surface energy additives on the fouling coefficient and scale adhesion are also being evaluated.

Field tests with flowing hypersaline brine under heat exchange conditions in conjunction with NREL were performed to evaluate the following coatings:

- Styrene/TMPTMA/SiC/antioxidant over zinc phosphate
- Styrene/TMPTMA/SiC over zinc phosphate
- Polyphenylene sulfide over zinc phosphate
- Polyphenylene sulfide/SiC over zinc phosphate

- Polyphenylene sulfide/Polytetrafluoroethylene/ SiC over zinc phosphate

Results of the field tests showed that all of the coatings prevented corrosion of the mild steel heat exchanger tubes. Scaling still occurred and hydrothermal oxidation of the coatings was observed. Addition of PTFE to PPS imparted reduced adhesion of scale to the coating. This resulted in easier scale removal by hydroblasting. The enhanced ability to remove scale is an important consideration since it increases time between cleaning cycles and thus reduced maintenance costs. Current research is examining the mechanisms of scale interaction with the candidate coatings and further field tests in high temperature, acidified brine are planned. 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: Thermally Conductive Composites, Polymers, Corrosion, Heat Transfer, Heat Exchanger Tubes, Scale Resistance

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

171. **ADVANCED HIGH TEMPERATURE GEOTHERMAL WELL CEMENTS**
$125,000
DOE Contact: R. LaSala, (202) 586-4198
BNL Contact: M.L. Allan, (516) 344-3060

Well cements that are chemically and thermally resistant to geothermal brines containing high concentrations of CO_2 are vital to ensuring well integrity and durability. This task focuses on formulating and testing calcium phosphate-based cements to withstand high temperature, high CO_2 and acidic conditions. Emphasis is being placed on phase chemistry, and the mechanical, physical, and chemical resistance properties of the cured materials.

Cost-shared R&D between BNL, Halliburton Services and Unocal to develop cementing materials produced by acid-base reactions between fly ash-blended calcium aluminate cements and phosphate-containing compounds was continued. Several candidate systems were evaluated. Studies of the cementing phases formed, microstructure developed, carbonation rate, and changes in strength after long term exposure to CO_2 solutions at 280°C were performed. Several wells in Indonesia were successfully completed with the developed cements. Ongoing research will continue to monitor the performance of the cements exposed in the Indonesian wells and examine how the acid resistance of calcium phosphate cements can be improved.

Keywords: Cements, Material Degradation, Strength, Drilling, Carbonation, Well Completions

172. **ELASTOMER/METAL BONDING**
$99,400
DOE Contact: R. LaSala, (202) 586-4198
BNL Contact: M.L. Allan, (516) 344-3060

If the goals for reducing the costs for geothermal wells are to be met, it is essential that a number of advanced high temperature elastomer-containing tools such as drillpipe protectors, blow-out-preventors, rotating head seals, and downhole drill motor stators become available. The lack of a hydrolytically stable chemical coupling system needed to bond high temperature elastomers to metal is an impediment to these goals. The objective for this activity was to identify and characterize one or more promising bonding systems. Contingent upon success, future work would involve establishment of cost-shared programs with tool manufactures to fabricate and test prototype components.

Different adhesives were evaluated for bonding ethylene propylene diene terpolymer (EPDM) to stainless steel substrates. These included hot melt polyphenyl-ethersulfone (PES), epoxy resin, polyurethane, polyamide, polyimide, and phenolformaldeyhde resin. The PES was found to maintain the best adhesion when the elastomer/metal joints were exposed to steam at 200°C. The EPDM-to-SS adhesive joint specimens were left intact after exposure for 70 days exposure and had a 180°-peel strength of 10.3 lb/in, corresponding to ~40 percent loss in bond strength over the unexposed control specimens. The main reason for loss of bond strength was accounted for the hydrothermal oxidation of PES adhesive, leading to the conformational transformation of sulfone groups within the PES into sulfonic acid derivative. This acid derivative favorably reacted with Fe in the SS to yield water-soluble $Fe_2(SO_4)_3$ reaction products. It is desirable to reduce the degree of hydrothermal oxidation to improve the long term durability of the adhesive. In addition, modification of PES with liquid crystalline polymers may be useful for improving toughness.

Keywords: Elastomers, Adhesion, Drillpipe Protectors, Bonding

173. **ADVANCED COATING MATERIALS**
$188,800
DOE Contact: R. LaSala, (202) 586-4198
BNL Contact: M.L. Allan, (516) 344-3060

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 composites, developed in other parts of the Geothermal Materials Development Program, as corrosion protective systems for use in brine dominated geothermal electric generation processes. 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.

Several different coating types, application methods and end uses were explored. This included thermal sprayed Ni-Al coatings for safe ending heat exchanger tubes, slurry and CVD coatings for turbines and vent gas blowers and polyphenylene sulfide-based coatings for various components exposed to brine. The Ni-Al coatings were found to be subject to corrosion when coupled to thermally conductive liners on heat exchanger tubes. Therefore, polymer-based alternatives are being sought. Some of the slurry and CVD coatings showed promising potential for corrosion protection in geothermal brines. The addition of polytetrafluoroethylene to PPS coatings was investigated and found to be beneficial. Future work will explore PPS alloy and blend coatings and thermal spraying of PPS for in-situ application to components.

Keywords: Corrosion Protection, Polymers, Ceramics, Composites, Coatings, CVD, Plasma Spraying

174. **THERMALLY CONDUCTIVE CEMENTITIOUS GROUTS FOR GEOTHERMAL HEAT PUMPS**
$135,000
DOE Contact: R. LaSala, (202) 586-4198
BNL Contact: M.L. Allan, (516) 344-3060

Ground heat exchangers used with geothermal heat pumps (GHPs) rely on a backfill material to provide heat transfer between the polyethylene U-tube and surrounding formation. Critical properties of the backfill grout are thermal conductivity, cost, ease of placement, impermeability, shrinkage resistance, bonding to U-tube and formation, and durability. By increasing the thermal conductivity of the grouting material the required length of the heat exchanger can be decreased and this results in decreased installation costs in addition to improved GHP performance.

Brookhaven's research is focused on formulating economic superplasticized cement-silica sand grouts to meet the property requirements for backfilling GHP boreholes. The effects of sand gradation and proportion on properties such as thermal conductivity, permeability, shrinkage, coefficient of thermal expansion, bond strength, leach resistance and durability have been investigated. Thermal conductivities up to three times higher than conventional grouts were achieved. Cost analysis and the impact of the developed thermally conductive grouts on heat exchanger length design were conducted in collaboration with the University of Alabama and showed significant potential reduction in bore length.

Effort in FY98 concentrated on field demonstration of the grouts at Oklahoma State University and Sandia National Laboratories, investigation of how the bonding between U-loop and grout is affected by temperature and thermal cycles, potential means of enhancing bonding, freeze-thaw resistance of grout and the feasibility of using non-destructive methods for studying and verifying the bonding characteristics in the coupled loop/grout/formation system. The grout was used to complete a total of four 250 ft. boreholes which are currently under test. Bentonite grouts are also being tested at the same sites. Based on the first field test at OSU, the grout formulation was modified to improve pumpability for the test at Sandia. The Sandia tests will determine the performance of the grout in arid environments. The long-term field performance of the grouts will be assessed in FY99.

Based on the improved bonding characteristics, resistance to cracking under thermal cycles and reduced grout/U-loop coefficient of permeability, the New Jersey Department of Environmental Protection approved a particular formulation of superplasticized cement-sand grout for use in consolidated and unconsolidated formations. The DEP has requested further surveillance to confirm hydraulic sealing by the grout and this will be investigated in FY99. In-situ infiltration tests of grouted boreholes which will take into account the differences in temperatures in the loop legs and thermal gradients are proposed. BNL will also be involved in training loop installers in mixing the developed grouting material.

Keywords: Geothermal Heat Pumps, Cementitious Grouts, Backfill, Ground Heat Exchanger, Thermal Conductivity, Coefficient of Permeability

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.

HIGH TEMPERATURE SUPERCONDUCTIVITY FOR ELECTRIC SYSTEMS

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

175. THE SUPERCONDUCTIVITY PARTNERSHIP INITIATIVE

$14,500,000
DOE Contact: Jim Daley, (202) 586-1165

The Superconductivity Partnership Initiative (SPI) is an industry-led venture between the Department of Energy (DOE) and industrial consortia intended to accelerate the use of high temperature superconductivity (HTS) in energy applications. Each SPI team includes a vertical integration of non-competing companies that represent the entire spectrum of the research and development (R&D) cycle. That is, the teams include the ultimate user of the technology (an electric power company), as well as a major manufacturing company and a 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 amount includes DOE's share of the SPI design activities, as well as parallel HTS technology development that directly supports the SPI teams. In FY 1998, ongoing SPI efforts were supplemented by the initiation of several new projects resulting from a competitive solicitation issued in 1997. All of these projects will incorporate high-temperature superconducting wire.

Project subtasks are as follows:

A. Current Controller

The Current Controller project, led by General Atomics, continued with engineering design analysis, HTS magnet characterization, and prototype testing supported by Los Alamos National Laboratory (LANL). Field evaluation will occur at a Southern California Edison substation. Current controllers can be used on transmission and distribution systems to protect system components from damaging power surges caused by ground faults. Compared to conventional devices, HTS current controllers offer better protection and improved system flexibility, reliability and performance.

General Atomics Contact: Eddie Leung, (619) 455-4443

B. 1000 hp and 5000 hp Motors

The project, led by Rockwell Automation, advanced toward the objective of the development of a 1,000 horse-power (hp) HTS motor by 1999 and a 5,000 hp pre-commercial prototype HTS motor by 2001. Activities included modeling of heat transfer and flow stability, system analysis, and continued experimental studies of outgassing, engineering design analyses and characterization of component parts for the motor project. Superconducting motors can have a large impact on electrical energy utilization through reduced losses and size compared to conventional iron core motors. These reduced losses and the smaller size will be the driving force for the commercial introduction of superconducting motors in industrial applications.

Rockwell Automation Contact: David Driscoll, (216) 266-6002

C. Superconducting Transmission Cable

Southwire Company and Oak Ridge National Laboratory (ORNL) began construction of a 5 meter, single-phase demonstration HTS cable. As part of this effort, the conductor was fabricated, the cable testing laboratory at ORNL was completed, and the conductor, terminations, and vacuum-insulated pipe were assembled. This cable was tested at full current (1.25 kA) and voltage (12.5 kV), as well as at off-design conditions. Also, the conceptual design for a three-phase, 30 meter cable was completed.

Southwire Contact: R. L. Hughey, (770) 832-4984

D. Superconducting Transmission Cable

A team led by Pirelli Cables and Systems LLC began work on a two phase project to design, fabricate, install, and test a 120 meter, 3-phase, room-temperature dielectric HTS power system. Initial alternating current (AC) loss measurements were conducted on sections of the Pirelli cable. The HTS cable will lead to smaller, more efficient electricity transmission lines in utility networks.

Pirelli Contact: Muhjib Rahman, (803) 951-4010

E. Transformer

A team led by Waukesha Electric Systems, with members Intermagnetics General Corporation (IGC), ORNL, and Rochester Gas and Electric, completed the assembly and testing of the 1 MVA single-phase demonstration transformer. A full test plan was developed and implemented, culminating in a short-circuit test. In addition, conceptual design for a 5/10 MVA cryocooled HTS transformer was initiated. HTS transformers offer dramatically improved efficiency over existing large power transformers, with reduced fire risk and environmental impacts.

Waukesha Contact: Sam Mehta, (414) 547-0121

Keywords: Motor, Current Controller, Transmission Cable, Transformer

176. **THE 2ND GENERATION WIRE INITIATIVE**
$8,000,000
DOE Contact: Jim Daley, (202) 586-1165
Argonne National Laboratory Contact:
U. Balachandran, (630) 252-4250
Brookhaven National Laboratory Contact:
David Welch, (516) 282-3517
Los Alamos National Laboratory Contact:
Dean Peterson, (505) 665-3030
National Renewable Energy Laboratory
Contact: Richard Blaugher, (303) 384-6518
Oak Ridge National Laboratory Contact:
Robert Hawsey, (615) 574-8057
Sandia National Laboratory Contact:
Jim Voigt, (505) 845-9044
American Superconductor Contact:
Gilbert N. Riley, (508) 836-4200
Intermagnetics General Corp. Contact:
Paradeep Haldar, (518) 782-1122
Oxford Instruments, Inc. Contact:
K. R. Marken, (908) 541-1300
Oxford Superconducting Technology
Contact: Seung Hong, (732) 541-1300
3M Contact: Arnold Funkenbusch,
(651) 733-5071
University of Tennessee Space Institute
Contact: Joel Muehlhauser, (931) 393-7286
Stanford University Contact:
Robert H. Hammond, (415) 723-0169
Southwire Contact: R. L. Hughey,
(770) 832-4984

The 2nd generation Wire Initiative capitalizes on two processing breakthroughs announced in 1995 and 1996: the Ion-Beam Assisted Deposition (IBAD) process refined by LANL and the Rolling Assisted Biaxial Texturing (RABiTS) technique pioneered by ORNL. Since then, industry-led consortia have evolved to develop these techniques into viable commercial processes for making HTS wire. In FY 1998, this initiative funded collaborative research and development between the national laboratories and industry partners, and strategic research and development at the laboratories with a focus on improving the understanding of substrate preparation as well as buffer layer and superconductor deposition. Project subtasks are as follows:

A. Collaborative R&D Projects

(1) Metallo-Organic Chemical Vapor Deposition (MOCVD) - Investigation continued on the development of a MOCVD technique for deposition of long-length Yttrium-Barium-Copper Oxide (YBCO) conductors. The goal is to establish processing conditions to deposit buffer and superconducting layers on textured metallic substrates. The substrates, buffer, and superconducting layers will be characterized.

(2) Thick HTS films - Teams made significant progress in FY 1998 in the development of thick HTS films. The films will be deposited on flexible tapes containing oxide buffer layers deposited by IBAD. Continuing coated conductor efforts focused on studying novel buffers and improvements in the superconductor deposition.

(3) Substrate development - Efforts at producing long lengths (up to 100 m) of textured nickel tape with all the appropriate characteristics for subsequent film growth (buffer layer(s) and superconductor) were continued. Work on a two year project with the goal of producing 1 meter lengths of buffered, textured nickel (RABiTS) and YBCO on RABiTS with a target critical current density (J_c) of 80,000 A/cm^2 also got underway.

(4) IBAD Research - Program partners were completing the first phase of research on the IBAD approach. Electron beam evaporation is 3M's selected method of deposition of all the layers. ORNL worked to characterize bare, textured nickel and films grown by a variety of techniques, and

to develop buffer layer and superconductor deposition technology. ORNL continued pursuing a promising alternative to in-situ formation of the YBCO film, by electron beam co-evaporation of Y, Ba, and Cu. ORNL scientists worked on determining the thickness limits of epitaxial film formation, and assessing the feasibility of rapid precursor depositions for the ex-situ precursor reaction process.

(5) YBCO/RABiTS - Development and demonstration of the fabrication of lengths of YBCO/RABiTS using MOCVD technology continued. A major deliverable in FY 1998 was the demonstration of a 1 m length of YBCO, using a development reactor and pull-through tape transport. Mechanical and processing conditions needed to develop the desired surface texture and smoothness of the bare nickel were determined. In addition to providing samples of short and long-length RABiTS, program researchers continued to characterize products for uniformity of texture and electrical and mechanical properties.

B. Strategic 2nd Generation Wire Projects

Strategic projects continued to focus on the development of improved substrates for both IBAD and RABiTS processes, and deposition processes for buffer layers and the superconductor layer. Characterization of buffer and superconductor layers attempted to correlate processing parameters with final wire performance. Projects were active at all six national laboratories.

- University collaborations - Argonne National Lab continued with five active university collaborations: (1) Development of dielectric substrates for coated conductors (with Pennsylvania State University); (2) Development of stable MOCVD precursors for buffer and YBCO layers (with Northwestern University); (3) Pulsed laser deposition of YBCO on textured substrates (with Iowa State University); (4) Understanding the fundamentals of film growth in the MOCVD process (with the University of Illinois at Chicago); and (5) Kinetics of YBCO crystallization from melts (with the University of Houston).

- Wire Characterization - Program participants were completing the characterization of microstructural and superconducting properties of second-generation wire to improve understanding of J_c-limiting factors related to the formation and growth kinetics of high temperature superconductors.

- Oxide buffer layer research - Work on developing sol-gel derived oxide buffer layer systems continued in 1998. A variety of deposition and processing strategies were being investigated to develop a fundamental understanding of this deposition approach and to optimize film properties. Additionally, Sandia scientists worked on developing high-quality, solution-derived, 123-type superconducting films for coated conductor applications.

- Coated conductor processing - Research and development of YBCO and Thallium-Barium-Calcium-Copper Oxide (TBCCO) coated conductor processing continued in a variety of subtasks. Scale-up issues are being defined and addressed. Developing the capability to fabricate 1 to 2 m lengths of RABiTS, using electron beam evaporation and an existing ultra-high vacuum, reel-to-reel system remained a priority. Lengths of RABiTS were being provided for internal use as well as for various partners.

- PLD Deposition - A system and process for deposition of YBCO by Pulse Laser Deposition on moving substrates was being developed by the utilization of a radiant heating system, along with sample translation. Also, improved texture in substrates with reduced magnetism was under development. Deposition studies of TBCCO on RABiTS continued, and new RABiTS architectures, with conductive and simpler structures, were investigated.

- Process technology - DOE partners worked toward developing and demonstrating process technology needed for epitaxial growth of buffer layers by metalorganic decomposition. A specific objective of the project is to develop alkoxide precursor methods for deposition of buffer layers compatible with textured metallic substrates appropriate to long-length conductor manufacture and compatible with American Superconductor's YBCO deposition methods.

- UTSI - The University of Tennessee Space Institute conducted work on a variety of strategic wire projects. UTSI performed parametric evaluation and scale-up engineering for production of YBCO coatings on textured substrates by the sol-gel/solution-based processes. This work was done in cooperation with studies at ORNL. UTSI also was modeling layer interfaces in coated conductors and measuring microscopic properties relevant to cracking and other failures in film coatings. UTSI was working on real-time diagnostics (for manufacturing) to develop: (1) Raman scattering for crystalline structure measurement; (2) atomic absorption spectra measurements in support of MOCVD process; and (3) surface roughness measurement of rolled nickel substrate in support of the RABiTS process. This effort complements projects at Westinghouse and Midwest Superconductivity, Inc. UTSI also engaged in work to conduct cost/performance modeling of potential manufacturing processes to identify needs for research and development. In addition, UTSI coordinated efforts of Coated Conductor Steering Committee and to conduct a workshop on basic science needs for the development of 2nd generation wires.

Keywords: Superconductor, Coated Conductor, Buffer Layers, Deposition, Textured Substrate

177. **STRATEGIC RESEARCH**
$10,000,000
DOE Contact: Jim Daley, (202) 586-1165
Argonne National Laboratory Contact: U. Balachandran, (630) 252-4250
Brookhaven National Laboratory Contact: David Welch, (516) 282-3517
Los Alamos National Laboratory Contact: Dean Peterson, (505) 665-3030
National Renewable Energy Laboratory Contact: Richard Blaugher, (303) 384-6518
Oak Ridge National Laboratory Contact: Robert Hawsey, (615) 574-8057
Oxford Superconducting Technology Contact: Seung Hong, (732) 541-1300
University of Wisconsin Contact: David C. Larbalestier, (608) 263-2194

Strategic research and development projects in the program are crucial for the discovery of new technologies, such as RABiTS and magneto-optical imaging (MOI), that make the program a world leader in the race to bring HTS electric power technologies to market. Critical theoretical calculations, new material evaluation, and process development support the program's industry-directed Cooperative Research and Development Agreement (CRADA) work and the SPI application projects and provide a foundation for future collaborations and progress toward HTS commercialization by industry.

Work by all organizations in strategic research comprises a diverse set of topics from characterization techniques to wire processing to applications development. As these activities mature, they evolve into more cohesive efforts devoted to improving mechanical and electrical properties of wire and new devices.

Project subtasks are as follows:

A. Fundamental Studies

The program supports a broad range of activities which concentrate on the underlying principles of HTS and developing an understanding of how these principles affect final HTS material properties. Collaborators in the activities have worked on understanding reaction kinetics, effects of stoichiometry on the superconducting properties, introducing flux pinning centers, and monitoring current transport in HTS conductors.

B. Wire Development

(1) Sheathed tapes - Wire development efforts included activities in the development of Ag-sheathed Bi-2223 tapes with improved mechanical and superconducting properties. Reproducibility has been a key objective in this project.

(2) Flux pinning and J_c Research - Work continued toward improving the flux pinning and critical current density in zero applied fields for Bismuth-Strontium-Calcium-Copper Oxide (BSCCO) wire architectures. The effects of the metal(s) and oxide on phase and texture evolution at the interface were studied.

(3) Powder development and characterization - Work continued in powder development and characterization and in optimization of processing conditions for producing long lengths of BSCCO-2223 and 2212 wires. A variety of techniques were used to analyze the microstructure of the resultant conductor, and chemical techniques were used in troubleshooting. Wire performance measurements and ac loss measurements were conducted on short samples and small coils.

(4) Thallium Oxides - Efforts continued to focus on the development of prototype conductors based on the Tl-oxides. The realization of a biaxially textured Tl-1223 thick film tape, with technologically useful transport properties, is the primary objective for this effort. A suitable long-length substrate combined with an acceptable thick film process were being

developed to permit the fabrication of superconducting tapes.

(5) BSCCO research - Efforts to develop BSCCO tapes with improved critical current densities, particularly at high magnetic fields and temperatures, were continued. Activities included improving the deposition rate of YBCO films; optimizing the IBAD and intermediate buffer layer processing to improve wire production speed; correlating IBAD/YBCO texture with surface roughness; and developing substrate specifications for high critical current (I_c) coated conductors.

ORNL funded three new university research and development projects in FY 1998. Researchers at Stanford University began investigating ion-beam assisted deposition of buffer layers and in-situ deposition of YBCO by electron beam evaporation. The University of Wisconsin initiated research efforts on BSCCO critical currents and microstructures, YBCO coated conductor microstructure, and pulse tube cryocooler technology. Finally, researchers at the University of Houston began research into high-rate photon-assisted metallo-organic chemical vapor deposition for YBCO onto buffered, textured metallic substrates.

C. Device Development

The program supported a portfolio of innovative device and application development activities that provide the basis for full-scale prototypes to be built in conjunction with industry and could evolve into SPI projects.

- AC loss characterization - Attempts to characterize ac losses in HTS tapes, under conditions which simulate the electromagnetic conditions in utility devices, continued. Program participants worked to design and demonstrate a prototype current-limiter and a hysteresis motor.

- Magnetic separator research - Magnetic separator research continued examining how to develop applications in the separation of Kaolin clays and radioactive contaminants. Key efforts were determining the effects of new HTS coated conductors on selected power applications and a study of magnetic flux trapping and superconductor normalization phenomena.

- In FY 1998, a new project produced the first lengths of YBCO/RABiTS wires - The objective of this project is to develop YBCO wires and coils that will lead to greater understanding of the quench behavior of these new wires, and to produce a small demonstration motor for educational use.

Keywords: Superconducting Tapes, Flux Pinning, Thallium Conductor, Bismuth Conductor

OFFICE OF ENERGY RESEARCH

	FY 1998
Office of Energy Research - Grand Total	$494,475,355
Office of Basic Energy Sciences	$404,553,700
Division of Materials Sciences	$392,475,000
Division of Chemical Sciences	$ 5,333,000
Division of Engineering and Geosciences	$ 6,745,700
Engineering Sciences Research	$ 3,458,800
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 932,000
Fundamentals of Thermal Plasma Processing	500,000
Metal Transfer in Gas-Metal Arc Welding	155,000
Thermal Plasma Chemical Vapor Deposition of Advanced Materials	165,000
Research on Combustion-Driven HVOF Thermal Sprays	112,000
Materials Properties, Behavior, Characterization or Testing	$ 2,396,800
An Investigation of History-Dependent Damage in Time-Dependent Fracture Mechanics	100,000
Intelligent Control of Thermal Processes	500,000
Elastic-Plastic Fracture Analysis: Emphasis on Surface Flaws	500,000
Modeling and Analysis of Surface Cracks	200,000
Development of Measurement Capabilities for the Thermophysical Properties of Energy-Related Fluids	490,000
High-T_c Superconductor-Semiconductor Integration and Contact Technology	130,800
Transport Properties of Disordered Porous Media From the Microstructure	135,000
Stress and Stability Analysis of Surface Morphology of Elastic and Piezoelectric Materials	150,000
3-D Experimental Fracture Analysis at High Temperatures	79,000
Simulation and Analysis of Dynamic Failure of Ductile Materials	112,000
Device or Component Fabrication, Behavior or Testing	$ 130,000
Pulse Propagation in Inhomogeneous Optical Waveguides	130,000
Geosciences Research	$ 3,286,900
Materials Preparation, Synthesis , Deposition, Growth or Forming	$ 432,300
Solution-Reprecipitation of Calcite and Partitioning of Divalent Metals	140,800
Transition Metal Catalysis in the Generation of Petroleum and Natural Gas	110,900
Mineral Dissolution and Precipitation Kinetics: A Combined Atomic Scale and Macro-Scale Investigation	180,600
Materials Structure and Composition	$ 531,900
Reaction Mechanisms of Clay Minerals and Organic Diagenesis: An HRTEM/AEM Study	0
Infrared Spectroscopy and Hydrogen Isotope Geochemistry of Hydrous Silicate Glasses	146,000
Biomineralization: Systematics of Organic-Directed Controls on Carbonate Growth Morphologies and Kinetics Determined by *In situ* Atomic Force Microscopy	160,900
Reactions and Transport of Toxic Meals in Rock-Forming Silicates at 25°C	225,000

OFFICE OF ENERGY RESEARCH (continued)

	FY 1998
Office of Basic Energy Sciences (continued)	
Division of Engineering and Geosciences (continued)	
Geosciences Research (continued)	
Materials Properties, Behavior, Characterization or Testing	$ 2,322,700
Structure and Reactivity of Ferric Oxide and Oxyhydroxide Surfaces: Quantum Chemistry and Molecular Dynamics	240,000
Cation Diffusion Rates in Selected Minerals	200,000
Grain Boundary Transport and Related Processes in Natural Fine-Grained Aggregates	0
Thermodynamics of Minerals Stable Near the Earth's Surface	150,000
New Method for Determining Thermodynamic Properties of Carbonate Solid-Solution Minerals	137,900
Theoretical Studies of Metal Species in Solution and on Mineral Surfaces	46,800
Micrommechanics of Failure in Brittle Geomaterials	264,700
Three-Dimensional Imaging of Drill Core Samples Using Synchrotron-Computed Microtomography	200,000
Shear Strain Localization and Fracture Evolution in Rocks	443,000
Dissolution Rates and Surface Chemistry of Feldspar Glass and Crystal	199,700
Transport Phenomena in Fluid-Bearing Rocks	181,300
Cation Chemisorption at Oxide Surfaces and Oxide-Water Interfaces: X-ray Spectroscopic Studies and Modeling	259,300
Office of Advanced Scientific Computing Research	$78,732,655
Division of Technology Research	$78,732,655
Laboratory Technology Research Program	$ 6,182,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 2,537,000
High Performance Tailored Materials for Levitation and Permanent Magnet Technologies (ANL 97-02)	109,000
Alloy Design of $Nd_2Fe_{14}B$ Permanent Magnets (ORL 94-15)	165,000
Interfacial Interactions of Biological Polymers with Model Surfaces (PNL 97-21)	248,000
Improved Materials for Semiconductor Devices (PNL 98-17)	125,000
An Advanced Hard Carbon Plasma Deposition System with Application to the Magnetic Storage Industry (LBL 98-16)	250,000
Synthesis and Crystal Chemistry of Technologically Important Ceramic Membranes (ANL 97-06)	125,000
Development of Rapid Prototyping Technology for Bioceramic Applications (ANL 95-08)	95,000
Catalytic Production of Organic Chemicals Based on New Homogeneously Catalyzed Ionic Hydrogenation Technology (BNL 97-05)	235,000
Critical Vacancy-Driven Phenomena in High Energy Ion-Implanted Silicon (ORL 98-18)	125,000
Development of Buffer Layers Suitable for Deposition of Thick Superconducting $YBa_2Cu_3O_7$ Layers by Post-deposition Annealing Process (BNL 98-05)	125,000
New Materials for Rechargeable Lithium Batteries (BNL 98-04)	125,000
Nonconsumable Metal Anodes for Primary Magnesium Production (ANL 98-05)	210,000

OFFICE OF ENERGY RESEARCH (continued)

	FY 1998
Office of Advanced Scientific Computing Research (continued)	
Division of Technology Research (continued)	
Laboratory Technology Research Program (continued)	
Materials Preparation, Synthesis, Deposition, Growth or Forming (continued)	
Advanced Separations Technology for Efficient and Economical Recovery and Purification of Hydrogen Peroxide (ANL 98-07)	125,000
Smooth Diamond Films for Friction and Wear Applications and Chemically Protective Coatings (ANL 97-05)	325,000
Nanometer Characterization and Design of Molecular Lubrication for the Head-Disk Interface (LBL 98-10)	150,000
Device or Component Fabrication, Behavior or Testing	$2,385,000
Ionically Conductive Membranes for Oxygen Separation (LBL 97-03)	225,000
Light Emission Processes and Dopants in Solid State Light Sources (LBL 97-13)	250,000
Combinatorial Discovery and Optimization of Novel Materials for Advanced Electro-Optical Devices (LBL 97-18)	250,000
Development of a Thin Film Battery Powered Transdermal Medical Device (ORL 95-11)	165,000
Development of Multi-Channel ASICs for CdZnTe Gamma Detector Arrays (BNL 97-06)	191,000
Microcircuits and Sensors for Portable, Low-Power Data Collection and Transmission (BNL 97-07)	243,000
Microfabricated Instrumentation for Chemical Sensing in Industrial Process Control (ORL 97-08)	260,000
Automotive Underhood Thermal Management Analysis Using 3-D Coupled Thermal-Hydrodynamic Computer Models (ANL 98-14)	250,000
The Development of Rhenium-188-Labeled Radioactive Stents for Prevention of Restenosis after Coronary Balloon Angioplasty (ORL 98-31)	129,000
Near-Frictionless Carbon Coatings (ANL 98-03)	125,000
Development of High-Temperature Superconducting Wire Using RABiTS Coated Conductor Technologies (ORL 97-02)	260,000
Thin Film Thermal Barrier Coatings (PNL 95-07)	15,000
Thin Film Lithium Batteries (BNL 95-11)	22,000
Instrumentation and Facilities	$ 651,000
A Facility for Studying Micromagnetic Structures (LBL 95-12)	300,000
Controlled Nonisothermal Hot Forging Using Infrared for Microstructural Control (ORL 98-08)	226,000
Micro-organism Detection and Characterization (PNL 98-03)	125,000
Materials, Properties, Behavior, Characterization or Testing	$ 609,000
The Role of Yttrium in Improving the Oxidation Resistance in Advanced Single Crystal Nickel-based Superalloys for Turbine Applications (ORL 95-07)	30,000
Next Generation Corrosion Inhibitors for Steel in Concrete (BNL95-12)	74,000
Atomic Scale Structure of Ultrathin Magnetic Multilayers and Correlation with Resistance, Giant Magnetoresistance, and Spin-Dependent Tunneling (ORL 97-03)	255,000
Highly Dispersed Solid Acid Catalysts on Mesoporous Silica (PNL 97-28)	250,000

OFFICE OF ENERGY RESEARCH (continued)

	FY 1998
Office of Advanced Scientific Computing Research (continued)	
Division of Technology Research (continued)	
Advanced Energy Projects Program	$3,377,000
Device or Component Fabrication, Behavior or Testing	$1,288,000
Composite Magnetostrictive Materials for Advanced Automotive Magnetomechanical Sensors	270,000
Investigation of High Efficiency Multi Band Gap Multiple Quantum Well Solar Cells	225,000
Magnetically Enhanced Thermoelectric Cooling	250,000
Efficient Energy Up-Conversion of Infrared to Visible Light at Semiconductor Heterojunctions	243,000
Electrically Active Liquid Matrix Composites	300,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$1,370,000
Next Generation High-Temperature Structural Materials for Heat Exchangers and Heating Elements	297,000
Tritiated Porous Silicon: A Stand-Alone Power Source	260,000
Supported Molten Metal Catalysts: A New Class of Catalysts	240,000
Combinatorial Synthesis of High T_c Superconductors	250,000
Micro-Hollow Cathode Discharge Arrays: High Pressure, Nonthermal Plasma Sources	210,000
Experimental and Theoretical Investigation of Dual-Laser Ablation for Stoichiometric Large-Area Multicomponent Film Growth	113,000
Materials Properties, Behavior, Characterization or Testing	$ 719,000
Shape Memory Alloy Reinforcement of Metals	195,000
Exploitation of Room Temperature Molecule/ Polymer Magnets for Magnetic and Electromagnetic Interference Shielding and Electromagnetic Induction Applications	215,000
Molecular Surface Modification as a Means of Corrosion Control	309,000
Small Business Innovation Research Program	$65,576,205
Device or Component Fabrication, Behavior or Testing	$26,891,466
Phase I	$ 1,644,738
Ultra-High-Speed Photonic Add-Drop Multiplexers for Wave-Division-Multiplexed Networking	74,986
Screen-Printed Solar Cells Based on Nanocrystalline TiO_2 Films	75,000
An Improved Membrane Module Tubesheet for Industrial Separations	75,000
A Scalable Process for Thin, Defect-Free Zeolite Membranes	75,000
Micromachined Silicon Sensor for DNA Sequencing by Hybridization	74,996
Sharp Bandpass AlGaN p-i-n Photodiode Detectors for Ultraviolet B Irradiance Measurements	74,895
Robust Micromachined Silicon Carbide Environmental Sensors	74,957
Hand-Held Monitor for On-Site Detection of Heavy Metals in Water Using Microfabricated Detector Chips	74,996
AlGaN Ultraviolet Light Emitting Diodes for Fiber Optic Sensors	74,894
A Photocatalytic $Ti0_2$ Anode and Membrane Reactor for the Enhanced Destruction of Chloro-Organic Compounds in Water	75,000

OFFICE OF ENERGY RESEARCH (continued)

	FY 1998
Office of Advanced Scientific Computing Research (continued)	
Division of Technology Research (continued)	
Small Business Innovation Research Program (continued)	
Device or Component Fabrication, Behavior or Testing (continued)	
Phase I (continued)	
A Novel UV Photodetector Array	74,765
Large Area, Low-Cost APDs Using Planar Processing	75,000
Solid-State Neutron Detection with LiZnP	75,000
A New Large Area Monolithic Avalanche Photodiode Array Having Widespread Applications and Lower Manufacturing Costs	72,890
Gallium Arsenide p-i-n Detectors for High-sensitivity Imaging of Thermal Neutrons	74,932
Robust, Zirconium Carbide and Hafnium Carbide Field Emitter Cathodes for Accelerator and Beams Applications	75,000
Pulsed High Power Switch for the Next-Generation Electron-Positron Linear Collider	72,460
High-Voltage, Fast Turn-on and Turn-off Diamond Switch	75,000
Avalanching MRS Detectors for Scintillation Photodetection	74,967
A Simple and Direct Tungsten Brush Fabrication Technique	75,000
High Speed Acousto-Optic Tuner	75,000
Development of High Speed Mercury Cadmium Telluride Detector Arrays with Integral Readouts	75,000
Phase II (First Year)	$5,156,589
Shaft Weld Replacement with a Ceramic Locking Assembly Joint	689,156
Development of Economical Procedures for Producing and Processing Fine Grained SSM Feedstock via Mechanical Stirring	718,280
Corrosion Resistant Bipolar Plates for PEM Fuel Cells	749,999
High Brightness LEDs based on the (Al,Ga,In)N Materials System	749,154
Development of High Power RF Windows and Waveguide Components for the Next Linear Collider	750,000
Electrical Discharge Machining Application to the Development of mm-wave Accelerating Structures	750,000
Beryllium and Tungsten Brush Armor for Plasma Facing Components	750,000
Phase II (Second Year)	$20,090,139
Catalytic Membrane for High Temperature Hydrogen Separations	750,000
Advanced Coal Based Power System Components Using Reaction Bonded Silicon Carbide	749,449
A New Separation and Treatment Method for Soil and Groundwater Restoration	749,529
Continuous Analyzer for Monitoring Hydrogen Chloride and Chlorine During Site Cleanup Activity	749,701
Long-Life Electrical Neutron Generator	750,000
Passive Electronic Components from Nanostructured Materials	750,000
A Multicore Optical Fiber Sensor for Mass Transport and Particulates	749,991
Infrared Hollow Waveguide Organic Solvent Analyzer	749,929
Stratospheric Water Vapor Microsensor	750,000
Compact, Airborne Laser Multigas Sensor	600,443

OFFICE OF ENERGY RESEARCH (continued)

	FY 1998
Office of Advanced Scientific Computing Research (continued)	
Division of Technology Research (continued)	
Small Business Innovation Research Program (continued)	
Device or Component Fabrication, Behavior or Testing (continued)	
Phase II (Second Year) (continued)	
Microwave Radiometer for Passively and Remotely Measuring Atmospheric Water Vapor	738,746
Advanced Water Sensor for Unmanned Aerial Vehicles	750,000
High-Gain Monocapillary Optics	539,595
High Performance X-ray and Neutron Microfocusing Optics	517,510
Very Low Friction Small Radius Domed Cutters for Percussion Drill Bits	750,000
Development and Testing of a Jet Assisted Polycrystalline Diamond Drilling Bit	750,000
Advanced Low-Stress Bonding of Thermally Stable Polycrystalline Diamond Cutters to Tungsten Carbide Substrates	749,968
Nanocrystalline Superhard, Ductile Ceramic Coatings for Roller Cone Bit Bearings	749,707
Solid-State Ultracapacitors for Electric Vehicles and Consumer Electronics	750,000
High Surface Area Non-Oxide Ceramic Electrodes for Ultracapacitors	750,000
Wrappable Inorganic Electrical Insulators for Superconducting Magnets	750,000
Joining of Tungsten Armor Using Functional Gradients	750,000
Carbon Thermostructure for Silicon-Based Particle Detectors	750,000
High Performance Optical Detectors for Calorimetry	750,000
Coplanar CdZnTe p-i-n, Gamma-Ray Detectors for Nuclear Spectroscopy	745,571
Large Room Temperature $Cd_{1-x}Zn_xTe$ Detectors	750,000
In-Situ Nondestructive Measurements of Key Mechanical Properties of Reactor Pressure Vessels Using Innovative SSM Technology	600,000
Oxidation Induction Time Technology for Electric Cable Condition Monitoring and Life-Assessment	600,000
Materials, Properties, Behavior, Characterization or Testing	$9,187,263
Phase I	$ 224,968
Detection of Mercury at the Parts per Quadrillion Level Using Cavity Ringdown Spectroscopy	75,000
Low Cost Fine Particulate Stack Monitor	74,968
Instrument for Real Time Measurement of Scale Growth at High Temperature and Under Applied Load	75,000
Phase II (First Year)	$ 750,000
High Current Density High Repetition Rate Ferroelectric Cathode	750,000
Phase II (Second Year)	$8,212,295
Carbon Monoxide Tolerant Anodes for Proton Exchange Membrane (PEM) Fuel Cells	750,000
Low Cost Advanced Bipolar Plates for Proton Exchange Membrane Fuel Cells	720,000
Improved Bi-2223 Flux Pinning Through Chemical Doping	750,000
Low Cost Multifilament Composite Process	750,000

OFFICE OF ENERGY RESEARCH (continued)

	FY 1998
Office of Advanced Scientific Computing Research (continued)	
Division of Technology Research (continued)	
Small Business Innovation Research Program (continued)	
Materials, Properties, Behavior, Characterization or Testing (continued)	
Phase II (Second Year) (continued)	
Template-Mediated Synthesis of Periodic Membranes for Improved Liquid-Phase Separations	750,000
Novel Fiber-Based Adsorbent Technology	750,000
Metal-Binding Silica Materials for Wastewater Cleanup	750,000
Superhard Nanophase Cutter Materials for Rock Drilling Applications	750,000
Evaluation and Constitutive Modeling of Unidirectional SiC/SiC Composites with Engineered SiC Fiber Coatings Subjected to Neutron Irradiation	748,520
Innovative Fabrication of SiC/SiC Composites with High Through-the-Thickness Thermal Conductivity	750,000
High Numerical Aperture Scintillating Fibers	743,775
Materials, Preparation, Synthesis, Deposition, Growth or Forming	$29,497,476
Phase I	$4,048,807
Hybrid Multilayer Membranes for the Selective Separation of Hydrogen from Complex Gas Streams	75,000
Carbon Nanostructures from Coal-Derived Liquid Feedstocks	75,000
High Temperature Oxidation Resistant Alumina Coatings for Advanced Energy and Processing Systems	75,000
Adherent and Reliable Alumina Coating Development	75,000
Surface Tailored Nanophase Alumina Coatings for Oxidation Protection of Aluminide Intermetallics	75,000
Novel Net Shape Processing for the Fabrication of Boron-Doped Mo_5Si_3-Based Intermetallic Alloys for High Temperature Applications	75,000
Synthesis of Mesoporous Tin Oxide for Chemical Gas Sensors	75,000
Polyurethane-Clay Nanocomposite and Microcellular Foaming	74,954
Mesoporus Bimetallic Transition Metal Oxides as Solid Acid Catalysts	75,000
Barium Titanate/Polymer Nanoscale Composites with Controllable Architectures	75,000
Thin (<30 micron) Silicon-Film Solar Cells on Glass-Ceramic Substrates	75,000
Spectral Sensitization of Nanocrystalline TiO_2 by Dye Aggregates	74,965
Dye Sensitized TiO_2 Photoelectrochemical Cells with Polymer Electrolytes	75,000
High Resistivity Tin Oxide for CdTe PV Cell Electrodes	74,754
Manufacturable $CuIn(Ga)Se_2$-Based Solar Cells via Development of Co-Sputtered $CuInSe_2$ Absorber Layers	75,000
Materials and Processes for High-Performance Cadmium Telluride Photovoltaic Modules	75,000
Improved Non-Vacuum Processes for Forming CIS Films	75,000
High Capacity Lithium Battery Cathodes Based on V_2O_5 Xerogels	74774
Irreversibility Compensated Metal Oxide Anodes for Lithium-Ion Batteries	75,000
High Rate, High Capacity Anodes for Rechargeable Li Batteries	75,000
Nanostructured Manganese Dioxides for Li-Ion Batteries	75,000
A Mixed Metal Oxide Anode Material for High Energy Density Li-Ion Batteries	74,980
Novel Membranes for Organic/Organic Separations	75,000
Novel Low-Cost Zeolite Ceramic Membrane Module	75,000

OFFICE OF ENERGY RESEARCH (continued)

FY 1998

Office of Advanced Scientific Computing Research (continued)

Division of Technology Research (continued)

Small Business Innovation Research Program (continued)

Materials, Preparation, Synthesis, Deposition, Growth or Forming (continued)

Phase I (continued)

Supported Zeolite Membranes for Methanol-Water Separation	75,000
Mixed-Conducting Membranes for the Spontaneous Oxidative Dehydrogenation of Alkanes to Olefins	75,000
Novel Nanofiltration Membranes for the Separation of Solvent/Oil Mixtures	75,000
Separation of Hydrogen/Light Hydrocarbon Gas Mixtures	75,000
Aerogels with Glass-like Transparency for Cherenkov Detectors	74,926
An Artifical Pinning Center Approach to the Manufacture of High Field NbTaTi Superconducting Wire	75,000
Fabrication of Rare Earth Doped Nb_3Sn Superconductors	74,645
High Magnetic Field Tl-Based Superconducting Tape on Biaxially Textured Flexible Metallic Substrates	75,000
Novel BSCCO Composites for High-Field Superconductor Technology	75,000
Combustion Chemical Vapor Deposition of High Temperature Ceramic Insulator Coatings on Superconductor Wire	75,000
Technology to Produce Long Lengths of Nb_3Al Superconductor Wire	75,000
Production of Jelly-Roll Process Nb_3Al Multifilamentary Superconducting Wire Using Warm Hydrostatic Extrusion	74,991
Development of High Field, High Current Density Nb_3Sn Conductor with Engineered Microstructures	75,000
High Quantum Efficency Extended Wavelength Vacuum Photocathodes	75,000
Micromachined Ceramic Microchannel Plates	75,000
High Field Magnets for Plasma Fusion Confinement Systems	75,000
High Performance SiC/SiC Composites for Structural Fusion Reactor Components	74,952
Innovative, Low Viscosity, Radiation-Resistant Insulation Systems for Fusion Magnets	75,000
Beryllium Armored Aluminum Alloy Plasma Facing Components	75,000
High Strength, High Conductivity, Low Activation Copper Matrix Nanocomposite for Fusion Reactor First Wall Application	74,984
Insulating Coatings Development for Vanadium Alloys for Use in Fusion Systems	75,000
An Improved Reaction-Bonded Silicon Carbide Process for SiC/SiC Composites	75,000
Structural Materials & Insulating Coatings	75,000
Refractory Metal Wicks for Extended Lifetime in AMTEC Power Systems	74,955
The Short-Pulse Plasma Implantation/Coating Process for Extending the Life of Die Casting Dies	75,000
PVD Coating of Dies Using Superhard Nano-layered Composite Coatings	75,000
Development of an Innovative Laser Assisted Coating Process for Extending Lifetime of Metal Casting Dies	74,931
The Application of Plasma Assisted Chemical Vapor Deposition (PACVD) Coatings for Die Casting Dies	75,000
Micromechanically Compliant Coating for Die Casting Dies	75,000
Hard, Wear Resistant Coatings for Die-Casting Dies by an Advanced Filtered Cathodic Arc Deposition Process	74,996

OFFICE OF ENERGY RESEARCH (continued)

	FY 1998
Office of Advanced Scientific Computing Research (continued)	
Division of Technology Research (continued)	
Small Business Innovation Research Program (continued)	
Materials, Preparation, Synthesis, Deposition, Growth or Forming (continued)	
Phase II (First Year)	$19,646,474
A Novel Reactive Joining Compound for High Temperature Applications	548,661
Development of Novel Boron-Based Multilayer Thin-Film	750,000
Advanced Plasma Surface Modification System	750,000
High-Flux, Low Energy Ion Source for High Rate Ion-Assisted Deposition of Hard Coatings	750,000
Semi-Solid Thermal Transformation to Produce Semi-Solid Formable Alloys	750,000
A Simple Process to Manufacture Grain Aligned Permanent Magnets	750,000
A Novel Technique for the Enhancement of Coercivity in High Energy Permanent Magnets	750,000
Stabilization of Nitride Magnet Material via Sol-Gel Route	750,000
A Combinatorial Approach to the Synthesis and Characterization of Novel Anode Materials for Direct Methanol Fuel Cells	750,000
Low Cost Deposition of Buffer Layers for Manufacturable YBCO HTS Conductors	750,000
Buffer Layers on Textured Nickel Using Commercially Viable CCVD Processing	750,000
Development of Efficient and Practical Passive Solar Building Systems with High Recycled Content Using the Preplaced Aggregate Concrete Technology	750,000
Heterogeneous Hydroformylation of Alkenes with Syngas	750,000
Tubular SOFC with Deposited Nano-Scale YSZ Electrolyte	749,943
High Speed Long Wavelength Infrared Detector Array/Preamplifier Development	750,000
Development of Cadmium Germanium Arsenide Crystals	750,000
An Easily Dispersed Reactive Coating for Surface Decontamination	736,111
Rapid Quench Nb_3Al for High Field Accelerator Applications	750,000
Ultra-Lightweight Carbon-Carbon Cooling Structure For Pixel and Silicon Strip Detectors	673,759
Development of Scintillators and Waveshifters for Detection of Ionizing Radiation	750,000
Phase II (Second Year)	$5,802,195
An Attrition-Resistant Zinc Titante Sorbent for a Transport Reactor	750,000
A Light Scattering Based Sensor for On-Line Monitoring of Fiber Diameter Distribution During Fiberglass Manufacturing	561,744
Novel Use of Gas Jet Plasma to Prepare Amorphous Silicon Alloy	750,000
High Rate Deposition of Transparent Conducting Zinc Oxide Using Activated Oxygen for Photovoltaic Manufacturing Cost Reduction	744,962
Development of Optimal SnO_2 Contacts for CdTe Photovoltaic Applications	750,000
Large Area, Low Cost Processing for CIS Photovoltaics	750,000
Improved Processes for Forming CIS Films	750,000
Ultrafast Polysilylene Scintillators	745,489

OFFICE OF ENERGY RESEARCH (continued)

	FY 1998
Office of Advanced Scientific Computing Research (continued)	
Division of Technology Research (continued)	
Small Business Technology Transfer Research Program	$3,597,450
Device or Component Fabrication, Behavior or Testing	$1,799,392
Phase I	$ 300,000
Novel Ultracapacitor: WN Aerogel Electrode with Polyoxometalate Polymers Electrolyte	100,000
High Energy and Power Ultracapacitors Utilizing Novel Type III Polymers and Non-Aqueous Electrolytes	100,000
A Low Cost High Performance Uranium Plutonium Detector	100,000
Phase II (First Year)	$999,392
Novel Thin Film Scintillator for Intermediate Energy Photons Detection and Imaging	499,392
Advanced Ceramic Hot Gas Filters	500,000
Phase II (Second Year)	$500,000
A Flywheel Motor Alternator for Hybrid Electric Vehicles	500,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$1,798,058
Phase I	$299,021
High Flux Ceramic Membrane for Hydrogen Separation	99,994
A Zeolite Membrane for Separation of Hydrogen from Process Streams	100,000
Boron Carbide Coatings for Enhanced Performance of Radio-Frequency Antennas in Magnetic Fusion Devices	99,027
Phase II (First Year)	$999,060
New High-Performance GaSb-Based Thermophotovoltaic (TPV) Devices	499,060
High Efficiency Magnetic Refrigerators as Alternate Environmentally Safe Commercial Refrigeration Devices	500,000
Phase II (Second Year)	$499,977
Cabled Monofilament Subelements for Improved Multifilament Niobium Tin Performance and Reduced Cost	499,977

OFFICE OF ENERGY RESEARCH (continued)

	FY 1998
Office of Fusion Energy Sciences	$11,189,000
Materials Properties, Behavior, Characterization or Testing	$11,189,000
Structural Materials Development	675,000
Modeling Irradiation Effects in Solids	50,000
Fusion Systems Materials	3,408,000
Structural Materials for Fusion Systems	950,000
Development of Radiation-hardened Ceramic Composites for Fusion Applications	21,000
Mechanisms of Plastic and Fracture Instability for Alloy Development of Fusion Materials	120,000
Damage Analysis and Fundamental Studies for Fusion Reactor Materials Development	200,000
International Thermonuclear Experimental Reactor (Iter) Materials Development for Plasma Facing Components	5,000,000
ITER Materials Evaluation	365,000
ITER Structural Materials Evaluation	200,000
Structural Materials Development for the Conduit of Iter Cable-in-conduit-conductors	200,000

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 Biological and Environmental Research - Medical Sciences Division

- 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 230 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 47 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 technologically 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 1997 (published October 1998). This 190-page publication contains program descriptions for 517 research programs that were funded in Fiscal Year 1997 by the Division of Materials Sciences. Five cross-cutting indices identify all 517 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/SC-0001. 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 on 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, electrochemical energy storage and conversion research and materials precursor chemistry. The operating budget for FY 1997 for materials-related programs was $5,333,000 and was allocated to 26 projects in heterogeneous catalysis, electrochemical energy storage and conversion research 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 Chemical Engineering Science program supports fundamental research in electrochemical energy storage and conversion 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 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 Summaries of FY 1998 Research in the Chemical Sciences (www.er.doe.gov/production/bes/chmhome.html) for summaries of all funded 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

178. FUNDAMENTALS OF THERMAL PLASMA PROCESSING
$500,000
DOE Contact: Robert E. Price, (301) 903-5822
INEL 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 graded 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 form a natural progression and will be pursued sequentially in the above order, but with significant overlap.

Keywords: Plasma Processing, Functionally Graded Materials

179. METAL TRANSFER IN GAS-METAL ARC WELDING
$155,000
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 were 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

180. **THERMAL PLASMA CHEMICAL VAPOR DEPOSITION OF ADVANCED MATERIALS**
$165,000
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

181. **RESEARCH ON COMBUSTION-DRIVEN HVOF THERMAL SPRAYS**
$112,000
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

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

182. **AN INVESTIGATION OF HISTORY-DEPENDENT DAMAGE IN TIME-DEPENDENT FRACTURE MECHANICS**
$100,000
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 attempts to predict the crack growth and failure response of material components exposed to high temperature conditions. However, micro- mechanical 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 micro-mechanics 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

183. **INTELLIGENT CONTROL OF THERMAL PROCESSES**
$500,000
DOE Contact: Robert E. Price, (301) 903-5822
INEL Contact: H. Smartt, (208) 526-8333

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 trajectory 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

184. **ELASTIC-PLASTIC FRACTURE ANALYSIS: EMPHASIS ON SURFACE FLAWS**
$500,000
DOE Contact: Robert E. Price, (301) 903-5822
INEL 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

185. **MODELING AND ANALYSIS OF SURFACE CRACKS**
$200,000
DOE Contact: Robert E. Price, (301) 903-5822
MIT Contacts: David M. Parks, (617) 253-0033 and F. A. McClintock, (617) 253-2219

This project is 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 under-matched 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

186. **DEVELOPMENT OF MEASUREMENT CAPABILITIES FOR THE THERMOPHYSICAL PROPERTIES OF ENERGY-RELATED FLUIDS**
$490,000
DOE Contact: Robert E. Price, (301) 903-5822
National Institute of Standards 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

187. **HIGH-T_c SUPERCONDUCTOR-SEMICONDUCTOR INTEGRATION AND CONTACT TECHNOLOGY**
$130,800
DOE Contact: Robert E. Price, (301) 903-5822
National Institute of Standards and Technology Contacts: 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 is 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

188. **TRANSPORT PROPERTIES OF DISORDERED POROUS MEDIA FROM THE MICROSTRUCTURE**
$135,000
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).

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 correlation functions have been extracted from them.

Keywords: Porous Media, Transport Properties

189. **STRESS AND STABILITY ANALYSIS OF SURFACE MORPHOLOGY OF ELASTIC AND PIEZOELECTRIC MATERIALS**
$150,000
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 solids. 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. 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 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 stability of these arrays under application of applied stresses is now underway.

Keywords: Surfaces, Interfaces, Stress Analysis, Piezoelectrics

190. **3-D EXPERIMENTAL FRACTURE ANALYSIS AT HIGH TEMPERATURES**
$79,000
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, ≈ 2 mm, and 2024-T3 aluminum, compact (CT) of large crack growth, ≈ 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 ≈ 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

191. **SIMULATION AND ANALYSIS OF DYNAMIC FAILURE OF DUCTILE MATERIALS**
$112,000
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 of 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

192. **PULSE PROPAGATION IN INHOMOGENEOUS OPTICAL WAVEGUIDES**
$130,000
DOE Contact: Robert E. Price, (301) 903-5822
University of Maryland Contact: C. Menyuk, (301) 455-3501

This project is focused in two areas. The first is the study of randomly varying birefringence in optical fibers and its impact on both soliton and NRZ communications. A set of equations have been derived (modified Manakov equations) that allow simulation of 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. Benchmarking of these codes has 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, analytical methods based on the theory of stochastic differential equations are being used 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, using a Green's function approach to determine the rate at which radiation leaks from the quasi-phase-matched guides. Future investigations 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

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 involve elements relevant to several different energy objectives. The DOE contact for this Program is Nicholas B. Woodward (301) 903-5822.

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

193. **SOLUTION-REPRECIPITATION OF CALCITE AND PARTITIONING OF DIVALENT METALS**
$140,800
DOE Contact: N. B. Woodward, (301) 903-5822
University of Chicago Contact: Frank M. Richter, (773) 702-8118

The proposed research is to investigate the exchange of metals (principally Sr and Cd) between $CaCO_3$ and fluids, at a fundamental level necessary for basing thermodynamic and kinetic treatments of dissolution/reprecipitation. The proposed measurements of precipitation rates and exchange of Sr and Cd with calcite solid-solutions will serve as the basis for developing a more general treatment of governing mechanisms and kinetics of dispersion of tracers and contaminants uptake/release in calcite, the predominant constituents of limestones. Laboratory measurements of exchange rates are to be complemented with analyses of the record of calcite-fluid exchange obtained from natural samples, in order to help determine a mechanistic understanding of the exchange rates over both short and longer time periods accessible in the sedimentary record.

Keywords: Carbonate Minerals, Dissolution and Precipitation Mechanisms

194. **TRANSITION METAL CATALYSIS IN THE GENERATION OF PETROLEUM AND NATURAL GAS**
$110,900
DOE Contact: N. B. Woodward, (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 kerogeneous 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

195. **MINERAL DISSOLUTION AND PRECIPITATION KINETICS: A COMBINED ATOMIC-SCALE AND MACRO-SCALE INVESTIGATION**
$180,600
DOE Contact: N. B. Woodward, (301) 903-5822
University of Wyoming Contact:
Carrick M. Eggleston, (307) 766-6769
LLNL Contact: Kevin G. Knauss,
(510) 422-1372

The project combines atomic-scale and macroscale 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 nature of the reactive interface.

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

MATERIALS STRUCTURE AND COMPOSITION

196. **REACTION MECHANISMS OF CLAY MINERALS AND ORGANIC DIAGENESIS: AN HRTEM/AEM STUDY**
$0
DOE Contact: N. B. Woodward,
(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

197. **INFRARED SPECTROSCOPY AND HYDROGEN ISOTOPE GEOCHEMISTRY OF HYDROUS SILICATE GLASSES**
$146,000
DOE Contact: N. B. Woodward, (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 un-derstand oxygen self-diffusion in silicate minerals and glasses and enhanced oxygen diffusion under hydrothermal conditions.

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

198. **BIOMINERALIZATION: SYSTEMATICS OF ORGANIC-DIRECTED CONTROLS ON CARBONATE GROWTH MORPHOLOGIES AND KINETICS DETERMINED BY *IN SITU* ATOMIC FORCE MICROSCOPY**
$160,900
DOE Contact: N.B. Woodward, (301) 903-5822
Georgia Institute of Technology Contact:
P. Dove, (404) 894-6043
LLNL Contact: James DeYoreo, (510) 423-4240

The research is to investigate biomineralization mechanisms of dissolution and precipitation reactions of the two common calcium carbonate polymorphs, calcite and (metastable) aragonite. Experiments have been undertaken 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 have been made under *in aquo* conditions. The combination of proposed 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

199. **REACTIONS AND TRANSPORT OF TOXIC METALS IN ROCK-FORMING SILICATES AT 25°C**
$225,000
DOE Contact: N. B. Woodward, (301) 903-5822
Johns Hopkins University 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 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 microns) of silicates in thin sections with X-ray photoelectron spectroscopy (XPS).

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

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

200. **STRUCTURE AND REACTIVITY OF FERRIC OXIDE AND OXYHYDROXIDE SURFACES: QUANTUM CHEMISTRY AND MOLECULAR DYNAMICS**
$240,000
DOE Contact: N. B. Woodward, (301) 903-5822
PNNL 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 Hydroxides

201. **CATION DIFFUSION RATES IN SELECTED MINERALS**
$200,000
DOE Contact: N. B. Woodward, (301) 903-5822
SNL Contacts: Randall T. Cygan, H. R. Westrich
and Diana Fisler, (505) 844-7216

Objectives of this research are to determine experimental cation diffusion coefficients for pyroxene and carbonate 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 used to measure the relative slow diffusion of Mg^{2+}, Mn^{2+}, and Ca^{2+} in pyroxenes and carbonates. 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. The experimental work has been complemented by atomistic simulations of calcium self-diffusion in calcite. Lattice energy, defect formation energies, and activation energy for a cation vacancy migration have been calculated, providing the mechanism and favored direction of migration of cations in the calcite structure. Results suggest that relaxation of atomic sites in the vicinity of a cation vacancy is a significant contribution to the energy for the migration of cations.

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

202. **GRAIN BOUNDARY TRANSPORT AND RELATED PROCESSES IN NATURAL FINE-GRAINED AGGREGATES**
$0
DOE Contact: N. B. Woodward, (301) 903-5822
Brown University Contacts: R.A. Yund, (401) 863-1931 and J.R. Farver

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

203. **THERMODYNAMICS OF MINERALS STABLE NEAR THE EARTH'S SURFACE**
$150,000
DOE Contact: N. B. Woodward, (301) 903-5822
University of California, Davis Contact: A. Navrotsky, (916) 752-9307

The objective of this research is to determine the enthalpies of formation of hydrous minerals and carbonates using high temperature solution calorimetry. Systematics in energetics of ionic substitutions are sought in order to predict the thermodynamics of complex multicomponent minerals. Mixing properties of mica, amphibole, clay, zeolite, and carbonate solid solutions are also analyzed. New calorimetric measurements confirm significant differences in enthalpy between the ordered and disordered carbonate solution series. Investigation of the energetics of ion exchange and hydration in zeolites is continuing, building on this group's recently published solution enthalpies of a suite of Ca-zeolites and their ion-exchanged forms. Using drop solution calorimetry, the study of energetics of polytypism of the kaolin minerals has been extended to several differently crystallized kaolinites and the minerals nacrite and halloysite. Enthalpies of formation in the illite/smectite system have been measured for the first time, providing good coverage of sedimentary sequences with different proportions of mixed layer compounds. Measurements on natural illite/smectite samples will be complemented with thermochemical measurements on selected synthetic compositional series to address the effects of various levels of impurities, and should provide constraints on the energetics of diagenetic processes.

Keywords: Thermochemistry, Solution Calorimetry, Zeolites, Carbonate Minerals, Clay Minerals

204. **NEW METHOD FOR DETERMINING THERMODYNAMIC PROPERTIES OF CARBONATE SOLID-SOLUTION MINERALS**
$137,900
DOE Contact: N. B. Woodward, (301) 803-5822
University of California, Davis Contacts: 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

205. **THEORETICAL STUDIES OF METAL SPECIES IN SOLUTION AND ON MINERAL SURFACES**
$46,800
DOE Contact: N. B. Woodward, (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. This involves the evaluation of structures, stabilities and spectral properties of heavy metal sulfide species, such as $As(SH)_3$, $Sb(SH)_3$ and $Au(SH)_2^{-1}$, both in aqueous solution and adsorbed on mineral surfaces and the interaction of flotation collector molecules with sulfide mineral surfaces. Predicted properties of As hydroxides provide a check for systematic comparison with experimental data and with results for the corresponding sulfides. Calculations have been completed on possible +2 oxidation state sulfur oxides and on surface relaxation in ZnS. Studies are in progress on the Hg sulfides and some methyl-Hg species. Analysis of aluminosilicate cage structures with single and double 4-ring geometries, is underway, with the goal of synthesizing new mineral-related compounds as candidate flotation collectors with improved efficiency.

Keywords: Surface Complexation, Gold Sulfides, Metal Transport

206. **MICROMECHANICS OF FAILURE IN BRITTLE GEOMATERIALS**
$264,700
DOE Contact: N. B. Woodward, (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

207. **THREE-DIMENSIONAL IMAGING OF DRILL CORE SAMPLES USING SYNCHROTRON-COMPUTED MICROTOMOGRAPHY**
$200,000
DOE Contact: N. B. Woodward, (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

208. **SHEAR STRAIN LOCALIZATION AND FRACTURE EVOLUTION IN ROCKS**
$443,000
DOE Contact: N. B. Woodward, (301) 903-5822
Northwestern University Contact: J .W. Rudnicki, (708) 491-3411
SNL Contact: W. Olsson, (505) 844-7344

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

209. **DISSOLUTION RATES AND SURFACE CHEMISTRY OF FELDSPAR GLASS AND CRYSTAL**
$199,700
DOE Contact: N. B. Woodward, (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

210. **TRANSPORT PHENOMENA IN FLUID-BEARING ROCKS**
$181,300
DOE Contact: N. B. Woodward, (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

211. **CATION CHEMISORPTION AT OXIDE SURFACES AND OXIDE-WATER INTERFACES: X-RAY SPECTROSCOPIC STUDIES AND MODELING**
$259,300
DOE Contact: N. B. Woodward, (301) 903-5822
Stanford University Contacts: G. E. Brown and
G. A. Parks, (415) 723-9168

This project concerns reactions and reaction mechanisms between metal ions in aqueous solution and oxide surfaces representative of those found in the Earth's crust as an aid to developing both quantitative understanding of the geochemistry of mineral surfaces and the macroscopic models required to predict the fate of contaminants in earth surface environments. The objectives of this research are: (1) to characterize sorption reactions by determining composition, molecular-scale structure, and bonding of the surface complexes produced using direct sorption measurements, synchrotron-based X-ray absorption fine structure (XAFS) spectroscopy, X-ray photoelectron spectroscopy (XPS), and UV/Vis/IR spectroscopy; (2) to investigate how these properties are affected by the solid surface, the composition of the aqueous solution, the presence or simple organic ligands containing functional groups common in more complex humic and fulvic substances, and time; and (3) to develop molecular-level and macroscopic models of sorption processes.

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

OFFICE OF ADVANCED SCIENTIFIC COMPUTING RESEARCH

DIVISION OF TECHNOLOGY RESEARCH

LABORATORY TECHNOLOGY RESEARCH PROGRAM

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

212. HIGH PERFORMANCE TAILORED MATERIALS FOR LEVITATION AND PERMANENT MAGNET TECHNOLOGIES (ANL 97-02)

$109,000
DOE Contact: Walter M. Polansky, (301) 903-5995
ANL Contact: George W. Crabtree, (630) 252-5509

The objective of this project is to develop high performance bulk materials for superconducting technologies, including levitation, frictionless bearings, motors, generators, and trapped field magnets. The goal is being addressed on three levels: application of basic materials research tools and techniques to explore and understand the flux pinning mechanisms in the (RE)BCO family of superconductors, development of novel processing techniques to optimize materials performance, and integration of these techniques to produce prototype materials suitable for commercial application. The project has achieved significant successes in all three of its objectives. First, basic materials research tools such as magnetization measurements (using SQUID, vibrating sample magnetometer (VSM), and miniature Hall probes), magneto-optical imaging, and scanning electron microscopy (SEM) have revealed the materials characteristics and processing conditions leading to high performance. The project has identified processing variables, such as the high temperature growth rate, the post-growth low temperature oxygen anneal, and rare earth composition of the starting materials, which are key factors in the ultimate performance of the materials. Second, new processing techniques making extensive use of this basic research information have been developed which control the materials performance at low and high magnetic field. For example, the peak performance field can be adjusted to any value between zero and 5 Tesla. Third, new fabrication techniques have been developed which allow the manufacture of large scale monolithic components of arbitrary shape. These fabrication techniques are based on novel multiple seeding procedures and innovative joining technology conceived and developed as part of this project. Test devices such as solenoids and rings have been fabricated and tested. In the remaining years of the project, further improvements in materials performance will be made, and simpler and more effective fabrication procedures will be developed. This project provides high performance materials for a new generation of bulk superconducting applications. The new processing allows tailoring materials to high field applications like trapped field magnets or motor components, or to low field applications like levitation or frictionless bearings. The development of monolithic fabrication procedures enables qualitatively new applications, such as motor components or shielding enclosures free of detrimental grain boundaries which limit current flow. This project supports the DOE mission to create new materials technology for the applications of superconductivity.

Keywords: Superconductors, Permanent Magnets, Processing Techniques, Materials Performance

213. ALLOY DESIGN OF $Nd_2Fe_{14}B$ PERMANENT MAGNETS (ORL 94-15)

$165,000
DOE Contact: Walter M. Polansky, (301) 903-5995
ORNL Contact: Joseph A. Horton, (423) 574-5575

The objective of this project is to improve the room temperature fracture toughness and fracture strength of neodymium-based permanent magnets. Demanding motor applications, such as a prototype electric vehicle drive motor with a 150 mm diameter neodymium magnet and spun at 10,000 rpm, need an improvement in these properties to produce acceptable failure rates for commercial use. This project is one of the first studies emphasizing mechanical properties of rare earth permanent magnets. Based on a survey of commercially available material produced by two different processes, melt spinning and powder metallurgy, and a survey of experimental alloys produced by Magnequench, the project has determined that the toughness is a function of both grain size and the composition and distribution of certain grain boundary phases. Processing variables were studied to optimize magnets with Magnequench's current composition and processing methods. A third processing route utilizing gas atomized magnet powder was investigated, and bulk magnets were successfully produced. In other tetragonal intermetallics, cleavage on basal planes is often observed. Cleavage fracture surfaces in single crystals of $Nd_2Fe_{14}B$ were analyzed by X-ray diffraction and atomic force microscopy and found to have a random orientation and some curvature. Auger electron spectroscopy analysis of the fracture surface chemistry showed that the large grained sintered materials cleave, while in the small grained hot-pressed Magnequench MQII magnets, fracture is largely intergranular. In the as melt spun material, fracture is either by cleavage or there is no grain boundary eutectic phase present. Microstructural analysis of a new grade of Magnequench powder, termed B+, was performed. A much greater uniformity of grain size and shape through the thickness of the ribbon resulted in a magnetic powder with higher energy products. A correlation of crystallographic texture, magnetic anisotropy, press direction, microstructure, and fracture toughness is underway in order to understand the preferred directionality of some of the failure situations. This project supports DOE's basic science programs in alloy and ceramic science.

Keywords: Alloy Design, Permanent Magnet, Fracture Properties, Needymium Magnet, Rare Earth Magnets

214. **INTERFACIAL INTERACTIONS OF BIOLOGICAL POLYMERS WITH MODEL SURFACES (PNL 97-21)**
$248,000
DOE Contact: Walter M. Polansky, (301) 903-5995
PNNL Contact: Allison Campbell, (509) 375-2180

The goal of this project is to apply state-of-the-art methods to design, synthesize and characterize systems for adsorption experiments. Specifically, molecular beam epitaxy, chemical vapor deposition and self-assembling monolayer surfaces with controlled properties such as chemistry, topography and heterogeneity will be constructed. The project will also develop, for the first time, CVD methods for producing controlled surfaces of the biologically relevant calcium oxalate, carbonate, and phosphate systems. Biological polymers of human serum albumin, Protein G and fibrinogen will be used in the adsorption experiments. These provide excellent models in that they exhibit a range of structures, sizes, and chemistries. State-of-the-art techniques of neutron scattering and reflectometry, quartz crystal microbalance, liquid chromatography/ mass spectroscopy, and atomic force microscopy will be employed to study adsorption *in situ*. Information on adsorption kinetics, isotherms, and protein conformation will be obtained in real time. Finally, solid state NMR experiments will be conducted that aim to identify the specific protein residues that are interacting with the surface. This investigation will provide molecular level information on specific interactions that has not yet been obtained. To date, an *in situ* quartz crystal microbalance (QCM) and screw-in flow-through cell interfaced with a syringe pump has been constructed. The absorption of fibrinogen and albumin was examined onto self-assembling monolayers attached to gold electrodes deposited onto quartz crystals. *In situ* protein adsorption kinetics was examined using the QCM, and *ex situ* protein adsorption amounts were determined by ellipsometry. The most significant result from this study was that the OH surface resulted in reduced fibrinogen adsorbed. This is of interest because fibrinogen is considered to be a very sticky protein and is difficult to keep off surfaces. The project has identified a method for studying the adsorption/desorption of proteins on various surfaces. Two classes of binding to various weak ion exchange supports have been quantified. By studying the behavior of the proteins on the chromatographic surface, the project has obtained information suggesting possible mechanisms of protein unfolding, kinetics of the adsorption/desorption process. From the data, structural characteristics of the protein in near-physiological environments have been deduced. The project is contributing to achieving DOE's mission in fundamental science, while also providing knowledge and technology to potentially enable the development of improved materials for use in health care.

Keywords: Interfacial Interactions, Biological Polymers, Model Surfaces, Design Synthesis and Characterization, Vapor Deposition

215. **IMPROVED MATERIALS FOR SEMICONDUCTOR DEVICES (PNL 98-17)**
$125,000
DOE Contact: Walter M. Polansky, (301) 903-5995
PNNL Contact: Suresh Baskaran, (509) 375-6483

The increasingly higher performance required of semiconductor devices has resulted in a need for new materials to reduce the capacitance between metal conductor lines (interconnects) on semiconductors. The ability of a material to reduce capacitance losses is defined by its dielectric constant, and the development of interlevel dielectric materials with much lower dielectric constants than what is currently available is the focus of considerable attention within the semiconductor industry. In addition to improving electrical performance (power consumption, signal speed, and propagation noise), such materials offer the potential of significant reductions (~$500M annually) in fabrication costs for semiconductors. The project will develop mesoporous silica dielectric films. The controlled, highly porous structure of these films make them good candidates to obtain the types of properties the semiconductor industry is seeking in low k dielectrics. Pacific Northwest National Laboratory (PNNL) will focus on the design and synthesis of the new materials, including pore design, pore characterization, surface modification, and initial process development. SEMATECH will be responsible for extensive characterization of film performance and evaluation in relation to interconnect processing for semiconductors. SEMATECH hopes to identify low k dielectric materials capable of being utilized by its member companies in the manufacture of higher performance semiconductor devices. DOE missions will benefit through an improved understanding of mesoporous materials that also have energy-related applications in catalysis and sensing, and environmental applications in chemical separations. Experiments have been initiated to increase film thickness and minimize surface topography due to the spin coating process. Using nuclear reaction analysis and the Rutherford backcattering facility at the Environmental Molecular Sciences Laboratory, porosity was determined for surfactant-based films with a range of porosity from approximately 20 percent to about 60 percent. Ideally, from both performance and integration standpoints, films should contain high porosity with isolated pores. Therefore, PNNL researchers have also begun investigation of a synthesis approach for films with closed porosity using new soluble pore-formers.

Keywords: Semiconducting, Devices, Interconnects, Silica Dielectric Film, Semitech

216. **AN ADVANCED HARD CARBON PLASMA DEPOSITION SYSTEM WITH APPLICATION TO THE MAGNETIC STORAGE INDUSTRY (LBL 98-16)**
$250,000
DOE Contact: Walter M. Polansky,
(301) 903-5995
LBNL Contact: Andre Anders, (510) 486-6745

The goal of this project is to develop a novel plasma deposition system used to coat computer hard disks and read/write heads with ultra-thin, diamond-like carbon films that can be implemented on an industrial scale. The project will combine the commercial and basic research strengths of CSC and Lawrence Berkeley National Laboratory, respectively, to develop next generation, filtered arc deposition equipment. Project objectives include: couple the plasma source and macro-particle filter to complete macro-particle suppression; improve plasma transmission (hopefully double the rate compared to present efforts); trap macro-particles within the filter; and design a compact system that can be directly plugged into existing sputter coating facilities. The system will be reasonably priced and able to coat large areas. It is anticipated that the technology developed in this project will become a key tool for next generation high-density magnetic storage media, a multi-billion dollar market in which U.S. companies currently maintain a market leadership position. The coating system is of vital interest to the U.S. computer industry. Many of the top names in the magnetic storage industry have voiced their support for a filtered cathodic arc system for advanced carbon coating. The project supports the DOE mission in advanced materials, specifically synthesis and processing by ions and plasmas.

Keywords: Plasma Deposition System, Arc Deposition Equipment, Macroparticle Deposition, High Density Magnetic Storage Coatings

217. **SYNTHESIS AND CRYSTAL CHEMISTRY OF TECHNOLOGICALLY IMPORTANT CERAMIC MEMBRANES (ANL 97-06)**
$125,000
DOE Contact: Walter M. Polansky,
(301) 903-5995
ANL Contact: James D. Jorgensen,
(630) 252-5513

Achieving the conversion of natural gas to synthesis gas (syngas) using oxygen-permeable ceramic membranes would bring vast resources of natural gas within our economic reach. This new technology depends on the development of suitable ceramic membrane materials whose performance is then demonstrated in prototype reactors. This project includes the development of suitable membrane materials at ANL, and the construction of a prototype reactor to evaluate the materials performance and demonstrate the viability of the process at AMOCO. A suitable ceramic membrane material, that demonstrates the potential for the desired performance, has been developed in previous work. However, the exact chemical composition and crystal structure of this material is not known. Neutron and X-ray diffraction techniques will be used to determine this information. This will allow the synthesis and processing of the membrane material to be optimized to produce the best performance. *In situ* neutron diffraction at elevated temperature in conditions that simulate the environment in a working syngas reactor will be used to study aspects of the materials related to achieving the longest possible working lifetime. Existing laboratory and pilot plant facilities will be upgraded and modified to facilitate testing of the ceramic membranes under increasingly rigorous conditions. This will provide a valid test of the suitability of the ceramic materials for use in large-scale reactors that convert natural gas into syngas and, at the same time, a useful test of the overall process.

Keywords: Natural Gas, Synthesis Gas (syngas), Ceramic Membranes, Testing of Membranes, Oxygen-Permeable Membranes

218. DEVELOPMENT OF RAPID PROTOTYPING TECHNOLOGY FOR BIOCERAMIC APPLICATIONS (ANL 95-08)
$ 95,000
DOE Contact: Walter M. Polansky, (301) 903-5995
ANL Contact: William A. Ellingson, (630) 252-5068

This project addresses the need to reduce medical costs associated with orthopaedic implant design, fabrication, and implantation, including medical costs for injury recovery time, as many situations require special implant configurations and designs. The approach is to reduce the cost of producing these complex implants using FDA approved bio-ceramic materials through two activities: (1) development of a new fabrication technology called "Rapid Prototyping" (also called Solid Freeform Fabrication) through use of FDA approved bioceramic materials, and (2) development of reverse engineering technology using 3-Dimensional X-ray Computed Tomographic Imaging (often called CAT scans in the press) and necessary advanced digital imaging methods. Tasks in the project include development of: (1) appropriate bioceramic feed stock for the rapid prototyping machine, (2) binder burn out and sintering schedules for the bioceramic materials, (3) machine parameters for proper fabrication of these materials, (4) digital image methods to allow digital files to be extracted from the "CAT" scan images to allow use by the rapid prototyping machine, (5) algorithms to allow digital image files as input to CAD software packages for design modifications, and (6) surgical implant procedures for these new implants. To date, selected bones (chosen by the industrial partners as being of importance), hand and forearm, have been used for high resolution X-ray imaging, and digital images have been obtained. The files have been extracted and modified to allow input to the rapid prototyping machine. (Feedstock materials for the rapid prototyping machine, using aluminum oxide, have been developed including binder burn out and sintering schedules.) The first hand bone and forearm bone have been fabricated using the feedstock material and the rapid prototyping machine. New bioceramic materials including hydroxyapetite/ tricalciumphosphate are now under development. Machine parameters, including thickness of layer, filament temperature, and cross-head speed, have been established for using the new feedstock material. The reverse engineering research is currently under study by the industrial partner for application. This project supports the DOE mission in materials research and medical applications.

Keywords: Rapid Prototyping, Bioceramics, Reverse Engineering, CAT Scans, Bones, CAD

219. CATALYTIC PRODUCTION OF ORGANIC CHEMICALS BASED ON NEW HOMOGENEOUSLY CATALYZED IONIC HYDROGENATION TECHNOLOGY (BNL 97-05)
$235,000
DOE Contact: Walter M. Polansky, (301) 903-5995
BNL Contact: Morris Bullock, (516) 344-4315

This project will focus on the development of new technology for the production of organic chemicals of commercial interest, based on fundamental research at BNL exploring the reactivity of transition metal hydride complexes. The scientific objectives are to explore the feasibility, scope, and selectivity of catalytic *ionic* hydrogenation technology. In these reactions, H_2 is added to an organic chemical sequentially, in the form of a proton (H^+) followed by hydride (H^-). The project plans to discover transition metal complexes that can carry out these functions catalytically, with hydrogen (H_2) being the ultimate source of both the proton and hydride. Homogeneously catalyzed ionic hydrogenations offer the possibility of enabling efficient and selective hydrogenation processes for organic transformations that are difficult to achieve by conventional methods. Initial work will focus on attempts to develop prototype metal systems capable of catalytic hydrogenation of ketones. Tungsten systems with weakly coordinating counterions will be investigated first, since preliminary results have indicated that such systems have the requisite ability to form cationic tungsten dihydride complexes upon reaction with H_2. A key issue to be addressed will be the relative binding strength of different ligands to the metal, and measurements of this type may require high pressure nuclear magnetic resonance experiments at DuPont. When a successfully functioning catalytic system is developed, optimization will be attempted by systematic variation of ligands and the metal. Further elaborations will later attempt to utilize these methods in asymmetric hydrogenations to produce commercially viable processes. This project supports the fundamental

DOE mission in understanding the mechanisms for catalysis and the chemical conversion of materials from biomass.

Keywords: Catalytic Production, Ionic Hydrogenation, Hydrogen, Organic Transformations, Catalysis

220. **CRITICAL VACANCY-DRIVEN PHENOMENA IN HIGH ENERGY ION-IMPLANTED SILICON (ORL 98-18)**
$125,000
DOE Contact: Walter M. Polansky, (301) 903-5995
ORNL Contact: Tony E. Haynes, (423) 576-2858

High-energy (MeV) ion implantation is now being rapidly introduced into integrated circuit manufacturing because it promises process simplification and improved device performance. However, high-energy implantation introduces an imbalance of excess vacancies and vacancy cluster defects in the near surface region of a silicon crystal, which can cause problems during subsequent processing. The objective of this project is to develop sufficient understanding of the physical mechanisms underlying the evolution of these defects and interactions with dopant atoms to enable accurate prediction and control of dopant diffusion and defect configurations during processing. By teaming Oak Ridge National Laboratory with Bell Labs and Brookhaven National Laboratory, the project has access to a suite of new, complementary capabilities for experiments and modeling that promises to elucidate the vacancy behavior. To accomplish the project's objective, a systematic method to generate large, controllable, and spatially isolated vacancy concentrations in silicon will be developed using high-energy implantation. This method will permit unprecedented flexibility and sensitivity in experiments designed to measure interactions involving vacancies and vacancy clusters. The evolution of vacancy profiles during thermal treatments will be monitored by conventional techniques such as positron annihilation spectroscopy, as well as some new methods that have just been developed by this team over the last 1-3 years. For instance, the team has just demonstrated a new method to measure X-ray diffuse scattering in cross section using submicron beam at the Advanced Photon Source at Argonne National Laboratory, as well as a method to measure vacancy cluster depth profiles by labeling them with gold atoms. For a better understanding, the experimental results will be modeled using computer simulations developed at Bell Labs. Improved physical models and simulation parameters will be derived in this project that will reduce the development time and cost for the introduction of new high energy implant processes into manufacturing. This project will directly benefit the telecommunications and microelectronics industries, and contribute to improvements in cost and performance for a wide range of high-tech products, from computers and cellular phones to digital television. This project supports the DOE mission in advanced processing of electronic materials.

Keywords: Ion Implantation, Vacancies, Defects, Dopant Atoms, Silicon Integrated Circuits

221. **DEVELOPMENT OF BUFFER LAYERS SUITABLE FOR DEPOSITION OF THICK SUPERCONDUCTING $YBa_2Cu_3O_7$ LAYERS BY POST-DEPOSITION ANNEALING PROCESS (BNL 98-05)**
$125,000
DOE Contact: Walter M. Polansky, (301) 903-5995
BNL Contact: M. Suenaga, (516) 344-3518

The goal of this project is to develop a textured buffer layer on top of a metallic substrate, e.g., a textured Ni, which is compatible with the Brookhaven National Laboratory method of fabricating thick $YBa_2Cu_3O_7$ films a post-deposition annealing method. In order to accomplish this, the project has started: (1) the purchase and installation of a textured measurement attachment to an existing X-ray apparatus (This makes it possible to determine the degree of the texture of the buffer layer as well as the substrate and $YBa_2Cu_3O_7$ layers.), and (2) testing of the chemical compatibility of CeO_2 with $YBa_2Cu_3O_7$ layers at the high temperature required for the formation of $YBa_2Cu_3O_7$ layers. A texture measuring attachment to a X-ray diffractometer was purchased and was installed such that a texture analysis of the rolled tapes, the buffer, or the superconducting films can be determined. This unit has been delivered and installed, and the process of a final acceptance of the unit is being performed. Since the post-deposition annealing process for growing thick (>5 μm) $YBa_2Cu_3O_7$ involves heat treating $YBa_2Cu_3O_7$ precursor films in a moist atmosphere at high temperatures (>725° C), it is important to select a buffer layer material which does not interfere with the growth of $YBa_2Cu_3O_7$. In order to study this, the project has initially deposited a $YBa_2Cu_3O_7$ precursor film on a CeO_2 buffered single crystalline $LaAlO_3$ and heat treated it to form a $YBa_2Cu_3O_7$ layer on top of the CeO_2. Note that CeO_2 is a well-known buffer layer which is used in conjunction with pulsed laser deposition of $YBa_2Cu_3O_7$. Although a significant reaction takes place between the $YBa_2Cu_3O_7$ and CeO_2 layers if they are heat-treated above 750°C, the reaction appears to be sufficiently minimized by keeping the reaction temperature below 735°C. A further study is being conducted to see the extent of the reaction, and other possible candidates for the buffer materials are being examined. If this project is successful, the superconducting tapes will be used in electrical utility systems, greatly increasing the efficiency of power transmission. This project supports DOE's mission through increased energy efficiency.

Keywords: Superconducting Oxides, Buffer Layers, Deposition of Thick Film, YBCO Buffer Layers, Electrical Utility Systems

222. NEW MATERIALS FOR RECHARGEABLE LITHIUM BATTERIES (BNL 98-04)
$125,000
DOE Contact: Walter M. Polansky, (301) 903-5995
BNL Contact: X. Q. Yang, (516) 344-3663

The goal of this project is to develop new electrolyte and cathode materials for rechargeable lithium batteries, especially for lithium ion and lithium polymer batteries. Enhancing performance, reducing cost, and replacing toxic materials by environmentally benign materials, are strategic goals of DOE in lithium battery research. This project will address these goals on two important material studies, namely the new electrolytes and new cathode materials. For the new electrolyte materials, additive organic lithium salts, and plasticizers which have been developed by Brookhaven National Laboratory (BNL) will be evaluated by Gould Electronics for potential use in commercial battery cells. New additive compounds for lithium battery electrolytes have been synthesized by BNL. Preliminary studies of using these compounds together with lithium fluoride salt in lithium battery electrolytes are very promising. These compounds will be further studied by Gould. For the cathode material studies, the project will develop new superior characterization methods, especially *in situ* techniques utilizing the National Synchrotron Light Source. *In situ* X-ray absorption and X-ray diffraction spectroscopy will be used to study the relationship between performance and the structural characteristics of intercalation compounds such as $LiNiO_2$, $LiCoO_2$, and $LiMn_2O_4$ spinel. Using samples supplied by Gould, very interesting results have been collected through pilot experiments. If the research is successful, the less expensive and more environmentally friendly lithium battery materials (lithium fluoride salt for electrolyte and $LiMn_2O_4$ for cathode) will be developed for commercial applications. This project supports the DOE mission to develop the capability to discover technologically, economically, and environmentally desirable new materials and processes, and the instruments and national user facilities necessary for achieving such progress.

Keywords: Lithium Batteries, Rechargeable, Lithium Ion and Polymers, Electrolytes, Electrodes, New Matrix

223. NONCONSUMABLE METAL ANODES FOR PRIMARY MAGNESIUM PRODUCTION (ANL 98-05)
$210,000
DOE Contact: Walter M. Polansky, (301) 903-5995
ANL Contact: Michael J. Pellin, (630) 252-3510

This project will develop a nonconsumable metal anode to replace consumable carbon anodes now used in commercial electrolysis cells for primary magnesium production. The use and manufacture of consumable carbon anodes, which must be constantly replaced, is costly, energy consuming, and occasions unwanted gaseous emissions such as CO_2 and HCl. In support of the DOE mission for energy efficient, environmentally sound industrial processes, ANL has identified certain metal alloys that are promising candidate materials for nonconsumable anodes. Such alloys form self-limiting surface oxide films that are thin enough to allow current to pass, yet thick enough to prevent attack of the underlying metal. These alloys are dynamic in that the more volatile, reactive components segregate to the surface at rates sufficient to reform the protective film as it dissolves in the chloride melt. The project will form surface films on candidate alloys and investigate them using surface analysis instruments and techniques. Promising alloys will be tested as anodes in bench-scale magnesium electrolysis cells. Cell operation will be monitored and interrupted at key points to remove the anode and investigate its surface film. If desirable, the anode film thickness and strain during electrolysis in specially designed cells will be studied. Alloys identified as optimal will be subject to long-term bench-scale tests by Dow Chemical Company, and then tested in full-scale cells at Dow's production facility in Freeport, Texas. Successful completion of this work will result in increased U.S. competitiveness and lower magnesium prices which would, for example, allow magnesium to be used more widely in the transportation sector, resulting in lower costs there. If successful, stable anodes would reduce the operation cost of making magnesium by 20-30 percent and eliminate the emission of CO_2 and other halocarbon gases during magnesium production by eliminating the need for carbon anodes, now used to produce magnesium electrolytically. Moreover, this work will illuminate the mechanisms associated with film formation on alloys. An understanding of these mechanisms (e.g., surface segregation, near surface diffusion) will provide the basis for developing a new class of corrosion resistant materials that can find application in harsh chemical environments, for example as nonconsumable anodes for aluminum production.

Keywords: Magnesium Production, Metal Anodes, Metal Alloy, CO_2 Emissions, Corrosion Resistant, Film Formation

224. **ADVANCED SEPARATIONS TECHNOLOGY FOR EFFICIENT AND ECONOMICAL RECOVERY AND PURIFICATION OF HYDROGEN PEROXIDE (ANL 98-07)**
$125,000
DOE Contact: Walter M. Polansky, (301) 903-5995
ANL Contact: Edward J. St. Martin, (630) 252-5784

Hydrogen peroxide is an effective oxidant that could be used in many industrial processes. However, the current method for production is inefficient and too costly. Because the only byproduct of oxidation using hydrogen peroxide is water, it could become the ultimate green chemical for the manufacture of oxygenated petrochemicals. The objective of this project is to develop an efficient, economical and safe process for the manufacture of hydrogen peroxide that utilizes advanced membrane separations technology with improved catalysts and processing technology. Argonne National Laboratory will develop an economical separations process for aqueous hydrogen peroxide from organic hydrocarbon containing reaction mixtures based upon pervaporation membrane technology. UOP will provide proprietary hydrogenation catalysts that confer higher specificity and lower losses. Unitel Technologies will provide improved organic formulations and process development. The combination of these three developments in the new hydrogen peroxide process represents a radical departure that promises to significantly change the way hydrogen peroxide is made and used. Not only could this be a simpler, more benign, and less expensive process, but it would also allow the development of new commercial applications and markets for hydrogen peroxide that are currently not competitive. In addition, it could allow small-scale systems to be built on site thus enabling rapid increases in capacity and point of use plants. This project supports the DOE mission in advanced environmental technologies that use advanced membrane technologies for solving fundamental issues in chemical processing and pollution prevention.

Keywords: Hydrogen Peroxide, Separations Technologies, Electrolyte & Cathode Materials, Organic Salts, Commercial Batteries, Lithium Electrolytes

225. **SMOOTH DIAMOND FILMS FOR FRICTION AND WEAR APPLICATIONS AND CHEMICALLY PROTECTIVE COATINGS (ANL 97-05)**
$325,000
DOE Contact: Walter M. Polansky, (301) 903-5995
ANL Contact: Alan Krauss, (630) 252-3520

Diamond has a number of properties which, in principle, make it an exceptional material for a large number of applications. In particular, the extreme hardness (harder than any other known material), chemical inertness (it resists attack by almost all known acids and bases), and low coefficient of friction (comparable with that of Teflon™) make it an ideal candidate for a wide range of applications involving sliding or rolling contact between moving surfaces. However, conventional diamond chemical vapor deposition (CVD) methods produce coatings with extremely rough surfaces. This roughness has limited the development of diamond film technology for tribological applications, and penetration of diamond film technology into these markets has been disappointingly slow. This project concerns the use of a process developed at Argonne National Laboratory for the production of ultra-smooth diamond coatings on rotating and sliding mechanical parts in order to reduce energy consumption, improve product reliability, and reduce toxic emissions into the environment. Films produced by this process have been shown to possess tribological properties which eliminate the problems which have so far limited the use of diamond coatings for applications involving moving parts. The work to be performed addresses adaptation of the process for the production of diamond coatings that are 10-100 times smoother than those produced by existing processes. This technology will be applied to end face mechanical seals, used to prevent the leakage of gases and liquids in equipment with rotating shafts. The benefits obtained in terms of energy savings, increased productivity, reduced maintenance, and reduced release of environmentally hazardous materials for this single application will be substantial. The technology developed will also be directly applicable to may application in manufacturing and transportation, in most cases with similar benefits, supporting DOE's mission for developing environmentally safe energy efficient technologies for the industrial sector.

Keywords: Diamond Films, Friction and Wear, Chemically Protective Coatings, Chemical Vapor Deposition, Diamond Film Technology, Smooth Films

226. **NANOMETER CHARACTERIZATION AND DESIGN OF MOLECULAR LUBRICATION FOR THE HEAD-DISK INTERFACE (LBL 98-10)**
$150,000
DOE Contact: Walter M. Polansky, (301) 903-5995
LBNL Contact: Miquel Salmeron, (510) 486-6704

Information recording density in magnetic storage (hard disks) is currently increasing at an annual rate greater than 60 percent. In the quest for ever higher performance, the trend in the industry is toward even smaller head-to-disk spacing. This project will attempt to characterize and design molecular lubrication for the head-disk interface (HDI). The goal of this project is to design advanced lubricants with properties tailored for the next generation of magnetic storage devices. The read head of a hard disk "Flies" within 10 nanometers of the disk surface, which is protected from damage during accidental contacts by an approximately 2 nanometer thick lubricating film. Although current film thickness is now less than the length of one lubricant molecule, industry standard characterization methods, based on optical techniques, are limited to micron-scale lateral resolution. Liquids exhibit unique physical properties when confined between surfaces separated by molecular dimensions, which have been used to develop a scanning polarization-force microscopy technique that is applicable to ultra-thin liquid films. This is the first non-invasive technique capable of imaging the structure of liquid films with approximately 50 nanometer lateral resolution and sub-nanometer normal resolution. The unique characterization methods developed at LBNL will be used to correlate nanoscale structure and properties with microscale engineering measurements and to develop and verify the performance of optimized, tailored HDI lubricants. The techniques developed at LBNL for the nanometer scale characterization of ultra-thin liquid films and droplets will be applied to determine the actual nanoscale structure, properties, and response to local contacts of head-disk interface lubricants used to identify critical performance parameters, with the final goal of designing an HDI lubricant with optimized wetting and spreading properties tailored for future generations of ultra-high density storage devices. This project supports the DOE mission in the application of basic research developments in materials sciences to new technologies.

Keywords: Characterization and Design, Molecular Lubrication, Magnetic Disk Storage, Advanced Lubricants, Thick Lubricating Films, Nanoscale Structures

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

227. **IONICALLY CONDUCTIVE MEMBRANES FOR OXYGEN SEPARATION (LBL 97-03)**
$225,000
DOE Contact: Walter M. Polansky, (301) 903-5995
LBNL Contact: Steven J. Visco, (510) 486-5821

The global market for industrial oxygen is estimated at $20 billion annually. The dominant technology for the production of commercial oxygen is cryogenic distillation. The high capital equipment costs for cryogenic O_2 separation limits this technology to large installations. Accordingly, industrial suppliers of oxygen are highly motivated to develop technologies that can satisfy increasing demand for oxygen through smaller scale plants. One approach under development elsewhere is the use of mixed ionic-electronic ceramics; when such ceramic electrolytes are exposed to compressed air on one side and ambient pressure on the other, oxygen diffuses through the mixed conductor from the compressed side to the low pressure side due to the chemical potential gradient of oxygen across the membrane. The drawback to this technology is the need for a compressor, which raises issues of noise and reliability. Another problem is that permeation delivers ambient pressure oxygen. In contrast, we propose the efficient electrolytic extraction of oxygen from air using novel thin-film structures consisting of high strength ionic membranes supported on porous, catalytic electrodes. Using this technology, high purity O_2 can be electrochemically pressurized as an integral part of the separation process. The simplicity of operation of an electrolytic O_2 generator promises high reliability as well as low cost. Still, to survive as a commercial process, this approach must be cost-competitive to cryogenic production of O_2 Key to success is highly efficient operation (low power consumption) of the device along with low fabrication costs. Power losses in the electrolytic oxygen cell will be related to ohmic losses across the electrolyte membrane, charge transfer polarization at the electrode/electrolyte interfaces, and mass transfer polarization across the electrodes. The LBNL approach addresses the above issues in such a way that both scientific and technical success are likely. The LBNL team has initiated preparation of porous substrates suitable for colloidal deposition. High temperature furnaces are being installed for sintering of bilayer structures suitable for high oxygen flux in an electrolytic oxygen generator. LBNL is working closely with the industrial partner to ensure maximum productivity of this collaborative effort. This research supports the DOE mission in materials research and applications.

Keywords: Oxygen, Membranes, Separation, Ceramic Electrolytes, Catalytic Electrodes, Oxygen Generators

228. **LIGHT EMISSION PROCESSES AND DOPANTS IN SOLID STATE LIGHT SOURCES (LBL 97-13)**
$250,000
DOE Contact: Walter M. Polansky, (301) 903-5995
LBNL Contact: Eugene Haller, Eugene Haller, (510) 486-5294

Light emitting diodes (LEDs) functioning in the red and infrared have been manufactured in large quantities since the 1960s. However, until very recently, only very inefficient and dim LEDs were available in the green and, especially, in the blue. Although there are a handful of semiconducting materials with sufficiently wide bandgaps to function in principle in the blue region of the spectrum, fundamental material properties and limitations have prevented bright and efficient diodes from being made. Recently, breakthroughs in the heteroepitaxial growth of gallium nitride (GaN) and its alloys with indium and aluminum have changed the blue and green LED technology outlook. Formerly, it was believed that III-V nitride layers had too high a defect density to function as LEDs. Nevertheless, a Japanese company (Nichia) has developed a family of blue and green LEDs based on GaN that are bright and efficient. For the last three years, Japanese companies have been manufacturing and selling blue GaN LEDs in bulk quantities. This project is a collaboration with HP, the leading U.S. producer of LEDs, to investigate the fundamental light-emitting mechanism in GaN-based LEDs. HP is providing GaN and InGaN layers and structures grown with their metal-organic chemical vapor deposition (MOCVD) equipment. Joint work is being performed in four technical areas: (1) Doping-related strain effects in GaN and InGaN epitaxial layers, (2) Metal/GaN contacts, (3) Localization properties of dopants and defects, and (4) Carrier transport in layers and devices. In the first technical area, it has been shown that compressive film stress and Si concentration, which were found to be positively correlated in previous work, could be varied independently by appropriate changes in growth conditions. This is of considerable importance to HP, because reliable production of thick GaN layers had been limited by cracking induced by the Si dopant. In work related to the localization and transport topics, optical measurements have been performed in diamond anvil cells with p-doped GaN single crystals, GaN, AlGaN, and InGaN single layers, and GaN/InGaN multilayer structures. These results are being used to understand the mechanism of light production in III-V nitrides supporting DOE's mission in materials research.

Keywords: Light Emitting Diodes, Red and Infrared, Hetero Epitaxia, Blue and Green LEDS, GaN, Single and Multi

229. **COMBINATORIAL DISCOVERY AND OPTIMIZATION OF NOVEL MATERIALS FOR ADVANCED ELECTRO-OPTICAL DEVICES (LBL 97-18)**
$250,000
DOE Contact: Walter M. Polansky, (301) 903-5995
LBNL Contact: Xiao-Dong Xiang, (510) 486-4864

Advanced materials are the building blocks of the emerging photonic technologies which are the foundation for a new industrial base. Complex oxide ceramics (ternaries and higher order compounds) exhibit a wide range of technologically significant properties such as the electro-optic effect. The rapid expansion in the types of phenomena exhibited by modern advanced ceramics has revived interest in the use of complex oxides for advanced optical device applications. This project directly supports DOE's interests in materials research for advanced ceramic applications. However, due to the complexity of multi-component oxides, searching for new materials or optimization of existing materials has become a forbidding task for the materials community. This project will: (1) use the method of combinatorial synthesis and screening, recently developed at LBNL, to evaluate a wide range of oxide materials and compounds and optimize the advanced oxide materials for electro-optical devices; and (2) use heteroepitaxial thin film growth methods, developed at NZAT, to fabricate advanced oxide electro-optical devices based on search and optimization results. The goal of this project is to produce commercially viable advanced electro-optical devices. If successful, this project will play an important role in forming a strong foundation for the emerging large scale integrated optics device industry.

Keywords: Photonic Technologies, Oxide Ceramics, Multi-Component Oxides, Electro-Optical Devices, Synthesis, Thin Films

230. **DEVELOPMENT OF A THIN FILM BATTERY POWERED TRANSDERMAL MEDICAL DEVICE (ORL 95-11)**
$165,000
DOE Contact: Walter M. Polansky, (301) 903-5995
ORNL Contact: John B. Bates, (423) 574-6280

Heart and brain activity are monitored by measuring microvolt signals developed on the surface of the skin using transdermal electrodes. The first objective of this project was to develop a thin-film battery-powered preamplifier that would attach directly to these electrodes so that the small electrocardiogram (EKG) and electroencephalogram (ECG) signals could be amplified before transmission to the recording unit. These "active" electrodes will eliminate the effect of interference from ac pickup in the long cables from the recording unit and improve the reliability in diagnosing heart or brain malfunctions. By incorporating batteries into the circuit to power the amplifiers, no change to existing EKG or ECG recording equipment is required. A thin-film lithium battery was developed that exceeds the requirements of Teledyne's transdermal-electrode application. The battery, which is based on a $LiCoO_2$ cathode, was fabricated directly onto the backside of the multi-chip modules developed by Teledyne as a prototype electrode preamplifier. This was the first demonstration of integration of thin-film batteries into electronic devices. When developed, the active electrodes will significantly improve the reliability of EKG and ECG diagnostic measurements and thereby help to improve the quality of patient care at a lower cost. The second objective of this project is to demonstrate manufacturing of thin-film batteries in a pilot scale facility at Teledyne. The cathode and electrolyte films deposited at Teledyne are being shipped to ORNL for a comparison of their properties with those grown at ORNL. To date, Teledyne has fabricated excellent $LiCoO_2$ cathode films over areas nearly 40 times larger than possible at ORNL. Batteries fabricated at Teledyne will be evaluated at ORNL. If they meet the rigid requirements of the medical device, full-scale manufacturing will follow. Teledyne has licensed ORNL's thin-film battery technology for application in medical devices. The work performed in this project supports DOE's Basic Energy Sciences programs in advanced battery technology and advanced ceramics.

Keywords: Thin-Film Batteries, Transdermal Medical Devices, Lithium, Multi-Chip Modules

231. **DEVELOPMENT OF MULTI-CHANNEL ASICS FOR CdZnTe GAMMA DETECTOR ARRAYS (BNL 97-06)**
$191,000
DOE Contact: Walter M. Polansky, (301) 903-5995
BNL Contact: Paul O'Connor, (516) 344-7577

The objective of this project is to develop an X-ray imaging module consisting of a multi-element Cadmium Zinc Telluride (CZT) detector and a CMOS application-specific integrated circuit (ASIC). The module will detect X and gamma rays in the energy range from 20-150 keV in the photon counting mode. The electronics must be compatible with the CZT detector characteristics and at a minimum preamplify and shape the pulse signals from the detector elements. There is currently a large need for solid state gamma and X-ray imaging capability for both medical and industrial applications. In industry, a need exists for imaging food products for foreign matter, non-contact, high speed weighing of consumer products to ensure minimum weight compliance and multi-energy high speed imaging of manufactured products to detect subtle defects. Solid state CZT arrays offer the possibility of reducing the weight and bulkiness of existing nuclear medicine cameras based on NaI scintillators and photomultiplier angular camera technology. Small hand-held imaging devices show promise for locating cancer tissue during surgery through the use of monoclonal antibodies tagged with radioactive tracers. For security screening, CZT arrays when used with multi-energy X-rays can detect explosives and other contraband. The technical approach consists of the evaluation of the performance of various existing BNL circuits with CZT arrays, adapting the existing design so that the front end and shaping parameters are ideally matched to the CZT detectors, producing a prototype array of a certain size by tiling arrays and ASIC circuits, developing a 64 or greater channel ASIC for larger substrates (or finer pitch), and configuring existing building blocks to build a multiplexing and image processing ASIC. The development of these solid-state detectors will benefit DOE mission areas in time-resolved X-ray crystallography, nuclear medicine, and extended X-ray absorption.

Keywords: ASICs, CdZnTe Detector Arrays, Solid State Detectors

232. **MICROCIRCUITS AND SENSORS FOR PORTABLE, LOW-POWER DATA COLLECTION AND TRANSMISSION (BNL 97-07)**
$243,000
DOE Contact: Walter M. Polansky, (301) 903-5995
BNL Contact: Paul O'Connor, (516) 344-7577

The objective of this project is to design, fabricate and test two novel devices for data collection and transmission: an optical photosensor array and a 2.4 GHz, single-chip, frequency-agile radio transceiver. Both devices can be processed in a standard CMOS integrated circuit process. CMOS technology has advanced to the point where many conventional electronics systems can be fully integrated on a single chip. Up to now the vast majority of these chips perform purely electronic functions. In this project we propose to investigate two integrated circuits with sensors which can process information in the form of radio-frequency waves and optical images. Our project goal is to develop an inexpensive single-chip frequency agile RF transceiver operating at the 2.4 GHz range—a universally accepted unlicensed band—with data rates up to 250 Kbps and an approximate range of 50 feet. We have previously demonstrated successful circuit blocks and will be seeking to use a higher performance CMOS 0.35 micron process to achieve lower power consumption and higher integration density. For the optoelectronic imaging portion of this project, we will investigate the "active pixel" architecture. This architecture uses photodiode sensors which can be made in a native CMOS process. The imaging array requirements (pixel size and count, spectral responsivity, speed, signal-to-noise ratio, dynamic range, linearity, crosstalk, and power consumption) will first be specified based on a knowledge of the 2D bar code reader system. We plan to model alternative photodetectors using the semiconductor device simulation codes currently used at BNL for silicon radiation detector development. This project supports the DOE mission in advanced semiconductor research for development of crosscutting sensor technologies.

Keywords: Data Collection and Transmissions, CMOS Process, Integrated Circuits, Microcircuits, Sensors, Imaging Arrays

233. **MICROFABRICATED INSTRUMENTATION FOR CHEMICAL SENSING IN INDUSTRIAL PROCESS CONTROL (ORL 97-08)**
$260,000
DOE Contact: Walter M. Polansky, (301) 903-5995
ORNL Contact: J. Michael Ramsey, (423) 574-5662

The monitoring of chemical constituents in manufacturing processes is of economic importance to most industries. The monitoring and control of chemical constituents may also be of importance for product quality control or, in the case of process effluents, of environmental concern. The most common approach now employed for chemical process control is to collect samples which are returned to a conventional chemical analysis laboratory. The objective of this project is to demonstrate the use of microfabricated structures, referred to as "lab-on-a-chip" devices, that accomplish chemical measurement tasks that emulate those performed in the conventional laboratory. The devices envisioned could be used as hand portable chemical-analysis instruments where samples are analyzed in the field or as emplaced sensors for continuous "real-time" monitoring. This project will focus on the development of filtration elements and solid phase extraction elements that can be monolithically integrated onto electrophoresis and chromatographic structures pioneered at ORNL. Successful demonstration of these additional functional elements on integrated microfabricated devices will allow lab-on-a-chip technologies to address real world samples that would be encountered in process-control environments. The resultant technology will have broad application to industrial environmental monitoring problems such as monitoring municipal water supplies, waste-water effluent from industrial facilities, or monitoring of run-off from agricultural activities. The technology will also be adaptable to manufacturing process control scenarios. This project supports DOE missions in environmental quality and energy efficiency.

Keywords: Microfabricated Instrumentation, Chemical Sensing, Industrial Process Control, Lab-On-A-Chip Devices, Chemical Analysis, Environmental Monitoring

234. **AUTOMOTIVE UNDERHOOD THERMAL MANAGEMENT ANALYSIS USING 3-D COUPLED THERMAL-HYDRODYNAMIC COMPUTER MODELS (ANL 98-14)**
$250,000
DOE Contact: Walter M. Polansky, (301) 903-5995
ANL Contact: David P. Weber, (630) 252-4576

The underhood of most contemporary vehicles presents an adverse environment for the operation of sensitive components. Aerodynamic, package and styling requirements reduce the size of the under-hood compartment and the size of the front openings, while new components are constantly added in an already congested space. These trends lead to a reduction in the available under-hood cooling flow and to increased temperature levels. Such levels, under adverse operating conditions, can cause the malfunction or failure of sensitive components. Early diagnosis and remedy of such potential problems during the design stage can significantly reduce the design time and cost, as well as increase the vehicle reliability. The vehicle manufacturers have recognized that it is desirable to replace the current practice of building and testing expensive prototypes with a numerical approach that can quickly and effectively analyze various designs and direct the designers toward the most efficient solution. The goal of this project is to develop and integrate thermal models for convective, conductive, and radiative heat transport, and to develop models for critical heat management system components including fan and heat exchangers. Substantial effort will be placed on improving the numerical solution algorithms for modeling the behavior of these three-dimensional thermal-hydraulics systems on state-of-the-art massively parallel computers. Extensive verification and validation of the resulting models will be performed by comparison to detailed thermal-hydraulics systems on state-of-the-art massively parallel comuters. Extensive verification and validation of the resulting models will be performed by comparison to detailed thermal and flow measurements and industry standard computational solutions. The development of a state-of-the-art commercial software product may be useful beyond the automotive thermal management analysis provided by this project. Applications in transportation, power generation, chemical and food processing, building and environment engineering, mechanical engineering, electronics, and the oil and gas industries can be expected. This project will also develop the ability to numerically test alternative under-hood automotive configuratations. As more and more electronic components are added to the engine in an ever decreasing space, the need to understand and manage the thermal loads under the hood become critical. This will reduce the necessity of costly experimentation and prototyping and result in faster time to market as well as reduce costs. This project supports the DOE mission to develop and apply advanced numerical algorithms and modeling on massively parallel computers.

Keywords: Automotive, Thermal Management, Computer Models, Massively Parallel Computers, Commercial Software

235. **THE DEVELOPMENT OF RHENIUM-188-LABELED RADIOACTIVE STENTS FOR PREVENTION OF RESTENOSIS AFTER CORONARY BALLOON ANGIOPLASTY (ORL 98-31)**
$129,000
DOE Contact: Walter M. Polansky, (301) 903-5995
ORNL Contact: F. F. Knapp, Jr., (423) 574-6225

Two approaches for restoring blood flow to the heart are "coronary bypass graft surgery" and "coronary angioplasty" a less expensive clinical procedure, where inflation of a small balloon in the blocked artery restores blood flow. Over 400,000 coronary angioplasties are performed annually in the United States. The reformation of arterial blockage (restenosis) following angioplasty, however, is a major clinical problem since the biological response to this vessel damage is stimulation of accelerated growth of arterial smooth muscle cells. Estimates from the American Heart Association indicate a restenosis incidence as high as 39-40 percent. Therefore, over 120,000 patients per year with coronary restenosis would benefit from methods which would inhibit restenosis of coronary arteries after the angioplasty procedure. The purpose of this project is to develop a new strategy using radioactive stent structures for coronary artery therapy to inhibit restenosis following coronary balloon angioplasty. The use of short-lived radioactive stents is expected to provide a "platform" to keep the vessel open so sufficient radiation to the vessel wall can inhibit restenosis. In addition, this approach will use the same widely used technology for placement of stents by high-pressure balloon expansion. The only difference is that the stent will be radioactive, which requires the institution of radiation protection procedures but does not require new equipment or technical procedures The objective of this project is the development of fabrication methods which are convenient, economical, routine, capable of being performed in hospitals and other user facilities, and capable of incorporating a choice of radioisotopes such as rhenium-188 which have appropriate dosages required for this application. This project supports DOE's mission of promoting beneficial applications of nuclear technology in human health.

Keywords: Rhenium-188, Radioactive Stents, Coronary Balloon Angioplasty, Arteries, Arterial Blockage, Nuclear Technology

236. **NEAR-FRICTIONLESS CARBON COATINGS (ANL 98-03)**
$125,000
DOE Contact: Walter M. Polansky, (301) 903-5995
ANL Contact: Ali Erdemir, (630) 252-6571

Numerous industrial applications involve the use of mechanical devices containing components that slide or roll against one another. The efficiency and durability of these components are often limited by the friction and wear properties of the materials used to fabricate the components. For example, Diesel Technology Company (DTC) and Stirling Thermal Motors (STM) develop advanced energy conversion systems and engine components that will contribute significantly to reducing oil imports and improving air quality by reducing engine emissions. Fuel injection systems being designed and developed by Diesel Technology for use in heavy-duty diesel engines will require tighter tolerances to run on low-lubricity fuels at higher operating pressures needed to achieve emissions and efficiency goals. Since materials used in current fuel injection systems will not survive under these aggravated conditions, new materials and/or coatings are needed. Similarly, Stirling engines being designed by Stirling Thermal Motors will operate under tribological conditions (e.g., speeds, temperatures, loads, and working fluids) not commonly encountered, and will require advanced materials, coatings, and lubricants to ensure long-term durability. Argonne will work with Front-Edge Technologies (FET) to commercialize Argonne's technology for fuel injection systems and Stirling engine components being developed by DTC and STM. The objectives of this project are to: (1) advance the basic understanding of the physical/chemical and tribological processes controlling the friction and wear behavior of the new carbon films, (2) demonstrate the ability of these coatings to improve the friction and wear performance of materials and components being developed by Diesel Technology and Stirling Thermal Motors, and (3) demonstrate that the coating technology can be scaled-up to coat large numbers of components on a cost-competitive basis. If successful, the NFC technology will have a significant impact not only on the technology being pursued by DTC and STM, but also in other applications found in the aerospace, biomedical, and manufacturing sectors. It builds on expertise at Argonne in tribology, coatings, and materials characterization. This project supports DOE missions in advanced materials and sustainable environments, reducing U.S. dependence on foreign oil imports, and improving U.S. air quality. This project won an R&D Award in 1998.

Keywords: Carbon Coatings, Friction and Wear, Fuel Injection, New Materials, Coatings, Tribology

237. **DEVELOPMENT OF HIGH-TEMPERATURE SUPERCONDUCTING WIRE USING RABiTS COATED CONDUCTOR TECHNOLOGIES (ORL 97-02)**
$260,000
DOE Contact: Walter M. Polansky, (301) 903-5995
ORNL Contact: David K. Christen, (423) 574-6269

High-temperature superconducting (HTS) materials hold promise for greatly improved energy efficiency in a number of power applications related to the production, distribution, storage, and utilization of electric energy. This project is directed at developing a new route to the fabrication of high-temperature superconducting wires for such power applications. The approach is based upon a recent breakthrough, referred to as RABiTS (Rolling Assisted Biaxially Textured Substrates), at the Oak Ridge National Laboratory (ORNL). The approach exploits the growth of crystalline biaxially-aligned coatings on long-length oriented metal tapes that are produced by simple thermomechanical processing. The achievement of biaxial texture is essential for the transport of large, loss-free electric currents, especially in the presence of magnetic fields. In the RABiTS approach, passivating "buffer" layers are deposited by electron beam and sputter deposition, and HTS coatings are deposited by electron-beam evaporation. The project is determining the scientific and technical feasibility of making long-length coated conductors that can provide operating characteristics that are currently unattainable by electrical conductor, including present prototype HTS tapes that utilize the "power-in-silver-tube" fabrication approach. ORNL research focuses on both the simplification and optimization of oxide buffer layers on reactive metals in general, and specifically is developing a simplified *ex situ* approach to the co-evaporation and processing of the superconductor coatings. Recent advances at ORNL using this approach have resulted in short-segment prototype conductors with critical current densities of over a million amps/cm at liquid nitrogen temperature. 3M is actively developing the scale-up of these techniques for the production of long-length tapes in a "continuous" process. 3M has established experience base in high-rate deposition of many materials in manufacturing technologies. Southwire is the leading U.S. manufacturer of utility wire and cable and is a retailer of under ground transmission lines capable of 2-5 times the power transfer into urban areas, without the need for additional rights-of-way and without significant losses to resistance. Other applications, such as power transformers, motors, current limiters, and magnetic energy storage, are projected to produce markets of tens-of-billions of dollars per year. This project supports DOE's mission to develop high-temperature superconductors.

Keywords: High Temperature Superconducting Materials, Superconducting Wire, RABiTS Technology, Fabrication, Reactive Metals, Magnetic Energy/Storage, Power Transformer and Motors, Current Limiters

238. **THIN FILM THERMAL BARRIER COATINGS (PNL 95-07)**
$15,000
DOE Contact: Walter M. Polansky, (301) 903-5995
PNNL Contact: Edward L. Courtright, (590) 375-6926

The objective of this project is to demonstrate the feasibility of reducing the thermal conductivity of zirconia base thermal barrier coatings with nanoscale multi-layer designs. If improved thermal barriers can be developed, both aircraft and land-based stationary gas turbines can be operated at higher temperatures, resulting in better efficiency and substantial energy savings, contributing to DOE's energy conservation mission. Multi-layer coatings can be designed to maximize infrared reflectivity while taking advantage of the phonon scattering that occurs at interfaces. The thermal dynamic stability issues that affect durability, reliability, and life-cycle performance are being investigated. Independent thermal diffusivity measurements performed by the National Institute of Standards and Technology on coatings made of alternating layers of zirconia and alumina, developed in the project, have shown that nanoscale multi-layers do significantly lower thermal conductivity compared to baseline coating. The multi-layers have also been found to retain their improved thermal performance even after extended exposure at 1200°C for 1000 hours or more. Adherence has been found to be substrate dependent, and such issues are currently being addressed. While the coatings appear to have good intrinsic toughness, process parameters such as deposition rate, rotational speeds, and temperature must be carefully controlled to obtain this characteristic.

Keywords: Thin Film Coatings, Multi-layer Coatings, Thermal Barriers, Aircraft and Stationary Turbines, Thermal Conductivity, Energy Conservation, Zirconia and Alumina Coatings

239. **THIN FILM LITHIUM BATTERIES (BNL 95-11)**
$ 22,000
DOE Contact: Walter M. Polansky, (301) 903-5995
BNL Contact: James McBreen, (516) 344-4513

This project is focused on low-cost electrolytes and cathode materials for thin-film lithium ion batteries. Present commercial batteries use $LiCoO_2$ which gives the most consistent performance and life but is expensive. Lower-cost materials would broaden applications beyond the present high-end applications such as laptop computers and camcorders. Possible lower cost substitutes are $LiMn_2O_4$ or $LiNiO_2$. Reproducibility and cycle life of these materials is a problem. In this project, Brookhaven National Laboratory has evaluated several types of $LiMn_2O_4$ and $LiNiO_2$ as well as mixed transition metal lithium oxides. Extensive *in situ* X-ray absorption (XAS) studies were done on these materials at the National Synchrotron Light Source. This was supplemented by both *in situ* and *ex situ* X-ray diffraction (XRD) studies. The results of these studies were correlated with material stability of cycling. The results of tests in small lithium cells showed that the most critical parameters in determining material stability were the temperature of preparation, the stoichiometry, and the use of dopants. This project supports DOE's missions in energy efficiency and alternative energy sources.

Keywords: Thin-Films, Thin-Film Batteries, Lithium Ions, Lithium Spinels, Energy Efficiency, Alternate Energy Sources

INSTRUMENTATION AND FACILITIES

240. **A FACILITY FOR STUDYING MICROMAGNETIC STRUCTURES (LBL 95-12)**
$300,000
DOE Contact: Walter M. Polansky, (301) 903-5995
LBNL Contact: Howard Padmore, (510) 486-5787

The objective 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 Advanced Light Source at Lawrence Berkeley National Laboratory, and 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 (X-MCD). 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. IBM will use the information from the studies to advance the technology of high-density information storage, thereby assisting the development of new products such as non-volatile magnetic random access memories. The PEEM1 Microscope has been fully commissioned, and its spatial resolution has been demonstrated at 0.3μm. The utilization of this microscope has continued in order to develop the application of photoemission microscopy to thin film materials science. Work on understanding the dewetting of layered polymer systems has continued, as has work on surface reactions induced in the lubricated surfaces of the disc-head interface in commercial magnetic disc drives. This is leading to a better understanding of the optimization of lubricants for reduction of wear. Beamline 7.3.1 is complete and has met its goals of focused spot size and intensity. The polarization chopping system was also installed, commissioned, and is now driven from the beamline control system. The new 30 KV microscope is now working, and is being commissioned under full computer control of all functions. The project's initial work has shown the resolution to be better than 50 nm as shown by analysis of the imaging of single 100 nm gold colloid particles, and the domain structure of 18μm square iron thin film pads (passivated by a thin surface layer of SiC) has been imaged. These show excellent elemental and magnetic contrast, with complete contrast reversal with use of left/right circularly polarized light. The sample transfer system has been installed, and now the work of using the microscope to study the growth and magnetic structure of layered magnetic thin films can begin. The project supports DOE's mission to develop improved materials.

Keywords: Microscopic Imaging, Magnetics, Information Storage, Layered Thin Films, Photo-Emission Microscopy, Micro Magnetic Structures

241. **CONTROLLED NONISOTHERMAL HOT FORGING USING INFRARED FOR MICROSTRUCTURAL CONTROL (ORL 98-08)**
$226,000
DOE Contact: Walter M. Polansky, (301) 903-5995
ORNL Contacts: Craig A. Blue and Howard Padmore, (423) 574-4357

Hot forging is a widely used method for making metal parts from automobile and aircraft components to hand tools. Forging is a plastic deforming of metal into desired shapes by compression, usually with one or more dies to control the shape. Forging is a $50 billion industry in the U.S. and employees 400,000 people. The heating of metal pieces prior to forging consumes large quantities of energy. Current heating practices require that an entire billet be heated to a uniform temperature prior to forging, even though only a portion of that material requires heating to that high temperature to achieve the desired plastic deformation. The goal of this project is to demonstrate the use of infrared heating to achieve controlled local heating of steel forging billets to permit forging with reduced heating requirements and with improved control of properties in the finished part. Infrared heating makes use of quartz halogen lamps to provide rapid radiant heating of metal surfaces in an easily controlled manner. This provides the means for controlled rapid local heating superior to heating methods currently used in the forging industry. In this project, experimental studies of the heating and forging processes will be combined with computer modeling of the process to demonstrate the application of this new technology to a variety of forging applications. These include forging restrikes in which the forged part is rapidly reheated and immediately forged again to produce more complex shapes which are not now forged economically. The structure and properties of material forged with this new method will be characterized. The results will be incorporated into the computer models currently in widespread use in the industry so that optimal forging conditions, and cost and energy benefits, can be predicted for each new part. The development and use of this technology will result in reduced manufacturing costs for a wide range of consumer goods. It will also reduce energy consumption in the forging industry resulting in low consumption of fossil fuels and less emission from electric power generating plants. This project support DOE's mission to develop energy efficient industrial processes.

Keywords: Hot Forging, Infrared Heating, Energy Savings

242. **MICRO-ORGANISM DETECTION AND CHARACTERIZATION (PNL 98-03)**
$125,000
DOE Contact: Walter M. Polansky, (301) 903-5995
PNNL Contacts: Darrell P. Chandler and Howard Padmore, (509) 376-8644

Rapid and accurate detection of Micro-organisms is important in a number of health-related and environmental application, such as food safety, wastewater treatment, disease diagnosis, forensics, and bioremediation monitoring. Recently, genosensor technology has been developed within context of clinical diagnostics to detect up to 10^6 *different* gene targets simultaneously. Such technology has the potential to significantly improve Micro-organism detection and characterization in environmental samples. However, the widespread application of this technology has been limited by the costs and time required for sample preparation and analysis. The objective of this project is to develop a versatile, fully integrated, automated, high throughput gene-based detector for broad application in health related and environmental fields. Pacific Northwest National Laboratory is utilizing its expertise in nucleic acid extraction and characterization from environmental samples, micromachining technology, and microfluidic systems and combing them with proprietary, patented nucleic acid concentration principles, surface chemistries, and detection arrays from Genometrix. The project is directed towards the development of a prototype, integrated detector that can be further enhanced by Genometrix for commercial application, while also contributing to achieving DOE mission objectives in biological research and environmental remediation. The project's first objectives include the synthesis and testing of novel microbead matrices and surface chemistries for their nucleic acid binding properties within several crude environmental nucleic acid extracts (aerosol, wastewater, soil, subsurface sediment), and applying a low-density genosensor array for the quantitative analysis of micro-organisms in an industrial wastewater processing stream. These experiments will represent samples and provide the technical/conceptual foundation for physically coupling a nucleic acid purification module directly to a genosensor array/reader for point-of-use devices for health-related and environmental applications.

Keywords: Micro-Organism Detection and Characterization, Clinical Diagnostics, Micromachining Technology

MATERIALS, PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

243. **THE ROLE OF YTTRIUM IN IMPROVING THE OXIDATION RESISTANCE IN ADVANCED SINGLE CRYSTAL NICKEL-BASED SUPERALLOYS FOR TURBINE APPLICATIONS (ORL 95-07)**
$30,000
DOE Contact: Walter M. Polansky, (301) 903-5995
ORNL Contacts: Edward A. Kenik, (423) 574-5066

The focus of this project is the examination of the role of yttrium and other alloying elements in the micro-structure and oxidation performance of improved single crystal nickel-based superalloys for advanced turbine applications. The microstructure and microchemistry of these alloys and their surface oxides are being measured with state-of-the-art microanalytical techniques (atom probe field ion microscopy and electron microscopy) and then correlated with burner rig and engine test oxidation performance. Recent results have dealt with distribution of alloying elements between the superalloy and the oxide scale, including the formation of Ta oxides in the scale, the oxidation of near-surface HfC particles to HfO, and the segregation of reactive elements to oxide grain boundaries. The overall 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. Anticipated improvements from these modified alloys include enhanced durability in the operating environments at the high temperatures required to improve energy efficiency. In addition, the availability of alloys capable of higher temperature operation will minimize the need for expensive coatings in some applications. These alloys are primarily used for the turbine components in engines which are exposed to the most extreme temperatures. These studies are relevant to both commercial land-based (energy-production) and advanced aircraft turbines used by a wide range of U.S. industries. This project supports DOE's missions in increased energy efficiency and reduced fuel consumption.

Keywords: Yttrium, Microstructure and Oxidation, Alloy Modification, Turbine Components, Energy Efficiency, Reduced Fuel Consumption

244. **NEXT GENERATION CORROSION INHIBITORS FOR STEEL IN CONCRETE (BNL95-12)**
$74,000
DOE Contact: Walter M. Polansky, (301) 903-5995
BNL Contact: Hugh Isaacs, (516) 344-4516

Steel-reinforced concrete is the most widely used construction material in the world. This is almost an ideal composite, with the steel providing tensile strength and the alkaline concrete imparting passivity to the steel. However, passivity can be compromised by the ingress of chlorides from a marine environment or from de-icing salts. To address this problem, corrosion inhibitors are added to the concrete mixture, usually as simple inorganic anions (e.g., nitrite). Both the mechanism of corrosion in a concrete environment and the action of inhibition are not well understood. The goal of this project is to elucidate the action of corrosion and the behavior of inhibitors. The objective of the study will ultimately be to develop more effective inhibition, possibly by the use of mixed anodic/cathodic inhibitors or altering the form in which the inhibitors are added. Corrosion measurements are being made of the anodic and cathodic kinetics taking place in concrete, which describe the processes occurring with and without inhibitors. Nitrite inhibitors have been found to display different degrees of effectiveness at various stages during the development of corrosion. In sufficient quantities, the inhibitors maintain passivity. However, they apparently have little action on the very early stages of passivity breakdown. At a later stage, when corrosion is well developed, corrosion is again influenced by nitrite additions. Very small quantities distinctly reduce the corrosion rates, whereas large additions again act to produce passivity and no corrosion. Efforts are now underway to define more closely the critical factors determining the differences in behavior. X-ray absorption near edge measurements will also be performed to examine the effect (if any) of inhibitors on the structure and chemistry of the passive oxide. Research in this area supports the DOE mission in materials characterization and processing.

Keywords: Steel-Reinforced Concrete, Corrosion, Corrosion Inhibitors, Passivation

245. **ATOMIC SCALE STRUCTURE OF ULTRATHIN MAGNETIC MULTILAYERS AND CORRELATION WITH RESISTANCE, GIANT MAGNETORESISTANCE, AND SPIN-DEPENDENT TUNNELING (ORL 97-03)**
$255,000
DOE Contact: Walter M. Polansky, (301) 903-5995
ORNL Contact: William H. Butler, (423) 574-4845

Giant Magnetoresistance (GMR) and Spin-Dependent Tunneling (SDT) are two recently discovered phenomena that are providing important new insights into how spin affects the transport of electrons in materials. These phenomena have the potential to spark revolutionary advances in several important technologies and both require the controlled deposition of ultrathin films. In order to realize the scientific and technological potential of these phenomena, it is necessary to relate the spin-dependent transport properties to the spin-dependent electronic structure of the deposited structures. Since spin dependent transport is very sensitive to structure at that scale, an understanding of the deposited structures at the atomic scale is required to accomplish that goal. Recent advances in electronic structure theory allow the calculation of spin-dependent transport. The missing key, however, is atomic-scale characterization of the deposited films. Through a close collaboration between theory and experiment, the objective of this project is to determine the physical, chemical, and magnetic structure of GMR and SDT films and to relate their structure to their magnetic and transport properties. This will be achieved by combining a uniquely powerful set of characterization tools, (X-ray Reflection and Diffraction, Atom-Probe Microscopy, Z-Contrast Electron Microscopy with Electron Energy Loss Spectroscopy, and Electron Holography) with first-principles computer codes that are capable of calculating the spin-dependent conductivity for realistic systems. The industrial partners (Honeywell Solid State Electronics Center and Nonvolatile Electronics Inc.) are uniquely qualified to optimize their deposition processes and to relate the structures they deposit to the observed spin-dependent transport. Success in this project should lead to better read sensors for magnetic disk drives, a new type of non-volatile radiation-resistant magnetic random access memory device, and better position and motion sensors for numerous industrial, transportation, and consumer product applications. Additionally, this work enhances DOE's basic materials sciences programs in magnetic structures and advanced characterization methods.

Keywords: Giant Magnetoresistance, Spin-Dependent Tunneling, Electron Transport, Magnetic Multilayers, Atomic Scale Structures

246. **HIGHLY DISPERSED SOLID ACID CATALYSTS ON MESOPOROUS SILICA (PNL 97-28)**
$250,000
DOE Contact: Walter M. Polansky, (301) 903-5995
PNNL Contact: Yong Wang, (509) 376-5117

This project will develop new materials optimized for use as solid acid catalysts by coupling the advanced characteristics of mesoporous silica with the superacidic properties of tungstophosphoric acid and sulfated zirconia. The surface of mesoporous silica will be functionalized to accommodate the dispersion of tungstophosphoric acid and sulfated zirconia. This approach should produce a new class of highly active, shape selective, and robust solid superacid materials. The novel catalysts will be tested with the alkylation and isomerization reactions in the bench and pilot scale testing unit. The goal is to exceed the performance characteristics of existing solid superacid catalysts, thereby enabling the chemical and petrochemical industries to replace homogeneous acid catalysts. This will contribute to DOE's mission to reduce environmental impacts in the energy sector. Homogeneous acid catalysts such as sulfuric acid and aluminum chloride are currently used to catalyze many industrially important reactions. Although these homogeneous acid catalysts are efficient, they are not environmentally benign and create many operational problems. These problems can be mitigated with solid acid catalysts. Tungstophosphoric acid and sulfated zirconia are two solid acid catalysts with super acidity. Low catalytic efficiency is the common problem with these two catalysts. In addition, it is difficult to disperse tungstophosphoric acid on supports due to its large cluster size,, and sulfated zirconia generally suffers rapid deactivation. These problems can be minimized with the superior characteristics of mesoporous silica. This work will enhance understanding of how the mesoporous support properties and acid grafting strategy influence reactivity, yields, selectivity, thermal stability, coking, and regeneration of the solid acid catalysts. In FY 1998, efforts were conducted to define the specific catalyst properties of interest. Synthesis and functionalization of the mesoporous silica supports was also initiated.

Keywords: Solid Acid Catalyst, Mesoporous Silica, Tungstophosphoric Acid, Sulfated Zirconia

ADVANCED ENERGY PROJECTS PROGRAM

The Advanced Energy Projects program (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 program 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

247. **COMPOSITE MAGNETOSTRICTIVE MATERIALS FOR ADVANCED AUTOMOTIVE MAGNETOMECHANICAL SENSORS**
$270,000
DOE Contact: Walter M. 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 Nm without malfunctioning or significantly changing sensitivity over the normal operating range of +/-10 Nm. Analysis of the relationship between the magneto-mechanical 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 promising 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

248. **INVESTIGATION OF HIGH EFFICIENCY MULTI BAND GAP MULTIPLE QUANTUM WELL SOLAR CELLS**
$225,000
DOE Contact: Walter M. Polansky, (301) 903-5995
City College of City University of New York Contact: Robert Alfano, (212) 650-5532

This project will investigate and develop multiple quantum well (MQW) solar cells which are expected to reach much higher efficiency than that obtained from conventional bulk solar cells by reducing radiative and nonradiative relaxation processes through resonant tunneling. The maximum energy conversion efficiency of a conventional bulk solar cell is limited to less than ~33 percent because of its single band gap. Using a novel MQW-based solar cell with multi band gaps, one expects to enhance the maximum energy efficiency to ~72 percent. These high efficiency MQW solar cells have the potential of being widely used in compact computers, space power supplies, micro-scale motors, consumer products, home electronic devices, guide signs, and other renewable energy applications. In preliminary studies, carrier dynamics and band gap structures for GaAs, InP and their alloys have been measured, and the resonant tunneling time and the barrier potential design criteria for achieving maximum energy conversion efficiency in MQW structures have been calculated. Based on these measurements and calculations, several GaAs- and InP-based MQW solar cell structures have been designed and fabricated using the MBE facility at CCNY. The current-voltage (I-V) characteristics of the fabricated GaAs/AlGaAs MQW solar cells have been measured, and an enhancement of energy efficiency for the MQW solar cells over that of the conventional bulk solar cells has been observed. This project will enhance these studies and develop high efficiency multiband gap MQW solar cells. Resonant tunneling times for GaAs/AlGaAs and InGaAs/InP MQW structures will be investigated to make sure that the resonant tunneling process dominates photocarrier collection. The I-V characteristics will be measured and the energy efficiencies for GaAs/AlGaAs and InGaAs/InP MQW solar cells with different well and barrier configurations will be investigated to select the best one. Multi-unit GaAs-and InP-based MQW solar cells will be studied to further increase the range of the band gaps and the energy efficiency. The target for the energy efficiency improvement is at least 150 percent for MQW solar cells over the conventional bulk solar cells. Industrial evaluations will be made by two companies (Applied Solar Energy in California and Plasma Physics in New York) during this project to determine the scientific and commercial potential of the MQW solar cells.

Keywords: Solar Cells, Photovoltaic, Quantum Well, GaAs/AlGaAs, InGaAs/InP

249. **MAGNETICALLY ENHANCED THERMOELECTRIC COOLING**
$250,000
DOE Contact: Walter M. Polansky, (301) 903-5995
LANL 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 $Nd_2Fe_{14}B$ permanent magnets, open the way for development of new ultra-high-performance, all solid-state Ettinghausen refrigerators. Studies of such coolers using modern materials will be initiated to engineer the world's best solid-state cryocooler.

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

250. **EFFICIENT ENERGY UP-CONVERSION OF INFRARED TO VISIBLE LIGHT AT SEMICONDUCTOR HETEROJUNCTIONS**
$243,000
DOE Contact: Walter M. Polansky, (301) 903-5995
NREL Contact: Hyeonsik M. Cheong, (303) 384-6484

A recently-discovered energy up-conversion phenomenon in semiconductor heterostructures will be studied. This phenomenon could be used to make light emitting devices that emit a wide range of colors and even multiple colors or white light. Possible applications for such devices are energy-efficient multi-color displays or a white light source to replace incandescent lamps in some areas. The principal advantage of such devices would be that multiple elements of these up-conversion structures with different emission colors, as well as the excitation source for the up-conversion, can be grown *monolithically* on a single wafer. When $GaAs/AlGaInP_2$ heterostructures are excited with a near-infrared laser at 1.52 eV (815 nm), electrons and holes are created in the lower-band-gap material (GaAs). Some of these electrons and holes are excited to the higher-band-gap material ($AlGaInP_2$), and then radiatively recombine at the band gap of $AlGaInP_2$, giving up-converted luminescence in red, orange, or green depending on the aluminum concentration in the $AlGaInP_2$ alloy. The objective of the study is to demonstrate the feasibility of the devices utilizing this novel phenomenon of up-conversion. In order to achieve this, we will examine various semiconductor heterostructures to find the optimal semiconductor heterostructure system that give the highest up-conversion efficiency. This will require sophisticated band-structure engineering using a number of different semiconductors including GaAs, AlGaAs, $GaInP_2$, and $AlGaInP_2$. We will also perform a systematic study of the mechanism for this up-conversion using both cw and ultrafast optical spectroscopies. The final phase of this project will be devoted to realization of a prototype device in which either vertical-cavity surface-emitting laser structure or a pn junction is used to excite up-conversion luminescence.

Keywords: Light Emitting Diodes, GaAs, AlGaAs, $GaInP_2$, $AlGaInP_2$, Energy Up Conversion, LED

251. **ELECTRICALLY ACTIVE LIQUID MATRIX COMPOSITES**
$300,000
DOE Contact: Walter M. Polansky, (301) 903-5995
ORNL Contact: Robert J. Lauf, (423) 574-5176

Varistors are nonlinear electrical resistors used to protect electrical equipment from the damaging effects of power surges. ZnO varistors are made by standard ceramic processes and are generally formed into cylinders or disks electroded on the end faces. Failure modes include catastrophic fracture, thermal runaway, and slow degradation of electrical properties. "Moldable" surge protective materials, comprising metal and semiconductor particles dispersed in a silicone rubber matrix, are not as nonlinear as ZnO but can be formed into a number of devices by injection molding. The material fails when an arc punches through at one point, leaving a carbonized, conductive path to ground. It has recently been shown that a slurry of metal, insulating, and semiconducting particles in dielectric oil can exhibit the same nonlinearity as the moldable rubber compositions, but with the added features that it is self-healing, thixotropic, and its I-V characteristics can serve as an excellent model system with which to study the poorly-understood electrical phenomena that occur in moldable varistors. This project will: (1) determine the compositional limits for optimal electrical properties and relate these findings to theoretical percolation models; (2) determine the rheological properties of the experimental materials and identify promising avenues for improving them; and (3) determine the dielectric constants and the temperature dependence of key electrical properties.

Keywords: Liquid Matrix Composites, Surge Protectors, Varistors, ZnO

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

252. **NEXT GENERATION HIGH-TEMPERATURE STRUCTURAL MATERIALS FOR HEAT EXCHANGERS AND HEATING ELEMENTS**
$297,000
DOE Contact:Walter M. Polansky, (301) 903-5995
Iowa State University Contact: Mufit Akinc, (515) 294-0744

The project is centered on the development of a new generation of electrical furnace heating elements and heat exchangers. Existing materials for heat exchangers and heating elements are limited by their mechanical and/or oxidative stability at high temperatures. $MoSi_2$ is limited by its low creep strength above 1000°C whereas other metallic or intermetallic materials are limited to about 1000°C. Increasing the temperature capability of existing heat exchangers and heating elements by several hundred degrees and/or providing alternative furnace designs will provide significant energy efficiencies as well as ecological benefits. Recent work in our laboratory shows that boron doped Mo_5Si_3 exhibits outstanding oxidative stability in addition to its excellent high temperature creep strength and high melting point. However, a number of scientific and technical issues remain to be elucidated. An integrated multi-disciplinary approach to synthesis and processing, microstructural, thermomechanical and electrical investigation of select compositions around Mo_5Si_3B is being pursued. The investigation will focus on establishing the fundamental relationship between composition, microstructure, and physical properties of B-doped Mo_5Si_3. In particular, select compositions will be synthesized and sintered to produce dense parts. A number of compositions will be studied for their stability in air and in corrosive atmospheres up to 1500°C. Thermomechanical properties of successful compositions will be investigated as a function of temperature and will be related to their microstructure. Thermoelectric properties such as thermal and electrical conductivity will be determined at temperatures up to 1500°C and above. Optimum compositions will be determined and process scale-up will be considered for heating element and heat exchanger applications.

Keywords: Heating Elements, Resistance Heaters, High Temperature Materials, $MoSi_2$, Mo_5Si_3B

253. **TRITIATED POROUS SILICON: A STAND-ALONE POWER SOURCE**
$260,000
DOE Contact: Walter M. Polansky, (301) 903-5995
ANL Contact: Carl E. Johnson, (630) 252-7533

Tritiated porous silicon could form the basis for a new class of stand-alone power sources that are rugged and portable and have high reliability over a very long period (>10 yr.). The tritium is covalently bonded to the silicon and, thus, cannot escape as a gas into the environment. This material would be able to provide the relatively low-level power requirement of many types of highly integrated devices in optoelectronics and sensor technology. The proposed research involves three tasks: (1) demonstrate the synthesis of tritiated porous silicon; (2) model the synthesis process; and (3) assess the optical activity of this novel material. The objective of this project is to attain proof-of-concept and lay the foundation for development of a commercial device. The data base resulting from the proposed work would provide a firm foundation for future engineering design efforts aimed at device development for specific applications.

Keywords: Porous Silicon, Power Supplies, Tritium

254. **SUPPORTED MOLTEN METAL CATALYSTS: A NEW CLASS OF CATALYSTS**
$240,000
DOE Contact: Walter M. 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 (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 elements, on porous refractory supports, much like supported microcrystallites of traditional solid catalysts. This technique could conceivably provide orders of magnitude higher surface area than that obtainable in conventional reactors containing molten metals in pool form while avoiding 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, initial work will concentrate on dehydrogenation and reforming reactions due to their commercial significance. Thus, dehydrogenation of methylcyclohexane and decalin and reforming of methylcyclopentane will be studied. These represent reactions of increasing complexity in catalytic reforming. The initial choice is 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

255. **COMBINATORIAL SYNTHESIS OF HIGH T_c SUPERCONDUCTORS**
$250,000
DOE Contact:Walter M. Polansky, (301) 903-5995
LBNL Contact: X. D. Xiang, (510) 486-6640

Currently, there is tremendous interest in materials such as high temperature superconductors, organic conductors, permanent magnets, nonlinear optical materials and zeolites. However, even though 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, quaternary, and higher order solid state compounds, in order to discover materials with novel electronic, optical, magnetic or mechanical properties. A new approach to materials discovery is being developed 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, 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

256. **MICRO-HOLLOW CATHODE DISCHARGE ARRAYS: HIGH PRESSURE, NONTHERMAL PLASMA SOURCES**
$210,000
DOE Contact: Walter M. 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 tens of microns, 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 is studying the physics of micro-hollow cathode discharge operation in a positive differential conductivity mode. Particularly, the conditions for discharge array operation at atmospheric pressure are being explored, concentrating on the electron energy distribution and the spectral emission of micro-hollow cathode discharges. This project is focusing 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 (VOCs).

Keywords: Plasma Sources, Hollow-Cathode Discharge

257. **EXPERIMENTAL AND THEORETICAL INVESTIGATION OF DUAL-LASER ABLATION FOR STOICHIOMETRIC LARGE-AREA MULTICOMPONENT FILM GROWTH**
$113,000
DOE Contact: Walter M. Polansky, (301) 903-5995
University of South Florida Contact: Sarath Witanachchi, (813) 974-2789

A novel dual-laser ablation process was recently discovered 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_2O_3 that were not possible with single excimer laser ablation. This provided the motivation for investigating 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. A systematic study will be used 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 will be used. 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 systems. 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

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

258. **SHAPE MEMORY ALLOY REINFORCEMENT OF METALS**
$195,000
DOE Contact: Walter M. Polansky, (301) 903-5995
ORNL Contact: Terry N. Tiegs, (423) 574-5173

A dispersed phase of shape memory alloy (SMA) has been employed to increase the hardness of a metal system. The hardness is well known to be directly related to the yield strength of the material and therefore a corresponding increase in the yield strength of the metal system is implied. The SMA works by generating an internal stress state in the matrix metal thereby increasing the stress required for yielding of the metal. The initial effort for the proof of principle used aluminum as the matrix material and NiTi for the shape memory alloy. The basic concept utilizes a dispersion of shape memory alloy particles in a metal matrix to induce internal stresses that increase the hardness and yield strength of the metal. The shape memory effect is a well known phenomenon observed in several material systems. When a SMA is mechanically deformed while below a specific transition temperature, it will return to its original shape, when the temperature is raised above the specific temperature. The shape memory alloy reinforcement of metals (SMART) works by: (1) taking a powder metallurgy-produced two-phase composite consisting of SMA particles dispersed in a metal matrix; (2) deforming the composite below the transition temperature; and (3) raising the temperature above the transition temperature to trigger the shape memory effect and induce internal stresses within the composite. Increasing the yield strength and hardness of materials is of considerable importance. Possible applications for SMART include high strength and lightweight structures for vehicles and industrial parts. Also these materials may be used for sensors and actuators where the reversibility of the shape memory effect could be utilized. To progress past the initial development stage for SMART, additional research and development is required. Such R&D would include development of optimum processing techniques, examination of the reinforcement-matrix interface, determination of the mechanical property envelope (including actual yield and ultimate tensile strength measurements) and survey of the corrosion resistance of this class of composites.

Keywords: Shape Memory Alloy, Composite Materials, Metal Matrix Composite

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

$215,000
DOE Contact: Walter M. 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. The first polymer (tetracyanoethylene)-based magnet that remained strongly magnetic up to 350 K (170°F) 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 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 of 13, 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. Preliminary results on modified Prussian Blue-type materials with vanadium replacing 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 T_c Prussian Blue-type magnetic materials, for shielding and induction applications from dc/low frequency to communications frequencies. The objective of this 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

260. MOLECULAR SURFACE MODIFICATION AS A MEANS OF CORROSION CONTROL

$309,000
DOE Contact: Walter M. 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 angstroms to 20 angstroms 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 this project 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

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

PHASE I

Ultra-High-Speed Photonic Add-Drop Multiplexers for Wave-Division Multiplexed Networking - DOE Contact George Seweryniak, (301) 903-0071; Intelligent Fiber Optic Systems Contact Dr. Behzad Moslehi, (650) 967-4107

Screen-Printed Solar Cells Based on Nanocrystalline TiO_2 Films - DOE Contact Yok Chen, (301) 903-3428; Radiation Monitoring Devices, Inc. Contact Dr. Gerald Entine, (617) 926-1167

An Improved Membrane Module Tubesheet for Industrial Separations - DOE Contact Charlie Russomanno, (202) 586-7543; TDA Research, Inc. Contact John D. Wright, (303) 940-2300

A Scalable Process for Thin, Defect-Free Zeolite Membranes - DOE Contact Charlie Russomanno, (202) 586-7543; TDA Research, Inc. Contact John D. Wright, (303) 940-2300

Micromachined Silicon Sensor for DNA Sequencing by Hybridization - DOE Contact Marvin Stodolsky, (301) 903-4475; TPL Inc. Contact Dr. William F. Hartman, (505) 342-4414

Sharp Bandpass AlGaN p-i-n Photodiode Detectors for Ultraviolet B Irradiance Measurements - DOE Contact Rick Petty, (301) 903-5548; SVT Associates, Inc. Contact Dr. Peter P. Chow, (612) 934-2100

Robust Micromachined Silicon Carbide Environmental Sensors - DOE Contact Rick Petty, (301) 903-5548; Boston Microsystems Inc. Contact Dr. Richard Mlcak, (617) 661-6075

Hand-Held Monitor for On-Site Detection of Heavy Metals in Water Using Microfabricated Detector Chips - DOE Contact Rick Petty, (301) 903-5548; Eltron Research, Inc. Contact Eileen E. Sammells, (303) 440-8008

AlGaN Ultraviolet Light Emitting Diodes for Fiber Optic Sensors - DOE Contact Rick Petty, (301) 903-5548; SVT Associates, Inc. Contact Dr. Peter P. Chow, (612) 934-2100

A Photocatalytic $Ti0_2$ Anode and Membrane Reactor for the Enhanced Destruction of Chloro-Organic Compounds in Water - DOE Contact Kamalendu Das, (304) 285-4065; Ceramem Corporation Contact Dr. Robert Goldsmith, (781) 899-4495

A Novel UV Photodetector Array - DOE Contact Dick Meyer, (301) 903-3613; NZ Applied Technologies, Inc. Contact Dr. Peter Norris, (781) 935-0300

Large Area, Low-Cost APDs Using Planar Processing - DOE Contact Dick Meyer, (301) 903-3613; Radiation Monitoring Devices, Inc. Contact Dr. Gerald Entine, (617) 926-1167

Solid-State Neutron Detection with LiZnP - DOE Contact Dick Meyer, (301) 903-3613; Radiation Monitoring Devices, Inc. Contact Dr. Gerald Entine, (617) 926-1167

A New Large Area Monolithic Avalanche Photodiode Array Having Widespread Applications and Lower Manufacturing Costs - DOE Contact Dick Meyer, (301) 903-3613; Silicon Power Corporation Contact Charles K. Fellows, (610) 407-4700

Gallium Arsenide p-i-n Detectors for High-sensitivity Imaging of Thermal Neutrons - DOE Contact Dick Meyer, (301) 903-3613; Spire Corporation Contact Dr. Everett S. McGinley, (781) 275-6000

Robust, Zirconium Carbide and Hafnium Carbide Field Emitter Cathodes for Accelerator and Beams Applications - DOE Contact Jerry Peters, (301) 903-5228; Creatv Microtech, Inc. Contact Dr. Cha-Mei Tang, (301) 983-1650

Pulsed High Power Switch for the Next-Generation Electron-Positron Linear Collider - DOE Contact Jerry Peters, (301) 903-5228; Triton Services, Inc., Electron Technology Div. Contact Stephen P. Black, (610) 252-7331

High-Voltage, Fast Turn-on and Turn-off Diamond Switch - DOE Contact Timothy E. Toohig, (301) 903-4115; Alameda Applied Sciences Corp. Contact Dr. Mahadevan Krishnan, (510) 483-4156

Avalanching MRS Detectors for Scintillation Photodetection - DOE Contact James L. Stone, (301) 903-0535; Cremat Contact Fred Olschner, (617) 926-0661

A Simple and Direct Tungsten Brush Fabrication Technique - DOE Contact Sam E. Berk, (301) 903-4171; Surmet Corporation Contact Dr. Suri A. Sastri, (781) 272-3250

High Speed Acousto-Optic Tuner - DOE Contact Carl Friesen, (208) 526-1765; Aurora Associates Contact Dr. Phoebe Chang, (408) 748-2960

Development of High Speed Mercury Cadmium Telluride Detector Arrays with Integral Readouts - DOE Contact Carl Friesen, (208) 526-1765; Fermionics Corporation Contact Dr. Peter C. C. Wang, (805) 582-0155

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

PHASE II (FIRST YEAR)

Shaft Weld Replacement with a Ceramic Locking Assembly Joint - DOE Contact Yok Chen, (301) 903-3428; Goss Engineers, Inc. Contact Gabrielle M. Goss, (303) 721-8783

Development of Economical Procedures for Producing and Processing Fine Grained SSM Feedstock via Mechanical Stirring - DOE Contact Yok Chen, (301) 903-3428; Formcast, Inc. Contact Charles Carlberg, (303) 778-6566

Corrosion Resistant Bipolar Plates for PEM Fuel Cells - DOE Contact Jim Merritt, (202) 586-0903; Physical Sciences Inc. Contact George E. Caledonia, (508) 689-0003

High Brightness LEDs based on the (Al,Ga,In)N Materials System - DOE Contact Karl Veith, (202) 586-6002; Advanced Technology Materials, Inc. Contact Dr. Duncan W. Brown, (203) 794-1100

Development of High Power RF Windows and Waveguide Components For the Next Linear Collider - DOE Contact Jerry Peters, (301) 903-5228; Calabazas Creek Research Contact Dr. R. Lawrence Ives, (408) 741-8680

Electrical Discharge Machining Application to the Development of mm-wave Accelerating Structures - DOE Contact Jerry Peters, (301) 903-5228; Ron Witherspoon, Inc. Contact Dr. Steven Schwartzkopf, (408) 370-6620

Beryllium and Tungsten Brush Armor for Plasma Facing Components - DOE Contact Sam E. Berk, (301) 903-4171; Plasma Processes, Inc. Contact Cheri McKechnie, (205) 851-7653

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

PHASE II (SECOND YEAR)

Catalytic Membrane for High Temperature Hydrogen Separations - DOE Contact Otis Mills, (412) 892-5890; Ceramem Corporation Contact Dr. Robert L. Goldsmith, (617) 899-0467

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 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

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

Passive Electronic Components from Nanostructured Materials - DOE Contact David Koegel, (301) 903-3159; Nanomaterials Research Corporation Contact Thomas Venable, (520) 294-7115

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

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 Microfocusing Optics - DOE Contact Tim Fitzsimmons, (301) 903-9830; Hirsch Scientific Contact Gregory Hirsch, (415) 359-3920

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

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

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

Joining of Tungsten Armor Using Functional Gradients - DOE Contact T. V. George, (301) 903-4957; Plasma Processes, Inc. Contact Cheri McKechnie, (205) 851-7653

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

High Performance Optical Detectors for Calorimetry - DOE Contact Robert Woods, (301) 903-3367; Radiation Monitoring Devices, Inc. Contact Dr. Gerald Entine, (617) 926-1167

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

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

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

PHASE I

Detection of Mercury at the Parts per Quadrillion Level Using Cavity Ringdown Spectroscopy - DOE Contact Thomas Brown, (412) 892-4691; ADA Technologies, Inc. Contact Dr. Daryl Roberts, (303) 792-5615

Low Cost Fine Particulate Stack Monitor - DOE Contact Thomas Brown, (412) 892-4691; Physical Sciences, Inc. Contact George E. Caledonia, (978) 689-0003

Instrument for Real Time Measurement of Scale Growth at High Temperature and Under Applied Load - DOE Contact Yok Chen, (301) 903-3428; Hypernex A Division Of Advanced Technology Materials, Inc. Contact Daniel P. Sharkey, (203) 794-1100

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

PHASE II (FIRST YEAR)

High Current Density High Repetition Rate Ferroelectric Cathode - DOE Contact Jerry Peters, (301) 903-5228; FM Technologies, Inc. Contact Dr. Frederick M. Mako, (703) 425-5111

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

PHASE II (SECOND YEAR)

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

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

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

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

Metal-Binding Silica Materials for Wastewater Cleanup - DOE Contact Kristine Bilenki, (301) 903-1687; TPL, Inc. Contact Jacqueline Taylor, (505) 343-8890

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

MATERIALS, PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

PHASE I

Hybrid Multilayer Membranes for the Selective Separation of Hydrogen from Complex Gas Streams - DOE Contact Kamalendu Das, (304) 285-4065; CCVD, Inc., DBA Microcoating Technologies Contact Jerome J. Schmitt, (770) 457-8400

Carbon Nanostructures from Coal-Derived Liquid Feedstocks - DOE Contact Richard Read, (412) 892-5721; TDA Research, Inc. Contact John D. Wright, (303) 940-2300

High Temperature Oxidation Resistant Alumina Coatings for Advanced Energy and Processing Systems - DOE Contact Yok Chen, (301) 903-3428; Plasma Processes, Inc. Contact Timothy McKechnie, (205) 851-7653

Adherent and Reliable Alumina Coating Development - DOE Contact Yok Chen, (301) 903-3428; Surmet Corporation Contact Dr. Suri A. Sastri, (781) 272-3250

Surface Tailored Nanophase Alumina Coatings for Oxidation Protection of Aluminide Intermetallics - DOE Contact Yok Chen, (301) 903-3428; TDA Research, Inc. Contact John D. Wright, (303) 940-2300

Novel Net Shape Processing for the Fabrication of Boron-Doped Mo_5Si_3-Based Intermetallic Alloys for High Temperature Applications - DOE Contact Yok Chen, (301) 903-3428; Micropyretics Heaters International, Inc. Contact Dr. Anu Vissa, (513) 772-0404

Synthesis of Mesoporous Tin Oxide for Chemical Gas Sensors - DOE Contact Yok Chen, (301) 903-3428; Ceramem Corporation Contact Dr. Robert Goldsmith, (781) 899-4495

Polyurethane-Clay Nanocomposite and Microcellular Foaming - DOE Contact Yok Chen, (301) 903-3428; Industrial Science And Technology Network, Inc. Contact Dr. Arthur Yang, (717) 843-0300

Mesoporus Bimetallic Transition Metal Oxides as Solid Acid Catalysts - DOE Contact Yok Chen, (301) 903-3428; T/J Technologies, Inc. Contact Leslie H. Alexander, (734) 213-1637

Barium Titanate/Polymer Nanoscale Composites with Controllable Architectures - DOE Contact Yok Chen, (301) 903-3428; TPL, Inc. Contact Dr. William F. Hartman, (505) 342-4414

Thin (<30 micron) Silicon-Film Solar Cells on Glass-Ceramic Substrate - DOE Contact Yok Chen, (301) 903-3428; Astropower, Inc. Contact Thomas J. Stiner, (302) 366-0400

Spectral Sensitization of Nanocrystalline TiO_2 by Dye Aggregates - DOE Contact Yok Chen, (301) 903-3428; Chemmotif, Inc. Contact Dr. Mark T. Spitler, (781) 229-8556

Dye Sensitized TiO_2 Photoelectrochemical Cells with Polymer Electrolytes - DOE Contact Yok Chen, (301) 903-3428; EIC Laboratories, Inc. Contact Dr. A. C. Makrides, (781) 769-9450

High Resistivity Tin Oxide for CdTe PV Cell Electrodes - DOE Contact Yok Chen, (301) 903-3428; ITN Energy Systems, Inc. Contact Janet L. Casteel, (303) 420-1141

Manufacturable $CuIn(Ga)Se_2$-Based Solar Cells via Development of Co-Sputtered $CuInSe_2$ Absorber Layers - DOE Contact Yok Chen, (301) 903-3428; Materials Research Group, Inc. Contact Dr. Pawan Bhat, (303) 425-6688

Materials and Processes for High-Performance Cadmium Telluride Photovoltaic Modules - DOE Contact Yok Chen, (301) 903-3428; Solar Cells, Inc. Contact Dan Sandwich, (419) 534-3377

Improved Non-Vacuum Processes for Forming CIS Films - DOE Contact Yok Chen, (301) 903-3428; Unisun Contact Dr. Chris Eberspacher, (805) 499-7840

High Capacity Lithium Battery Cathodes Based on V_2O_5 Xerogels - DOE Contact Susan Rogers, (202) 586-8997; Aveka, Inc. Contact Dr. Willie Hendrickson, (612) 730-1729

Irreversibility Compensated Metal Oxide Anodes for Lithium-Ion Batteries - DOE Contact Susan Rogers, (202) 586-8997; Covalent Associates, Inc. Contact Dr. K. M. Abraham, (781) 938-1140

High Rate, High Capacity Anodes for Rechargeable Li Batteries - DOE Contact Susan Rogers, (202) 586-8997; T/J Technologies, Inc. Contact Leslie H. Alexander, (734) 213-1637

Nanostructured Manganese Dioxides for Li-Ion Batteries - DOE Contact Susan Rogers, (202) 586-8997; US Nanocorp, Inc. Contact Dr. David E. Reisner, (203) 234-8024

A Mixed Metal Oxide Anode Material for High Energy Density Li-Ion Batteries - DOE Contact Susan Rogers, (202) 586-8997; Yardney Technical Products, Inc. Contact Dr. Thomas B. Reddy, (860) 599-1100

Novel Membranes for Organic/Organic Separations - DOE Contact Charlie Russomanno, (202) 586-7543; Bend Research, Inc. Contact Dr. Rod Ray, (541) 382-4100

Novel Low-Cost Zeolite Ceramic Membrane Module - DOE Contact Charlie Russomanno, (202) 586-7543; Ceramem Corporation Contact Dr. Robert L. Goldsmith, (781) 899-4495

Supported Zeolite Membranes for Methanol-Water Separation - DOE Contact Charlie Russomanno, (202) 586-7543; Crystals & Ceramics Technology, Inc. Contact Steven L. Ford, (317) 549-2715

Mixed-Conducting Membranes for the Spontaneous Oxidative Dehydrogenation of Alkanes to Olefins - DOE Contact Charlie Russomanno, (202) 586-7543; Eltron Research, Inc. Contact Eileen E. Sammells, (303) 440-8008

Novel Nanofiltration Membranes for the Separation of Solvent/Oil Mixtures - DOE Contact Charlie Russomanno, (202) 586-7543; Membrane Technology and Research, Inc. Contact E. G. Weiss, (650) 328-2228

Separation of Hydrogen/Light Hydrocarbon Gas Mixtures - DOE Contact Charlie Russomanno, (202) 586-7543; Membrane Technology and Research, Inc. Contact E. G. Weiss, (650) 328-2228

Aerogels with Glass-like Transparency for Cherenkov Detectors - DOE Contact Dick Meyer, (301) 903-3613; Aspen Systems, Inc. Contact Dr. Kang P. Lee, (508) 481-5058

An Artifical Pinning Center Approach to the Manufacture of High Field NbTaTi Superconducting Wire - DOE Contact Jerry Peters, (301) 903-5228; Alabama Cryogenic Engineering, Inc. Contact Mary T. Hendricks, (205) 536-8629

Fabrication of Rare Earth Doped Nb_3Sn Superconductors - DOE Contact Jerry Peters, (301) 903-5228; Alchemet, Inc. Contact Katherine L. Miller, (610) 566-5964

High Magnetic Field Tl-Based Superconducting Tape on Biaxially Textured Flexible Metallic Substrates - DOE Contact Jerry Peters, (301) 903-5228; AMBP Tech Corporation Contact Dr. Gary S. Tompa, (732) 885-5909

Novel BSCCO Composites for High-Field Superconductor Technology - DOE Contact Jerry Peters, (301) 903-5228; American Superconductor Corporation Contact Dr. Alexis P. Malozemoff, (508) 836-4200

Combustion Chemical Vapor Deposition of High Temperature Ceramic Insulator Coatings on Superconductor Wire - DOE Contact Jerry Peters, (301) 903-5228; CCVD, Inc., DBA Microcoating Technologies Contact Jerome J. Schmitt, (770) 457-8400

Develop Technology to Produce Long Lengths of Nb_3Al Superconductor Wire - DOE Contact Jerry Peters, (301) 903-5228; Innovare, Inc. Contact Dr. Alfred R. Austen, (610) 837-8830

Production of Jelly-Roll Process Nb_3Al Multifilamentary Superconducting Wire Using Warm Hydrostatic Extrusion - DOE Contact Jerry Peters, (301) 903-5228; Supercon, Inc. Contact Elaine Drew, (508) 842-0174

Development of High Field, High Current Density Nb_3Sn Conductor with Engineered Microstructures - DOE Contact Jerry Peters, (301) 903-5228; Supercon, Inc. Contact Elaine Drew, (508) 842-0174

High Quantum Efficiency Extended Wavelength Vacuum Photocathodes - DOE Contact James L. Stone, (301) 903-0535; Nano Systems Inc. Contact Robert Boerstler, (203) 811-2827

Micromachined Ceramic Microchannel Plates - DOE Contact James L. Stone, (301) 903-0535; Nanomaterials Research Corporation Contact Michelle Mikus, (520) 294-7115

High Field Magnets for Plasma Fusion Confinement Systems - DOE Contact T. V. George, (301) 903-4957; American Superconductor Corporation Contact Dr. Alexis P. Malozemoff, (508) 836-4200

High Performance SiC/SiC Composites for Structural Fusion Reactor Components - DOE Contact F. W. Wiffen, (301) 903-4963; Ceramic Composites, Inc. Contact Sharon S. Fehrenbacher, (410) 224-3710

Innovative, Low Viscosity, Radiation-Resistant Insulation Systems for Fusion Magnets - DOE Contact T. V. George, (301) 903-4957; Composite Technology Development, Inc. Contact Dr. Naseem A. Munshi, (303) 664-0394

Beryllium Armored Aluminum Alloy Plasma Facing Components - DOE Contact Sam E. Berk, (301) 903-4171; Plasma Processes, Inc. Contact Timothy Mckechnie, (205) 851-7653

High Strength, High Conductivity, Low Activation Copper Matrix Nanocomposite for Fusion Reactor First Wall Application - DOE Contact Sam E. Berk, (301) 903-4171; Supercon, Inc. Contact Elaine Drew, (508) 842-0174

Insulating Coatings Development for Vanadium Alloys for Use in Fusion Systems - DOE Contact F. W. Wiffen, (301) 903-4963; Surmet Corporation Contact Dr. Suri A. Sastri, (781) 272-3250

An Improved Reaction-Bonded Silicon Carbide Process for SiC/SiC Composites - DOE Contact F. W. Wiffen, (301) 903-4963; TDA Research, Inc. Contact John D. Wright, (303) 940-2300

Structural Materials & Insulating Coatings - DOE Contact F. W. Wiffen, (301) 903-4963; TPL, Inc. Contact Dr. William F. Hartman, (505) 342-4414

Refractory Metal Wicks for Extended Lifetime in AMTEC Power Systems - DOE Contact Bill Barnett, (301) 903-3097; Creare, Inc. Contact Robert A. Hickin, (603) 643-3800

The Short-Pulse Plasma Implantation/Coating Process for Extending the Life of Die Casting Dies - DOE Contact Ehr-Ping HuangFu, (202) 586-1493; First Point Scientific, Inc. Contact Dr. John Bayless, (818) 707-1131

PVD Coating of Dies Using Superhard Nano-layered Composite Coatings - DOE Contact Ehr-Ping HuangFu, (202) 586-1493; Hardhard Coating, Inc. Contact Bobby Oglesby, (812) 422-2356

Development of an Innovative Laser Assisted Coating Process for Extending Lifetime of Metal Casting Dies - DOE Contact Ehr-Ping HuangFu, (202) 586-1493; Karta Technology, Inc. Contact Thomas Tower, (210) 681-9102

The Application of Plasma Assisted Chemical Vapor Deposition (PACVD) Coatings for Die Casting Dies - DOE Contact Ehr-Ping HuangFu, (202) 586-1493; Materials and Electrochemical Research (MER) Contact Dr. J.C. Withers, (520) 574-1980

Micromechanically Compliant Coating for Die Casting Dies - DOE Contact Ehr-Ping HuangFu, (202) 586-1493; Surmet Corporation Contact Dr. Suri A. Sastri, (781) 272-3250

Hard, Wear Resistant Coatings for Die-Casting Dies by an Advanced Filtered Cathodic Arc Deposition Process - DOE Contact Ehr-Ping HuangFu, (202) 586-1493; UES, Inc. Contact Francis F. Williams, Jr., (937) 426-6900

MATERIALS, PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

PHASE II (FIRST YEAR)

A Novel Reactive Joining Compound for High Temperature Applications - DOE Contact Yok Chen, (301) 903-3428; Sienna Technologies, Inc. Contact Dr. Ender Savrun, (425) 485-7272

Development of Novel Boron-Based Multilayer Thin-Film - DOE Contact Yok Chen, (301) 903-3428; Front Edge Technology, Inc. Contact Stephen Denlinger, (818) 856-8979

Advanced Plasma Surface Modification System - DOE Contact Yok Chen, (301) 903-3428; ISM Technologies, Inc. Contact Robert J. Stinner, (619) 530-2332

High-Flux, Low Energy Ion Source for High Rate Ion-Assisted Deposition of Hard Coatings - DOE Contact Yok Chen, (301) 903-3428; Plasmaquest, Inc. Contact Dr. John E. Spencer, (972) 680-1811

Semi-Solid Thermal Transformation to Produce Semi-Solid Formable Alloys - DOE Contact Yok Chen, (301) 903-3428; Hot Metal Molding, Inc. Contact B. Wilcox, (541) 298-0814

A Simple Process to Manufacture Grain Aligned Permanent Magnets - DOE Contact Yok Chen , (301) 903-3428; Advanced Materials Corporation Contact Vijay K. Chandhok, (412) 268-5121

A Novel Technique for the Enhancement of Coercivity in High Energy Permanent Magnets - DOE Contact Yok Chen, (301) 903-3428; Advanced Materials Corporation Contact Dr. S.G. Sankar, (412) 268-5649

Stabilization of Nitride Magnet Material via Sol-Gel Route - DOE Contact Yok Chen, (301) 903-3428; Chemat Technology, Inc. Contact Jenny Sajoto, (818) 727-9786

A Combinatorial Approach to the Synthesis and Characterization of Novel Anode Materials For Direct Methanol Fuel Cells - DOE Contact JoAnn Milliken, (202) 586-2480; Symyx Technologies Contact Isy Goldwasser, (408) 328-3100

Low Cost Deposition of Buffer Layers for Manufacturable YBCO HTS Conductors - DOE Contact James Daley, (202) 586-1165; American Superconductor Corporation Contact Ramesh Ratan, (508) 836-4200

Buffer Layers on Textured Nickel Using Commercially Viable CCVD Processing - DOE Contact James Daley, (202) 586-1165; CCVD, Inc., DBA Microcoating Technologies Contact Jeffrey C. Moore, (770) 457-7767

Development of Efficient and Practical Passive Solar Building Systems with High Recycled Content Using the Preplaced Aggregate Concrete Technology - DOE Contact Mary Margaret Jenior, (202) 586-2998; DPD, Inc. Contact Faragnis Jamzadeh, (517) 349-5653

Heterogeneous Hydroformylation of Alkenes with Syngas - DOE Contact Donald Krastman, (412) 892-4720; TDA Research, Inc. Contact Michael E. Karpuk, (303) 940-2301

Tubular SOFC with Deposited Nano-Scale YSZ Electrolyte - DOE Contact Udaya Rao, (412) 892-4743; Nextech Materials, Ltd. Contact William J. Dawson, (614) 766-4895

High Speed Long Wavelength Infrared Detector Array/Preamplifier Development - DOE Contact Carl Friesen, (208) 526-1765; Fermionics Corporation Contact Dr. Peter C.C. Wang, (805) 582-0155

Development of Cadmium Germanium Arsenide Crystals - DOE Contact Carl Friesen, (208) 526-1765; Inrad, Inc. Contact James L. Greco, 201-767-1910

An Easily Dispersed Reactive Coating for Surface Decontamination - DOE Contact Carl Friesen, (208) 526-1765; Lynntech, Inc. Contact Dr. Oliver J. Murphy, (409) 693-0017

Rapid Quench Nb_3Al for High Field Accelerator Applications - DOE Contact Jerry Peters, (301) 903-5228; Plastronic, Inc. Contact Michael Tomsic, (937) 335-0656

Ultra-Lightweight Carbon-Carbon Cooling Structure For Pixel and Silicon Strip Detectors - DOE Contact Richard Plano, (301) 903-4801; Hytec, Inc. Contact William O. Miller, (505) 662-0080

Development of Scintillators and Waveshifters for Detection of Ionizing Radiation - DOE Contact Richard Plano, (301) 903-4801; Ludlum Measurements, Inc. Contact Donald G. Ludlum, (915) 235-5494

MATERIALS, PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

PHASE II (SECOND YEAR)

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

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

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

High Rate Deposition of Transparent Conducting Zinc Oxide Using Activated Oxygen for Photovoltaic Manufacturing Cost Reduction - DOE Contact Alec Bulawka, (202) 586-5633; 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

SMALL BUSINESS TECHNOLOGY TRANSFER RESEARCH PROGRAM

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

PHASE I

Novel Ultracapacitor: WN Aerogel Electrode with Polyoxometalate Polymers Electrolyte - DOE Contact Susan Rogers, (202) 586-8997; Chemat Technology, Inc. Contact Jenny Sajoto, (818) 727-9786

High Energy and Power Ultracapacitors Utilizing Novel Type III Polymers and Non-Aqueous Electrolytes - DOE Contact Susan Rogers, (202) 586-8997; Covalent Associates, Inc. Contact Dr. K.M. Abraham, (781) 938-1140

A Low Cost High Performance Uranium Plutonium Detector - DOE Contact Carl Friesen, (208) 526-1765; Photon Imaging, Inc. Contact Dr. Bradley E. Patt, (818) 709-2468

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

PHASE II (FIRST YEAR)

Novel Thin Film Scintillator for Intermediate Energy Photons Detection and Imaging - DOE Contact Dick Meyer, (301) 903-4398; NZ Applied Technologies, Inc. Contact Peter Norris, (617) 935-0300

Advanced Ceramic Hot Gas Filters - DOE Contact Theodore McMahon, (304) 285-4865; LoTec, Inc. Contact Mr Santosh Y. Limaye, (801) 483-3100

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

PHASE II (SECOND YEAR)

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

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

PHASE I

High Flux Ceramic Membrane for Hydrogen Separation - DOE Contact Kamalendu Das, (304) 285-4065; Harvest Energy Technology, Inc. Contact Dr. David Warren, (818) 767-3157

A Zeolite Membrane for Separation of Hydrogen from Process Streams - DOE Contact Kamalendu Das, (304) 285-4065; TDA Research, Inc. Contact Michael Karpuk, (303) 940-2345

Boron Carbide Coatings for Enhanced Performance of Radio-Frequency Antennas in Magnetic Fusion Devices -DOE Contact T. V. George, (301) 903-4957; Hy-tech Research Corporation Contact Dr. Robert Hazelton, (540) 639-4019

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

PHASE II (FIRST YEAR)

New High-Performance GaSb-Based Thermo-photovoltaic (TPV) Devices - DOE Contact David Koegel, (301) 903-3159; Astro Power, Inc. Contact Dr. Allen Barnett (302) 366-0400

High Efficiency Magnetic Refrigerators as Alternate Environmentally Safe Commercial Refrigeration Devices - DOE Contact David Koegel, (301) 903-3159; Materials and Electrochemical Research Corp. Contact Dr. R. O. Loutfy, (520) 574-1980

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

PHASE II (SECOND YEAR)

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

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 materials program in the United States is conducted with a high degree of international cooperation. Bilateral agreements with Japan and the Russian Federation enhance the ability of each party to mount fission reactor irradiation experiments. The Fusion Materials Agreement under the International Energy Agency (IEA) serves as a useful venue for the exchange of information and the coordination of programs of research on Fusion Materials. 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. A large part of the materials work sponsored by OFES is in support of the ITER collaboration.

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

261. STRUCTURAL MATERIALS DEVELOPMENT

$675,000
DOE Contact: F. W. Wiffen (301) 903-4963
ANL Contact: D. L. Smith (630) 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/ compatibility 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, including liquid lithium and helium.

Keywords: Vanadium, Compatibility, Lithium, Irradiation Effects, Alloy Development

262. MODELING IRRADIATION EFFECTS IN SOLIDS

$50,000
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

263. FUSION SYSTEMS MATERIALS

$3,408,000
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 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 and other test reactors, as partial simulation of the fusion environment.

Keywords: Ceramics, Steels, Vanadium, Silicon Carbide, Composites, Irradiation Effects, Electrical Properties

264. **STRUCTURAL MATERIALS FOR FUSION SYSTEMS**
$950,000
DOE Contact: F. W. Wiffen, (301) 903-4963
PNNL Contacts: R. J. Kurtz, (509) 373-7515

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

265. **DEVELOPMENT OF RADIATION-HARDENED CERAMIC COMPOSITES FOR FUSION APPLICATIONS**
$21,000
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

266. **MECHANISMS OF PLASTIC AND FRACTURE INSTABILITY FOR ALLOY DEVELOPMENT OF FUSION MATERIALS**
$120,000
DOE Contact: F. W. Wiffen, (301) 903-4963
UCLA Contact: N. M. Ghoniem, (310) 825-4866

This research is focussed on increasing the understanding of plastic instabilities and fracture processes in materials irradiated under projected fusion conditions. The effects of the many materials, irradiation, and mechanical loading parameters on the flow and fracture processes, especially embrittlement processes, will be evaluated and modeled to establish understanding of controlling mechanisms. Techniques in use include atomistic computer simulation, atomic cluster modeling, 3-D dislocation dynamics, and analysis using flow and fracture models. The goal is to develop the understanding needed to establish models and methods to extrapolate from the available data base to predict the behavior of structural components in future operating fusion power systems.

Key words: Irradiation Effects, Fracture, Mechanical Properties, Modeling

267. **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 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 fusion systems.

Keywords: Vanadium, Steels, Irradiation Effects Fracture

268. **INTERNATIONAL THERMONUCLEAR EXPERIMENTAL REACTOR (ITER) MATERIALS DEVELOPMENT FOR PLASMA FACING COMPONENTS**
$5,000,000
DOE Contact: S. Berk, (301) 903-4171
SNL Contact: M. Ulrickson, (505) 845-3020

Research activities include: improved techniques for joining beryllium or tungsten 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, tungsten 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, Tungsten, Carbon-Fiber Composite, Joining, Erosion, Thermal Fatigue

269. **ITER MATERIALS EVALUATION**
$365,000
DOE Contact: F. W. Wiffen, (301) 903-4963
ORNL Contacts: 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

270. **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

271. **STRUCTURAL MATERIALS DEVELOPMENT FOR THE CONDUIT OF ITER CABLE-IN-CONDUIT-CONDUCTORS**
$200,000
DOE Contact: T. V. George, (301) 903-4957
MIT Contact: J. Minervini, (617) 253-5503

The conduit material selected for the ITER cable-in-conduit-conductors is the high strength superalloy Incoloy Alloy 908, developed via collaboration between INCO Alloys International (IAI) and MIT. Using the materials provided by IAI, a significant database has been developed by materials properties characterization as well as industrial processing experience and coil winding experience. Work is continuing on alloy development to reduce the sensitivity of the material to Stress Accelerated Grain Boundary Oxidation (SAGBO).

Keywords: Conduit, Incoloy, Magnet Materials

OFFICE OF ENVIRONMENTAL MANAGEMENT

	FY 1998
Office of Environmental Management - Grand Total	$7,991,663
Materials Properties, Behavior, Characterization or Testing	$7,991,663
The Influence of Radiation and Multivalent Cation Additions on Phase Separation and Crystallization of Glass	241,000
Chemical and Ceramic Methods Toward Safe Storage of Actinides Using Monazite	429,000
Atmospheric-Pressure Plasma Cleaning of Contaminated Surfaces	404,000
Chemical Decomposition of High-Level Nuclear Waste Storage/Disposal Glasses Under Irradiation	163,000
Analysis of Surface Leaching Processes in Vitrified High-Level Nuclear Wastes Using In-Situ Raman Imaging and Atomistic Modeling	186,333
Investigation of Microscopic Radiation Damage in Waste Forms Using ODNMR and AEM Techniques	232,667
In-Situ Spectro-Electrochemical Studies of Radionuclide Contaminated Surface Films on Metals and the Mechanism of Their Formation and Dissolution	335,000
Determination of Transmutation Effects in Crystalline Waste Forms	304,328
Radiation Effects on Materials in the Near-Field of Nuclear Waste Respository	136,000
An Alternative Host Matrix Based on Iron Phosphate Glasses for the Vitrification of Specialized Nuclear Waste Forms	208,278
Microstructural Properties of High Level Waste Concentrates and Gels with Raman and Infrared Spectroscopies	155,000
Fundamental Thermodynamics of Actinide-Bearing Mineral Waste Forms	383,333
Optimization of Thermochemical, Kinetic, and Electrochemical Factors Governing Partitioning of Radionuclides During Melt Decontamination of Radioactively Contaminated Stainless Steel	400,000
Mechanism of Pitting Corrosion Prevention by Nitrite in Carbon Steel Exposed to Dilute Salt Solutions	216,667
Stability of High-Level Waste Forms	254,000
Radiation Effects in Nuclear Waste Materials	960,000
New Silicotitanate Waste Forms: Development and Characterization	400,000
Distribution & Solubility of Radionuclides & Neutron Absorbers in Waste Forms for Disposition of Plutonium Ash & Scraps, Excess Plutonium, and miscellaneous Spent Nuclear Fuels	600,000
Modeling of Diffusion of Plutonium in Other Metals and of Gaseous Species in Plutonium-Based Systems	145,000
Radionuclides Immobilization in the Phases Formed by Corrosion of Spent Nuclear Fuel: The Long-Term Assessment	160,321
Direct Investigations of the Immobilized of Radionuclides in the Alteration Phases of Spent Nuclear Fuel	260,829
Decontamination of Radionuclides from Concrete During and After Thermal Treatment	271,907
Mechanisms of Radionuclide-Hydroxycarboxylic Acid Interactions for Decontamination of Metallic Surfaces	383,333
Physical, Chemical and Structural Evolutioon of Zeolite-Containing Waste Forms Produced from Metakaolinite and Calcined HLW	170,000
Mechanisms and Kinetics of Organic Aging in High-Level Nuclear Wastes	300,000
Modeling of Spinel Settling in Waste Glass Melter	291,667

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.

The projects listed in this report are managed under the Environmental Management Research Program (EMSP). 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 current EMSP portfolio consists of 202 awards amounting to a total of $160 million in three-year funding. Twenty-six of those awards were in scientific disciplines related to materials issues that have potential to solve Environmental Management challenges. The 1998 component of materials research is estimated to amount to $7,991,663. The entire EMSP portfolio can be viewed on the World Wide Web at http://www.em.doe.gov/science.

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

272. **THE INFLUENCE OF RADIATION AND MULTIVALENT CATION ADDITIONS ON PHASE SEPARATION AND CRYSTALLIZATION OF GLASS**
$241,000
DOE Contact: Arnold Gritzke, (202) 586-3957
University of Arizona Contact:
Michael C. Weinberg, (520) 621-6909

Recent reviews which have dealt with critical issues regarding the suitability of glasses for nuclear waste disposal have identified liquid-liquid immiscibility and crystallization processes as having the potential to alter significantly storage behavior, especially chemical corrosion characteristics. These phase transformation processes can be abetted (or deterred) by radiation or the inclusion of small quantities of other components such as transition metals, rare earths, actinides, etc. Consequently, in order to minimize the chances for the occurrence of deleterious phase separation or crystallization, it is essential to examine the influence of these factors on phase transformation kinetics.

The major goal of this program is to study the influence of irradiation and multivalent cations and redox conditions upon the thermodynamics and kinetics of phase separation and crystallization in selected glass compositions. Any observed changes in transformation behavior will be related to structural modifications caused by radiation. Finally, guidelines will be developed to mitigate the deleterious effects of phase separation and crystallization by composition adjustments, based on the development of a database from ongoing and existing measurements and the development of appropriate models.

The characteristics of phase separation are being analyzed, experimentally, using SEM, EDS, HSEM, TEM, and SAXS. Crystallization is being studied using XRD, SEM, TEM, and optical microscopy. Structural changes are being examined using IR and Raman Spectroscopies and solid state NMR measurements.

Keywords: Radiation, Phase Separation, Crystallization, Glasses

273. **CHEMICAL AND CERAMIC METHODS TOWARD SAFE STORAGE OF ACTINIDES USING MONAZITE**
$429,000
DOE Contact: Arnold Gritzke, (202) 586-3957
Rockwell International Corporation Contact:
P.E.D. Morgan, (805) 373-4273
ORNL Contact: Lynn A. Boatner, (423) 574-5492

The program is investigating monazite ceramics for safe, secure, geologically tested, very long term, containment for actinides. The main outstanding fundamental research issues facing the use of monazite as a waste form necessitate the development of fundamental understanding of: 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 program is addressing these issues to serve as a knowledge base for using monazite as a nuclear waste form.

Keywords: Monazite, Waste Form, Sintering, Densification

274. **ATMOSPHERIC-PRESSURE PLASMA CLEANING OF CONTAMINATED SURFACES**
$404,000
DOE Contact: Arnold Gritzke, (202) 586-3957
University of California at Los Angeles Contact:
Robert F. Hicks, (310) 206-6865
LANL Contact: Gary Selwyn, (505) 667-7824

Decommissioning of transuranic waste (TRU) into low-level radioactive waste (LLW) represents the largest cleanup cost associated with the nuclear weapons complex. This project is developing a low-cost technology for converting TRU into LLW based on the selective plasma etching of plutonium and other actinides from contaminated structures. Plasma etching has already been used to remove Pu films from materials. However, this process is operated under vacuum, making it both expensive and difficult to apply to many nuclear wastes. A major breakthrough in this field was the demonstration of the operation of a g-mode, resonant-cavity, atmospheric-pressure plasma jet (APPJ). This jet etches kapton at between 10 and 15 m/hour, and tantalum at between 1 and 2 m/hour. Etching occurs below 373 K, so that delicate materials will not be destroyed by this process. The plasma jet may be used to selectively remove plutonium and other actinide elements by converting them into volatile compounds that are trapped by adsorption and filtration.

Since the jet operates outside a chamber, many nuclear wastes may be treated, including machinery, duct-work, concrete and other building materials. At LANL, the source physics is being studied using Stark-broadening, microwave interferometry, and laser-induced fluorescence (LIF). The metastables, neutrals and radical species produced with mixtures of NF3, CF4, C2F6, O2,He and Ar are being identified by LIF, optical emission spectroscopy (OES), laser Raman spectroscopy (LRS), coherent anti-Stokes Raman spectroscopy (CARS), and mass spectroscopy (MS). At UCLA, the elementary surface reactions of these species with tantalum and tungsten (surrogate metals for Pu) are being studied in ultrahigh vacuum using a supersonic molecular-beam coupled to the plasma jet. The surfaces are being characterized by X-ray photoemission (XPS), infrared spectroscopy (IR), low-energy electron diffraction (LEED), and scanning-tunneling microscopy (STM). In addition, plutonium etching experiments are being carried out at the Los Alamos Plutonium Facility.

Keywords: Plasma Etching, Plutonium

275. **CHEMICAL DECOMPOSITION OF HIGH-LEVEL NUCLEAR WASTE STORAGE/DISPOSAL GLASSES UNDER IRRADIATION**
$163,000
DOE Contact: Arnold Gritzke, (202) 586-3957
Naval Research Laboratory Contact:
David L. Griscom, (202) 404-7087

This project is addressing potential hazards of radiation-induced gas phase formation in borosilicate glasses intended for vitrification of high-level nuclear waste. The present research effort is designed to: (1) demonstrate unambiguously the nature(s) 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 chemical explosion, 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: Borosilicate Glass, Gas Phases, High Level Waste

276. **ANALYSIS OF SURFACE LEACHING PROCESSES IN VITRIFIED HIGH-LEVEL NUCLEAR WASTES USING IN-SITU RAMAN IMAGING AND ATOMISTIC MODELING**
$186,333
DOE Contact: Arnold Gritzke, (202) 586-3957
University of Florida Contact: Joseph H. Simmons, (352) 392-6679

This research combines a novel investigative technique with novel modeling studies to analyze leaching processes in glasses. Its utility is that it will provide both a means of conducting fundamental studies of the corrosion behavior of high valence and multivalent ions in the waste glass as well as a proven in-situ method for monitoring the chemical corrosion behavior of radioactive waste glasses, remotely and in burial sites. The research has three major thrusts: (1) the development of in-situ Raman Imaging Spectroscopy for a detailed examination of leaching processes and associated structural changes and mineral precipitates on the surface of borosilicate glasses loaded with simulated high-level nuclear wastes, (2) the application of this method to the analysis of transition states and their energetics during surface leaching by novel modeling studies, and by comparison with existing methods of IR, Auger XPS and SIMS spectroscopy, SEM, TEM and STM/AFM microscopy and BET surface analysis; and (3) the extension of in-situ Raman Imaging Spectroscopy for conducting remote tests on radioactive loaded samples, and for the examination of variations over the surface of large ingots. The research comprises fundamental studies of (1) the relationship between leaching processes and Raman spectroscopy, using both tests on simple liquids and quantum mechanical modeling; and (2) the examination of transition states in hydration processes involving the higher valence and multivalent ions and their use in predicting, with high accuracy, their solubility in aqueous solutions using both experimental and quantum mechanical modeling methods. The combination of these two studies has the potential to offer a novel method which has both in-situ and remote capabilities for the analysis of leaching processes on high-level radioactive waste glasses. This method makes possible tests on radioactive materials with greatly reduced personnel exposure, and makes possible the examination of leaching processes in real-time in burial sites. Finally, this method can be applied to the continuous monitoring of the conditions of glass boules during actual disposal conditions.

Keywords: High Level Waste, Leaching, Glass

277. **INVESTIGATION OF MICROSCOPIC RADIATION DAMAGE IN WASTE FORMS USING ODNMR AND AEM TECHNIQUES**
$232,667
DOE Contact: Arnold Gritzke, (202) 586-3957
Argonne National Laboratory Contact: Guokui Liu, (630) 252-4630

This project investigates the microscopic effects of radiation damage in crystalline and glass high level waste forms (HLW). Information about the nature of electronic interaction and the chemical bonding properties of radionuclides in damaged phases is being developed. Connections between the consequences of alpha and beta-decay processes and radionuclide release and chemical decomposition in waste forms are being established. Detailed studies focus on the microscopic effects of alpha-decay of the transuranic isotopes 238,239Pu, 241,243Am, and 243,244Cm and the beta- and alpha-decay of 249Bk(249Cf) doped into crystalline materials 10 to 30 years ago and currently prepared borosilicate glasses. 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 are being probed using nonlinear laser spectroscopic techniques, such as optically detected nuclear magnetic resonance (ODNMR), in concert with analytical electron microscopy (AEM) imaging and analysis and X-ray diffraction methods. Experimental information obtained using various techniques for the same materials is being compared and systematic measurements are being made after the samples undergo a series of annealing tests. Theoretical models based on electronic and nuclear interactions of the actinides and their surrounding ligands are being 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: High Level Waste, Radiation Damage

278. **IN-SITU SPECTRO-ELECTROCHEMICAL STUDIES OF RADIONUCLIDE CONTAMINATED SURFACE FILMS ON METALS AND THE MECHANISM OF THEIR FORMATION AND DISSOLUTION**
$335,000
DOE Contact: Arnold Gritzke, (202) 586-3957
Argonne National Laboratory Contact: Carlos A. Melendres, (630) 252-4346,
Northern Illinois University Contact: S. M. Mini, (815) 753-6484

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. This project seeks to expand our knowledge, while obtaining useful practical information, through the conduct of a systematic research activity that utilizes the unique facilities at Argonne National Laboratory, e.g., the Advanced Photon Source (APS) for X-ray absorption spectroscopy (XAS), as well as specialized laboratory facilities and instrumentation for carrying out experiments with radioactive materials. Formal collaboration with a university assures that a strong basic approach is taken in the analyses and methodologies used to achieve the desired goals.

The research consists of electrochemical studies of the corrosion and passivation behavior of iron, nickel, chromium, and stainless steel over a wide pH range and as a function of temperature from 25 to 95°C. The energetics and dynamics of film formation and dissolution and the effect of incorporation of heavy metal ions and radioactive elements are being investigated. Synchrotron X-ray absorption and vibrational (infrared and Raman) spectroscopic techniques are being used to define *in-situ* the structure and composition of the various oxide phases that are formed as a function of temperature.

Keywords: Surface Films, Metals, Piping, Waste Tanks

279. **DETERMINATION OF TRANSMUTATION EFFECTS IN CRYSTALLINE WASTE FORMS**
$304,328
DOE Contact: Arnold Gritzke, (202) 586-3957
Argonne National Laboratory Contact: Jeff Fortner, (630) 252-4479
PNNL Contact: Nancy J. Hess, (509) 375-2142

The objective of this study is to characterize the effects of transmutation in a candidate waste form for 137Cs by investigating samples of a cesium aluminosilicate mineral, pollucite, that have undergone "natural" decay of the Cs under ambient temperature while isolated from interfering chemical effects. There currently is no information on β-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. As a result, uncertainties arise about the viability of the waste form as a long-term storage media for nuclear waste. Information on the effects of transmutation from β-decay will give support to the selection of alternate waste forms for separated 137Cs and give information on the long-term behavior of candidate waste forms.

The approach is to nondestructively examine small stainless steel capsules containing pure pollucite. The contents of these capsules will be examined with XANES, XAFS, and small angle anomalous X-rays. The synchrotron facilities at Stanford and ANL will be utilized. The scientific team is comprised of members from PNNL, ANL, and LANL.

Keywords: Transmutation, Crystalline Waste Forms, Synchrotron Radiation Facilities

280. **RADIATION EFFECTS ON MATERIALS IN THE NEAR-FIELD OF NUCLEAR WASTE REPOSITORY**
$136,000
DOE Contact: Arnold Gritzke, (202) 586-3957
University of Michigan Contacts: Lu-Min Wang, (313) 647-8530 and Rodney C. Ewing, (313) 647-8529

Successful, demonstrated containment of radionuclides in the near-field can greatly reduce the complexity of the performance assessment analysis of a geologic repository. The chemical durability of the waste form, the corrosion rate of the canister, and the physical and chemical integrity of the back-fill provide important barriers to the release of radionuclides. However, near-field containment of radionuclides depends critically on the behavior of these materials in a radiation field.

A systematic study is being performed 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 (clays and zeolites); (3) back-fill materials (clays and zeolites). The work draws on over twenty years of experience in studying radiation effects in minerals and complex ceramics and utilizes an unusual combination of studies of natural phases of great age with ion beam and electron irradiations of synthetic phases under carefully controlled conditions.

Keywords: Radiation Effects, Near-field, Geologic Repository

281. **AN ALTERNATIVE HOST MATRIX BASED ON IRON PHOSPHATE GLASSES FOR THE VITRIFICATION OF SPECIALIZED NUCLEAR WASTE FORMS**
$208,278
DOE Contact: Arnold Gritzke, (202) 586-3957
University of Missouri-Rolla Contact: Delbert E. Day, (573) 341-4354

Borosilicate glass is the only material currently approved and being used to vitrify high level nuclear waste. Unfortunately, many high level nuclear waste feeds in the U.S. contain components which are chemically incompatible with borosilicate glasses. Current plans call for vitrifying even these problematic waste feeds in borosilicate glasses after the original waste feed has been pre-processed and/or diluted to compensate for the incompatibility. However, these pre-treatment processes, as well as the larger waste volumes resulting from dilution, will add billions of dollars to the DOE's cost of cleaning up the former nuclear weapons production facilities. Such additional costs may be avoided by developing a small number of alternative waste glasses which are suitable for vitrifying those specific waste feeds that are incompatible with borosilicate glasses.

An alternative waste form based on a new family of iron-phosphate glasses which appear to be well suited for many waste feeds, especially those which are incompatible with borosilicate glasses, has recently been developed.

More information on the atomic structure, valence states, nature of bonding, structure-property relationships, crystallization kinetics, and optimized melt processing conditions is needed for iron phosphate glasses and their waste forms. This research is using techniques such as EXAFS, XANES, XPS, X-ray and neutron diffraction, IR, SEM, Mössbauer spectroscopy and DTA/DSC to obtain the information needed to demonstrate that iron phosphate waste forms can meet the stringent requirements for nuclear waste disposal.

Keywords: Iron Phosphate Glasses, Vitrification, Nuclear Waste

282. **MICROSTRUCTURAL PROPERTIES OF HIGH LEVEL WASTE CONCENTRATES AND GELS WITH RAMAN AND INFRARED SPECTROSCOPIES**
$155,000
DOE Contact: Arnold Gritzke, (202) 586-3957
Los Alamos National Laboratory Contact: Stephen F. Agnew, (505) 665-1764

Nearly half of the high level radioactive waste stored at Hanford is composed of highly alkaline concentrates referred to as either salt cakes or Double-Shell Slurry (DSS), depending on their compositions and processing histories. The major components of these concentrates are water, sodium hydroxide, and sodium salts of nitrate, nitrite, aluminate, carbonate, phosphate, and sulfate. In addition, there are varying amounts of assorted organic salts such as EDTA, glycolate, and citrate. Although measurements of the bulk properties of these wastes, such as viscosity, gel point, density, etc., have been exhaustively reported in the past, little is known about how those macroscopic characteristics are related to the microscopic physical and chemical properties of the waste. Such characteristics as viscosity, solids volume percent, and gas retention can change dramatically with relatively small changes in composition and temperature and these same properties are important for the determination of safe storage conditions as well as in planning retrieval, pretreatment, and disposal of the wastes.

The aim of this work is to use FTIR, Raman, and NMR spectroscopies, along with thermophysical heats of gelation, to relate the microstructural, physical and chemical properties of these concentrates to their macroscopic characteristics. With this better understanding of macroscopic characteristics, the DOE will be in a better position to safely store these wastes as well as to be able to better plan for their retrieval, pretreatment, and final disposal. These microscopic properties are being related to the 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 Al 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.

Keywords: High Level Waste, Raman Spectroscopy, Infrared Spectroscopy

283. **FUNDAMENTAL THERMODYNAMICS OF ACTINIDE-BEARING MINERAL WASTE FORMS**
$383,333
DOE Contact: Arnold Gritzke, (202) 586-3957
Los Alamos National Laboratory Contact: Mark A. Williamson, (505) 667-4045
LLNL Contact: Bartley B. Ebbinghaus, (510) 422-8792
UC Davis Contact: Alexandra Navrotsky, (916) 752-3292

The end of the Cold War raised the need for the technical community to be concerned with the disposition of excess nuclear weapon material. The plutonium will either be converted into mixed-oxide fuel for use in nuclear reactors or immobilized in glass or ceramic waste forms and placed in a repository. The stability and behavior of plutonium in the ceramic materials as well as the phase behavior and stability of the ceramic material in the environment is not well established. In order to provide technically sound solutions to these issues, thermodynamic data are essential in developing an understanding of the chemistry and phase equilibria of the actinide-bearing mineral waste form materials proposed as immobilization matrices. Mineral materials of interest include zircon, zirconolite, and pyrochlore. High temperature solution calorimetry is one of the most powerful techniques, sometimes the only technique, for providing the fundamental thermodynamic data needed to establish optimum material fabrication parameters, and, more importantly, to understand and predict the behavior of the mineral materials in the environment. The purpose of this project is to experimentally determine the enthalpy of formation of actinide orthosilicates, the enthalpies of formation of actinide substituted zirconolite and pyrochlore, and develop an understanding of the bonding characteristics and stabilities of these materials.

Keywords: High Temperature Solution Calorimetry, Actinides

284. **OPTIMIZATION OF THERMOCHEMICAL, KINETIC, AND ELECTROCHEMICAL FACTORS GOVERNING PARTITIONING OF RADIONUCLIDES DURING MELT DECONTAMINATION OF RADIOACTIVELY CONTAMINATED STAINLESS STEEL**
$400,000
DOE Contact: Arnold Gritzke, (202) 586-3957
SNL Contact: James A. Van den Avyle, (505) 845-3105

Melt Decontamination represents an effective scrap metal recycling route for the estimated 1,200,000 tons of contaminated stainless steel and nickel currently within the DOE complex. At present, this material must be considered a substantial disposal liability. However, with appropriate recycling, this material may be regarded as an asset worth an estimated $5 billion. The goal of this project is to optimize a melt decontamination process through a basic understanding of the factors which govern the partitioning of various radionuclides between the metal, slag, and gas phases. Radionuclides which are captured by a slag phase may be stabilized by promoting the formation of synthetic minerals within a leach-resistant matrix. This research describes an integrated program of simulation and experimentation designed to investigate and optimize liquid metal techniques for the decontamination and recycling of radioactive scrap metal.

Keywords: Melt Decontamination, Radioactive Scrap Metal

285. **MECHANISM OF PITTING CORROSION PREVENTION BY NITRITE IN CARBON STEEL EXPOSED TO DILUTE SALT SOLUTIONS**
$216,667
DOE Contact: Arnold Gritzke, (202) 586-3957
Savannah River Technology Center Contact: Philip E. Zapp, (803) 725-2567
University of South Carolina Contact: John Van Zee, (803) 777-2285

The overall goal of this project is to develop a fundamental understanding of the role of nitrite in preventing the breakdown of protective oxide coating on steel and the onset of pitting. A fundamental understanding of the materials science and electrochemistry of the nitrite role is expected to lead to superior and more cost-effective corrosion prevention methods for storing and processing complex, industrially important salt solutions. One important application of this new information in the DOE complex involves the high-level radioactive waste solutions contained in carbon steel tanks.

There is an extensive base of engineering knowledge of corrosion prevention by nitrite in alkaline salt solutions containing various organic and inorganic aggressive species. This knowledge is empirical; effective nitrite concentrations have been related to solution composition and temperature through numerous laboratory tests. The role of nitrite has not been explained electrochemically in a general manner that permits the prediction of nitrite effectiveness in solutions of widely varied composition.

A model is being developed of the nitrite concentration required to prevent pitting corrosion in terms of the electrochemical and surface oxide properties of the carbon steel solution system for a wide range of solution compositions. Typical industrial salt solutions contain numerous ionic species and suspended insoluble compounds, as well as dissolved organic species.

Keywords: Pitting Corrosion, Nitrite, Carbon Steel

286. **STABILITY OF HIGH-LEVEL WASTE FORMS**
$254,000
DOE Contact: Arnold Gritzke, (202) 586-3957
Oak Ridge National Laboratory Contact:
Theodore M. Besmann, (423) 574-6852

The assessment of release of radionuclides from waste repositories depends substantially on the leaching behavior of the spent fuel or waste form. Assumed rates based on dissolution of specific phases (assumption of unit activity) will lead to potentially grossly overestimated values as well as possibly underestimated values, and are therefore difficult to defend. Current, experimentally-determined values are less than desirable since they depend on measurement of the leach rate under non-realistic conditions designed to accelerate processes that are geologic in time scale. With the possible consideration of a hot repository for the disposal of spent fuel and high-level waste forms, the materials will experience elevated temperatures (>100°C) for hundreds of years or longer, driving chemical and phase changes. The objective of the effort is to develop a basic understanding of the phase equilibria and solid solution behavior of the constituents of high-level waste forms and to model that behavior. The results of this effort will provide reaction path information for leaching/transport codes such as ESP, as well as basic insights into complex ceramic solution behavior, bonding in glasses, and crystal chemistry of the fluorite-structure uranium dioxide-fission product system.

Keywords: Spent Fuel, High Level Waste, Leaching, Transport

287. **RADIATION EFFECTS IN NUCLEAR WASTE MATERIALS**
$960,000
DOE Contact: Arnold Gritzke, (202) 586-3957
PNNL Contact: William J. Weber, (509) 375-2299
Argonne National Laboratory Contact:
R. B. Bircher, (630) 252-4996
LANL Contact: Michael A. Nastasi, (505) 667-7007
University of Michigan Contact: Rodney C. Ewing, (313) 647-8529

The objective of this multidisciplinary, multi-institutional research effort is to develop a fundamental understanding at the atomic, microscopic, and macroscopic levels of radiation effects in glass and ceramics that provides the underpinning science and models for evaluation and performance assessments of glass and ceramic waste forms for the immobilization and disposal of high-level tank waste, plutonium residues and scrap, surplus weapons plutonium, and other actinides. 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. This program exploits a variety of structural, optical, and spectroscopic probes to characterize the nature and behavior of the defects, defect aggregates, and phase transformations. Computer simulation techniques are used to determine defect production from ballistic and ionization interactions, calculate defect stability, energies of formation and migration, damage processes within an alpha-recoil cascade, and defect/gas diffusion and interaction.

Keywords: Glass, Ceramics, Radiation Effects

288. **NEW SILICOTITANATE WASTE FORMS: DEVELOPMENT AND CHARACTERIZATION**
$400,000
DOE Contact: Arnold Gritzke, (202) 586-3957
PNL Contact: Mari Lou Balmer, (509) 372-4693
SNL Contact: Tina Nenoff, (505) 844-0340
UC Davis Contact: Alexandra Navrotsky, (916) 752-3292

This program outlines a new strategy for disposing of crystalline silicotitanate (CST) ion exchangers by *in situ* heat treatment to produce an alternate waste form. New waste forms and disposal strategies specific to CST secondary waste that are developed in this work will offer an alternative to current disposal plans which call for recombining the separated Cs, Sr-loaded CST into the high activity waste streams then dissolving it in borosilicate glass. This research is predicated by work at Pacific Northwest National Laboratory that shows that thermally treated CSTs have durabilities better than borosilicate glass. The goal of the program is to reduce the costs associated with CST waste disposal, to minimize the risk of contamination to the environment during CST processing, and to provide DOE with technical alternatives for CST disposal. Because there is uncertainty in repository availability and in waste acceptance criteria, it is likely that Cs and Sr loaded ion exchangers will require short term storage at Hanford or that new scenarios for long term storage or disposal of nuclides with relatively short half lives (such as 137Cs and 90Sr) will arise.

This research synthetically explores both low and high temperature stable and metastable phases involving the key component elements. This allows for characterization of all potential by-products from thermal treatment of CSTs. The technical objective of the work is to (1) fully characterize the phase relationships, structures and thermodynamic and kinetic stabilities of crystalline silicotitanate waste forms, and (2) to establish a sound technical basis for understanding key waste form properties, such as melting temperatures and aqueous durability, based on an in-depth understanding of waste form structures and thermochemistry.

Keywords: Silicotitanate, Waste Form

289. **DISTRIBUTION & SOLUBILITY OF RADIONUCLIDES & NEUTRON ABSORBERS IN WASTE FORMS FOR DISPOSITION OF PLUTONIUM ASH & SCRAPS, EXCESS PLUTONIUM, AND MISCELLANEOUS SPENT NUCLEAR FUELS**
$600,000
DOE Contact: Arnold Gritzke, (202) 586-3957
PNNL Contact: Denis Strachan, (509) 376-0677
Australian Nuclear Science & Technology Organisation Contact: Eric R. Vance, 011-61-2-9717-3733
LBNL Contact: David K. Shuh, (510) 486-6937
University of Michigan Contact: Rodney C. Ewing, (313) 647-8529

The objective of this multi-institutional, multi-national research effort is to understand the distributions, solubilities, and releases of radionuclides and neutron absorbers in waste forms. The results will provide the underpinning knowledge for developing, evaluating, selecting, and matching waste forms for the safe disposal of various wastes associated with Pu, miscellaneous spent nuclear fuels (SNF), and other transuranic (TRU) wastes and for developing deterministic model for the long-term performance assessment of radionuclide containment.

The scope of this project includes: (1) systematically investigate the solubility and partition behavior of selected waste forms as a function of composition, temperature, and processing conditions with the goal of enhancing our understanding of the physics and chemistry of radionuclides and neutron absorbers in simplified waste forms; (2) determine the local structure of radionuclides and neutron absorbers waste forms in various phases: (a) develop a microscale characterization to determine what phases are presented and how key elements are partitioned among those phases using optical, scanning, and transmission microscopies and XRD; (b) develop a molecular level characterization to understand local coordination using EXAFS and NMR; (c) perform an atomic level characterization to determine oxidation state using XANES; (3) selectively study waste form properties with the emphasis on the release behaviors of neutron absorbers and radionuclides.

Keywords: Radionuclides, Neutron Absorbers, Solubility, Waste Form

290. **MODELING OF DIFFUSION OF PLUTONIUM IN OTHER METALS AND OF GASEOUS SPECIES IN PLUTONIUM-BASED SYSTEMS**
$145,000
DOE Contact: Arnold Gritzke, (202) 586-3957
West Virginia University Contact: Bernard R. Cooper, (304) 293-3423
University of Connecticut Contact: Gayanath Fernando, (860) 486-0442

The research is aimed at developing and utilizing computational-modeling-based methodology to treat two major problems. The first of these is to be able to predict the diffusion of plutonium from the surface into the interior of another metal such as uranium or stainless steel (fcc iron). The second is the more complicated situation of treating the diffusion of a gaseous species into plutonium-containing oxidized material, specifically the solid-state diffusion of O_2-driven by an oxygen gradient. The first class of problem, diffusion of plutonium into host metals, is pertinent to characterizing contamination and consequent clean-up procedures in situations where plutonium has been in contact with other metals for extended periods of time. The second situation is pertinent to complicated hydrogen generation mechanisms creating possibly catastrophic pressure in situations, such as storage barrels, where oxidized plutonium-containing material has been stored for long periods of time.

The investigation of thermally-activated diffusion makes use of transition state theory with dynamic corrections. In transition state theory the number of crossings of a specified counting surface that separates initial and final states is equated to the number of such crossings that occur in an equilibrium system. The use of ab-initio-based atomistic potentials allows efficient mapping of the pertinent energy barriers. Molecular dynamics can be used to treat realistically the nature of the hoppings as well as to correct for dynamical effects such as recrossings. Grain boundaries are simulated and incorporated into dynamic simulations to study the relative importance of grain boundary diffusion in allowing plutonium atoms to penetrate into the interior of the host metals.

The two main components of the modeling study are: (1) the treatment of diffusion and of the pertinent grain boundary modeling and (2) the development of physically accurate plutonium atomistic potentials. The physical quality of these potentials is the controlling quantity in determining the ability to be accurately predictive for the questions of interest.

Keywords: Diffusion, Plutonium, Modeling and Simulations

291. **RADIONUCLIDE IMMOBILIZATION IN THE PHASES FORMED BY CORROSION OF SPENT NUCLEAR FUEL: THE LONG-TERM ASSESSMENT**
$160,321
DOE Contact: Arnold Gritzke, (202) 586-3957
University of Michigan Contact: Rodney C. Ewing, (313) 647-8529

The UO_2 in spent nuclear fuel is not stable under oxidizing conditions. Under oxidizing conditions, the U(IV) has a strong tendency to exist as U(VI) in the uranyl molecule, UO_2^{2+}. The uranyl ions react with a wide variety of inorganic and organic anions to form complexes which are often highly soluble. The result is rather rapid dissolution of UO_2 and the formation of a wide variety of uranyl oxide hydrates, uranyl silicates and uranyl phosphates. The reaction rates for this transformation are rapid, essentially instantaneous on geologic time scales. Over the long term, and depending on the extent to which these phases can incorporate fission products and actinides, these alteration phases become the near-field source term.

Fortunately, previous investigations (experimental studies and field studies) have established that natural uraninites and their alteration products can be used as natural analogues to study the corrosion of UO_2 in spent nuclear fuel. This research program is addressing the following issues: (1) What are the long-term corrosion products of natural UO_2+x, uraninite, under oxidizing conditions? (2) What is the paragenesis or the reaction path of the phases that form during alteration? How is the paragenetic sequence formation related to the structures and compositions of these uranyl phases? (3) What is the trace element content (as compared to the original UO_2+x), and does the trace element content substantiate models developed to predict fission product and actinide incorporation into these phases? (4) Are these the phases that are predicted from reaction path models (e.g., EQ3/6) which will be used in performance assessments? (5) How persistent over time are the metastable phase assemblages that form? Will these phases serve as barriers to radionuclide release? (6) Based on the structures of these phases (mostly sheet structures) can the thermodynamic stabilities of these phases be estimated, or at least bounded, in such a way as to provide for a convincing and substantive performance assessment?

Keywords: Uranium Oxides, Minerology, Corrosion, Phase Stability

292. **DIRECT INVESTIGATIONS OF THE IMMOBILIZATION OF RADIONUCLIDES IN THE ALTERATION PHASES OF SPENT NUCLEAR FUEL**
$260,829
DOE Contact: Arnold Gritzke, (202) 586-3957
University of Notre Dame Contact: Peter C. Burns, (219) 631-5380
Argonne National Laboratory Contact: Dr. Robert J. Finch, (630) 252-9829
University of Missouri-Rolla Contact: David J. Wronkiewicz

DOE is the custodian of several thousand tons of spent nuclear fuel that is intended for geological disposal. The direct disposal of spent nuclear fuel or of mixed oxide fuel (fabricated for the disposal of excess weapons plutonium) requires a careful analysis of the role of spent fuel as a waste form. During burn-up, as much as four percent of the uranium in the fuel will have fissioned to produce stable and radioactive fission products (e.g., Sr, Cs, Tc, I, Mo, Se). In addition, transuranic elements (e.g., Np, Pu, Am, Cm) will have formed from uranium by neutron capture. These radionuclides are cause for concern if they are released in to the biosphere.

In an oxidizing environment, such as in the proposed geological repository at Yucca Mountain, Nevada, rapid alteration rates are expected for spent nuclear fuel, based upon experimental studies of UO_2 and spent nuclear fuel. The alteration involves matrix dissolution of the UO_2 and will release the radionuclides contained within the spent fuel. Researchers in the Chemical Technologies Division of Argonne National Laboratory have ongoing experiments on the oxidative dissolution of both UO_2 and spent nuclear fuel. In both cases, the samples are exposed, by slow dripping in contact with air, to water similar in composition to that found at the Yucca Mountain site. The alteration rate of the UO_2 and spent fuel in the experiments is appreciable, and the alteration products are primarily U6+ phases. The generally low concentrations of the fission products and transuranic elements in spent fuel will probably preclude them from forming separate phases. Rather, current research at Argonne National Laboratories indicates that some of these radionuclides are being incorporated into the U^{6+} phases, significantly impacting upon the future mobility of the radionuclides.

Approximately 20 minerals that contain U^{6+} are of importance for spent fuel disposal. There is currently inadequate data pertaining to the migration of radionuclides in a repository setting. Only a limited database exists that relates to the effects of alteration phases on the retardation of radionuclides, but this information is necessary in providing a radionuclide release estimate as required for performance assessment modeling. This project will characterize the incorporation of radionuclides into the alteration products to enable a more realistic estimate of the rate of radionuclide migration from the near field environment. An accurate assessment of realistic radionuclide solubilities in the repository will allow for the development of an effective and cost-efficient engineered barrier system. The alteration products of spent nuclear fuel will be studied to identify in which phases, and to what extent, the radionuclides of environmental concern are being incorporated.

Keywords: Uranium Oxides, Minerology, Phase Stability, Corrosion, Radionuclides

293. **DECONTAMINATION OF RADIONUCLIDES FROM CONCRETE DURING AND AFTER THERMAL TREATMENT**
$271,907
DOE Contact: Arnold Gritzke, (202) 586-3957
ORNL Contact: Brian P. Spalding, (423) 574-7265
Northwestern University Contact:
Zdenek P. Bazant, (847) 864-4752

The total area of contaminated concrete within all DOE facilities is estimated at 7.9 x $10^8 ft^2$ or approximately 18,000 acres with the major contaminating radionuclides being U, ^{90}SR, ^{60}Co, and ^{137}Cs (Dickerson et. al. 1995). Techniques to decontaminate concrete through the application of heat (including microwaves, infrared radiation, lasers, plasma torch, etc.) have centered on the generally known deterioration of concrete strength with imposed thermal stress. These strategies have all attempted to spall or scabble contaminated solids from the concrete surface and to maximize the particular technology's capability to that end. However, in addition to the imprecisely defined knowledge of the physical effects of specific heat treatments on concrete (final temperature, heating rate, and type of concrete aggregate), concomitant behavior of DOE's major radioactive contaminants (^{137}Cs, U, ^{90}Sr, and ^{60}Co) during thermal treatment is very poorly known. This research will determine the thermal effects between 100 and 1400°C on concrete engineering properties (compressive strength, strain, porosity, bulk density, and cracking), chemical properties (dehydration, mineral phase change, and solubility), and contaminant behavior as a function of final temperature, heating rate, and aggregate type (none, limestone, or silica); thermal effects on contaminants and concrete are depicted conceptually in Figure 1. Major effects on radionuclide transport via direct volatilization (particularly for ^{137}Cs and ^{60}Co) during heating are anticipated to lead to *in situ* decontamination techniques. Changes in the extractability of radionuclides from heat affected concrete will be measured, using short-lived radioisotopes, to ascertain changes in decontamination potential following thermal treatment. Detailed finite-element modeling of heat flow in concrete and resulting mechanical stresses (from pore pressure and thermal expansion) of optimal thermal treatments will be completed so that effects on laboratory-sized specimens can be extrapolated to field-scale thermal treatments on concrete mechanical properties and contaminant behavior. Expected results will be a thorough and detailed understanding of the thermal effects on concrete engineering properties and concomitant radionuclide behavior including a detailed empirical data base. Specific decontamination technologies using thermal stressing of concrete will then be able to predict their effects rather than continue with DOE's apparent present approach of supporting novel thermal technologies without either a basic understanding of the limits of thermal effects on concrete or the fate and behavior of key radionuclides.

Keywords: Concrete, Radionuclides, Decontamination

294. **MECHANISMS OF RADIONUCLIDE-HYDROXYCARBOXYLIC ACID INTERACTIONS FOR DECONTAMINATION OF METALLIC SURFACES**
$383,333
DOE Contact: Arnold Gritzke, (202) 586-3957
BNL Contact: A. J. Francis, (516) 344-4534
State University of New York at Stony Brook
Contact: Gary P. Halada, (516) 632-8526

This project addresses key fundamental issues involved in the use of simple and safe methods for the removal of radioactive contaminants from slightly contaminated steel and other surfaces at the DOE sites so that the metals can be reused. The objectives are to (1) determine the nature of the association of radionuclides U, Pu, Co and Sr with stainless steel, and (2) selectively remove the radionuclides using hydroxycarboxylic acids (citric acid and its analogs). The basic mechanisms involving coordination, complexation, dissolution and removal will be elucidated in a systematic manner.

This is a collaborative research project between Brookhaven National Laboratory (BNL) and the State University of New York at Stony Brook (SUNY-SB). This project is divided into three phases. In Phase I the basic mechanism of interaction of actinides with metal oxides on metallic surfaces will be investigated. Phase II will determine the interaction of hydroxycarboxylic acids citric, malic and tartaric acids with the actinide contaminated metallic surfaces. Phase III involves investigation of interaction of hydroxycarboxylic acid with actual contaminated samples from DOE sites and interpretation of results based on knowledge gained from Phases I and II. The nature of radionuclide association with representative metal oxides typically formed on metallic surfaces which have undergone oxidation characteristic of long term environmental exposure will be investigated. The rate and extent of incorporation of radionuclide into amorphous and crystalline forms of iron oxides (goethite, hematite, magnetite and lepidocrocite), and metallic coupons will be determined. Exposure of metallic coupons to radionuclides during and following accelerated aqueous corrosion will utilize standard electrochemical cells and equipment. Advanced spectroscopic techniques (XPS, XANES, EXAFS, EDX, SIMS, FTIR and LD-ITMS at PNNL) will be used to characterize the (1) nature of the radionuclide association with the metal oxides and contaminated surfaces, and (2) radionuclide-citrate complexes and mixed-metal (actinide-metal-citrate) complexes that have been removed from contaminated surfaces. In addition, the photochemical and biochemical degradation of the resulting actinide-organic complexes will be examined, with application to recovery of radionuclides in a concentrated form and reduction of secondary waste generation.

Keywords: Radionuclides, Decontamination, Actinides, Corrosion

295. **PHYSICAL, CHEMICAL AND STRUCTURAL EVOLUTION OF ZEOLITE-CONTAINING WASTE FORMS PRODUCED FROM METAKAOLINITE AND CALCINED HLW**
$170,000
DOE Contact: Arnold Gritzke, (202) 586-3957
Pennsylvania State University Contact:
Michael Grutzeck, (814) 863-2779
Savannah River Technology Center Contact:
Carol M. Jantzen, (803) 725-2374

Natural and synthetic zeolites are extremely versatile materials. They can adsorb a variety of liquids and gases, and also take part in cation exchange reactions. Zeolites are easy to make, they can be synthesized from a wide variety of natural and man made materials. One such combination is metakaolinite and sodium hydroxide solution. The objective of this research is to adapt this well known reaction for use in site remediation and clean-up of caustic waste solutions now in storage in tanks at Hanford and the Savannah River sites.

It has been established that a mixture of calcined equivalent ICPP waste (sodium aluminate/hydroxide solution containing 3:1 Na:Al) and fly ash and/or metakaolinite can be cured at various temperatures to produce a monolith containing Zeolite A (80°C) or Na-P1 plus hydroxysodalite (130°C) dispersed in an alkali aluminosilicate hydrate matrix. The zeolitization process is a simple one and as such could be a viable alternative for fixation of low activity waste (LAW) salts and calcines. Dissolution tests have shown these materials to have superior retention for alkali, alkaline earth and heavy metal ions.

The technology for synthesizing zeolites is well documented for pure starting materials, but relatively little is known about the process if metakaolinite is mixed with a complex mixture of oxides containing nearly every element in the periodic table. The purpose of the proposed work is to develop a clearer understanding of the advantages and limitations of producing a zeolite-containing waste form from calcined radioactive waste, i.e. the effect of processing variables, reaction kinetics, crystal and phase chemistry, and microstructure on their performance. To accomplish this, two waste forms representative of solutions in storage at the Hanford and Savannah River sites will be simulated. Because nitrate is detrimental to the process, the LAW will be calcined at various temperatures (w/wo sugar) to maximize the reactivity of the resultant mix of oxide phases while minimizing the loss of volatiles. The oxides will be mixed with varying amounts and types of metakaolinite, small amounts of other chemicals (alkali hydroxides and/or carbonates, zeolite seeds, templating agents) and enough water to make a paste. The paste will then be cured (in-can) at a variety of temperatures (80°-100°C). Once reaction rates for the process are established, MAS NMR and TEM will be used to study the atomic-level structure of the solids. X-ray diffraction will be used to examine the degree of crystallinity of the waste forms. An environmental SEM will be used to track the development of microstructure in real time. An electron microprobe will be used to analyze the phases in the waste form. Attempts will be made to relate changes in phase chemistry and microstructure to distribution coefficients and dissolution data. Compressive and bending strength tests will be used to determine mechanical behavior and standard leach tests will be used to determine the potential consequences of cation exchange reactions. Since simulated waste is not an adequate predictor, a major portion of the proposed work will be carried out at the Savannah River Technology Center, using actual LAW samples obtained from the Savannah River site.

Keywords: Zeolites, Radioactive Waste

296. MECHANISMS AND KINETICS OF ORGANIC AGING IN HIGH-LEVEL NUCLEAR WASTES

$300,000
DOE Contact: Arnold Gritzke, (202) 586-3957
Pacific Northwest National Laboratory Contact:
Donald M. Camaioni, (509) 375-2739

Highly radioactive wastes stored at Hanford and Savannah River DOE sites have unresolved questions relating to safety of the stored waste, as well as needs for safe, effective, and efficient waste processing to minimize the volume of high-level waste (HLW) streams for disposal. HLW undergoes constant irradiation from decaying radionuclides resulting in an array of radiation and thermochemical effects that directly impact issues concerning storage, retrieval, and pretreatment of the wastes. Heat from nuclear decay and from chemical processing (e.g., evaporation campaigns and tank transfers) drive thermal reactions of waste constituents, especially organic complexants. Radiolytic and thermochemical processes have been shown to degrade ("age") organic solutes into smaller fragments of lower energy content, reducing hazards associated with deflagration of nitrate organic mixtures while contributing to hazards such as the generation of toxic, flammable and potentially explosive gases (i.e., volatile organics, NH_3, H_2, and N_2O).

The goal of this project is to develop a fundamental understanding of organic aging and to assemble a model which describes and predicts the thermal and radiolytic aging of organic compounds in high level wastes. Kinetics will be measured and products and mechanisms of organic reactions occurring under conditions of waste storage, retrieval, and processing will be elucidated. Much emphasis will be placed on studying thermal effects, since organic reaction mechanisms and effects of varying conditions are uncertain. Organic complexants are of greatest concern regarding both safety and pretreatment since they have been found to degrade to gases, combust in dry wastes, and interfere with radionuclide separations. Therefore, efforts will focus on studying the reactions of these organic chemicals and associated degradation products.

Keywords: Oxidation, Organics, Radionuclides, Aging

297. MODELING OF SPINEL SETTLING IN WASTE GLASS MELTER

$291,667
DOE Contact: Arnold Gritzke, (202) 586-3957
Pacific Northwest National Laboratory Contact:
Pavel R. Hrma, (509) 376-5092
Czech Academy of Sciences Contact:
Lubomir Nemec, 011-420-2-24-310-371
Glass Service Ltd. Contact: Petr Schill,
011-420-657-611-439

The topic of this multi-institutional bi-national research is the formation and settling of spinel, the most common crystalline phase that precipitates in molten high-level waste (HLW) glass. For the majority of HLW streams, spinel formation in the HLW melter limits the waste fraction in glass because accumulation of spinel interferes with melter operation and shortens its lifetime. Hence, understanding spinel formation and behavior is important for HLW vitrification technology and economy, which call for the highest waste loading that is compatible with the quality and processability of the waste form.

Spinel is a product of an interaction between Cr_2O_3, Fe_2O_3, NiO, FeO, and other oxides, which are components of virtually all HLW streams at Hanford and Savannah River. Understanding and modeling the kinetics of spinel formation and the dynamics of spinel behavior in a waste glass melter will result in a reliable prediction and control of the rate of spinel settling and accumulation. The spinel settling rate will be predicted by mathematical modeling for which reliable experimental values of coefficients and material parameters will be obtained by laboratory studies. This approach combines the materials science, hydrodynamics, and mathematical modeling of spinel behavior in HLW glass melters.

Keywords: Spinel Formation, Equilibria, High-Level Waste Glass

OFFICE OF NUCLEAR ENERGY, SCIENCE AND TECHNOLOGY

	FY 1998
Office of Nuclear Energy, Science and Technology - Grand Total	$70,117,000
Office of Space and Defense Power Systems	$ 3,617,000
Space and National Security Programs	$ 3,617,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 3,537,000
Development of an Improved Process for the Manufacture of DOP-26 Iridium Alloy Blanks and Clad Vent Sets, Product Characterization and Exploratory Alloy Improvement Studies	1,940,000
Carbon-Bonded Carbon Fiber Insulation Production Maintenance, Manufacturing Process Development and Product Characterization	320,000
A New High Temperature Solar Cell/Selective Emitter for Thermo Photovoltaic (TPV) Systems	272,000
Carbon-Carbon Composites with Improved Mechanical and Thermal Characteristics for Radioisotope Power Systems	300,000
Enhancement of High Temperature Performance of Nd-Fe-B Permanent Magnets for Sterling Engine/Linear Alternator Power Generation	225,000
AMTEC Electrode and Beta" Alumina Solid Electrolyte Development	300,000
AMTEC Cell Assembly Process Development for Haynes-25 and for Niobium-1% Zirconium Cells	180,000
Materials Properties, Behavior, Characterization or Testing	$ 80,000
Emissivity Measurement and Sodium Compatibility Tests on AMTEC Cell Materials	80,000
Office of Naval Reactors	$66,500,000[1]

[1]This excludes $48.5 million for the cost of irradiation testing in the Advanced Test Reactor (ATR).

OFFICE OF NUCLEAR ENERGY, SCIENCE AND TECHNOLOGY

OFFICE OF SPACE AND DEFENSE POWER SYSTEMS

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 space nuclear reactor power and propulsion systems. During FY 1998, essentially all materials programs were aimed at: (1) transfer of clad vent set production operation from the Y-12 plant to Oak Ridge National Laboratory, (2) maintenance of iridium alloy and carbon bonded carbon fiber (CBCF) insulation radioisotope heat source material and components manufacturing capability, (3) continued improvement in heat source materials and their production processes and product characterization and (4) materials support for future terrestrial system applications and advanced high efficiency space power systems, particularly the alkali thermal to electric conversion (AMTEC) radioisotope power systems.

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

298. **DEVELOPMENT OF AN IMPROVED PROCESS FOR THE MANUFACTURE OF DOP-26 IRIDIUM ALLOY BLANKS AND CLAD VENT SETS, PRODUCT CHARACTERIZATION AND EXPLORATORY ALLOY IMPROVEMENT STUDIES**
$1,940,000
DOE Contact: W. Barnett, (301) 903-3097
ORNL Contacts: E. P. George, (423) 574-5085 and E. K. Ohriner, (423), 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 production of DOP-26 alloy blanks, foil and clad vent sets for the Cassini Mission. Production yields have continued to exceed our goals.

During FY 1997, production of DOP-26 iridium alloy blanks, foil and clad vent set hardware for the Cassini mission was completed. Transfer of the clad vent set manufacturing operation from the Y-12 plant to the Oak Ridge National Laboratory was continued. Iridium alloy manufacturing capabilities are being maintained in a production maintenance mode.

Iridium process improvement activities were continued. Bare rolling is ready for introduction into the sheet production process. Bare cup forming development was continued. Scale-up and evaluation of a new DOP-40 low thorium alloy (Ir-0.3 wt. % tungsten with dopant additions of 40 ppm cerium and 15 ppm thorium) was continued. A study of laser welding for fuel clad closure was initiated.

Keywords: Consumable Arc Melt, Extrusion, Noble Metal, Rolling, Forming

299. **CARBON-BONDED CARBON FIBER INSULATION PRODUCTION MAINTENANCE MANUFACTURING PROCESS DEVELOPMENT AND PRODUCT CHARACTERIZATION**
$320,000
DOE Contact: W. Barnett, (301) 903-3097
ORNL Contact: D. J. McGuire, (423) 574-4835

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 1998 program encompassed (1) continued maintenance of capability for both tube and plate billet production, (2) qualify a new X-ray inspection process and upgrade chemical analyses capability.

Keywords: Insulators/Thermal, High Temperature Service, Fibers

300. **A NEW HIGH TEMPERATURE SOLAR CELL/SELECTIVE EMITTER FOR THERMO PHOTOVOLTAIC (TPV) SYSTEMS**
$272,000
DOE Contact: W. Barnett, (301) 403-3097
Auburn University, Space Power Institute Contact: H. W. Brendhurst, (334) 844-5894

Selective rare earth emitters are being developed and matched with solar cells for TPV operation of 200°PC or higher.

Keywords: Selective Emitters, Solar Cells, Thermophotovoltaics

301. **CARBON-CARBON COMPOSITES WITH IMPROVED MECHANICAL AND THERMAL CHARACTERISTICS FOR RADIOISOTOPE POWER SYSTEMS**
$300,000
DOE Contact: W. Barnett, (301) 903-3097
Auburn University Contact: R. Zee, (334)844-3320
ORNL Contact: G. Romanowski, (423) 574-4838

Carbon-carbon composites having variations in cylindrical reinforcement architecture are being evaluated for replacement of the fine weave pierced fabric orthogonal structure currently being employed in the General Purpose Heat Source Graphite Impact Shell. Impact behaviors are being investigated.

Keywords: Carbon-Carbon, Impact Shell

302. **ENHANCEMENT OF HIGH TEMPERATURE PERFORMANCE OF Nd-Fe-B PERMANENT MAGNETS FOR STERLING ENGINE/LINEAR ALTERNATOR POWER GENERATION**
$225,000
DOE Contact: W. Barnett, (301) 903-3097
Iowa State University Contacts: F. McAllum, (515) 294-4726 and M. Russel, (515) 294-9225

Structure modifications via developed of functionally graded materials were persuaded to significantly enhance the Curie temperature with minimal degradation of the energy product.

Keywords: Permanent Magnets, Rare Earth Magnets

303. **AMTEC ELECTRODE AND BETA" ALUMINA SOLID ELECTROLYTE DEVELOPMENT**
$300,000
DOE Contact: W. Barnett, (301) 903-3097
Texas A&M University Contact: M. Schuler, (409) 845-8767

The development of improved performance electrode materials, principally iridium and mixed conductor electrode materials, was initiated for potentially improved performance AMTEC cells.

Keywords: Electrode Materials, AMTEC

304. **AMTEC CELL ASSEMBLY PROCESS DEVELOPMENT FOR HAYNES-25 NIOBIUM-1% ZIRCONIUM CELLS**
$180,000
DOE Contact: W. Barnett, (301) 903-3097
ORNL Contact: J. King, (923) 574-4807

Electron beam weld procedures and fixture were developed and applied to the manufacture of developmental AMTEC cell test hardware.

Keywords: Electron Beam Welding, AMTEC

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

305. **EMISSIVITY MEASUREMENT AND SODIUM COMPATIBILITY TESTS ON AMTEC CELL MATERIALS**
$80,000
DOE Contact: W. Barnett, (301) 903-3097

Emissivity measurements on AMTEC cell materials were conducted before and after sodium exposure tests.

Keywords: Emissivity, Sodium Compatibility, AMTEC

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 $115 million in FY1998. Approximately $48.5 million represents 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 1998
Office of Civilian Radioactive Waste Management - Grand Total	$23,848,000
Materials Properties, Behavior, Characterization or Testing	$23,848,000
Waste Packages	$23,848,000

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

306. **WASTE PACKAGES**
$23,848,00
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 and Viability Assessment design was completed in 1998. 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 1997. Interim examination of selected samples have been completed and documented in project reports. Waste form materials are also being evaluated for alteration and leaching under repository-relevant conditions. During 1998 additional materials were added to the test matrix based on an evaluation of alternate waste package design and materials configurations. This work was done in support of License Application Design Selection Alternatives Evaluation. To provide supporting test data for this design option, two new materials, titanium grade 7 and 316L stainless steel were added to the test matrix. In addition, a short-term test program was initiated to support waste package material degradation model development effort. The short-term test program focuses on stress corrosion cracking, hydrogen embrittlement, crevice corrosion, galvanic effects among the candidate materials and determination of the appropriate test environment that will represent saturated aqueous condition on the waste package surface.

Keywords: Yucca Mountain Repository, Waste Package, Engineered Barrier System

OFFICE OF DEFENSE PROGRAMS

	FY 1998
Office of Defense Programs - Grand Total	$67,591,200
The Weapons Research, Development and Test Program	$67,591,200
Sandia National Laboratories	$16,886,200
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 5,924,000
Materials Processing	2,999,000
Atomic-Scale Studies of Surface Defect Chemistry	*600,000*
Exploiting Lens Technology Through Novel Materials	545,000
Atomically-Engineered Nanostructures: An Interdisciplinary Approach to Properties	400,000
Enabling Science & Technology for Cold Spray Direct Fabrication Properties	330,000
Atomic-Level Studies of Surfactant-Directed Materials Growth	400,000
Freeforming of Ceramics and Composites from Colloidal Slurries	450,000
Laser-Assisted Arc Welding for Aluminum Alloys	200,000
Materials Properties, Behavior, Characterization or Testing	$ 8,367,600
Aging and Reliability	1,997,000
From Atom-Picoseconds to Centimeter-Years in Simulation and Experiment	700,000
Nanoscale Structures and Phenomena	1,070,000
Hardening and Tribological Improvement of Mems Ni Alloys by Ion Implantation	300,000
Corrosion Behavior of Plasma-Passivated Copper	400,000
In-Situ Stress Relaxation During Annealing of Amorphous Carbon Films	300,000
Physics of Photosensitivity in Novel Thin Films	250,000
The Shock Properties of PZT 95/5	300,000
The Properties and Physics of the Slim-Loop Ferroelectric PBZT-Bi	250,000
Catalytic Membrane Sensors	361,600
Photonic Band Gap Structures as a Gateway to Nano-Photonics	375,000
Molecular-Scale Lubricants for Micromachine Applications	475,000
The Initiation and Propagation of Nano-Scale Cracks at an Adhesive/Solid Interface	400,000
Fundamental Aspects of Micromachine Reliability	350,000
Intelligent Polymers for Nanodevice Performance Control	439,000
Quantum Dot Arrays	400,000
Device or Component Fabrication, Behavior or Testing	$ 1,257,600
Wide-Bandgap Compound Semiconductors to Enable Novel Semiconductor Devices Project	290,000
Scanning Probe-Based Processes for Nanometer-Scale Device Fabrication	442,600
Surface Micromachined Flexural Plate Wave Device Integrated on Silicon	525,000
Instrumentation and Facilities	$ 1,337,000
Advanced Analytical Techniques	998,000
Monolithic Structures for Nanoseparation Properties	339,000

OFFICE OF DEFENSE PROGRAMS (continued)

	FY 1998
The Weapons Research, Development and Test Program (continued)	
Los Alamos National Laboratory	$33,300,000
Materials Properties, Behavior, Characterization or Testing	$33,300,000
Rapid Solidification Processing	500,000
Neutron Diffraction	1,500,000
Dynamic Mechanical Properties of Weapons Materials	2,000,000
Materials Aging	11,000,000
Powder Characterization	300,000
Manufacturing Process Development	8,000,000
Component Fabrication	10,000,000
Lawrence Livermore National Laboratory	$17,405,000
Material Preparation, Synthesis, Deposition, Growth or Forming	$ 7,440,000
Engineered Nanostructure Laminates	2,000,000
KDP and DKDP Crystal Development and Production	4,000,000
Energetic Materials Strategic Chemistry	350,000
Cheetah Thermochemical Code	190,000
Explosives Development	900,000
Material Properties, Behavior, Characterization or Testing	$ 1,665,000
Interfaces, Adhesion, and Bonding	265,000
Laser Damage: Modeling and Characterization	400,000
KDP Characterization	1,000,000
Instrumentation and Facilities	$ 8,300,000
Scanning Tunneling Microscopy (STM), Atomic Force Microscopy (AFM), Near Field Scanning Optical Microscopy (NSOM)	250,000
Atomic Level Explosive Calculations	325,000
Metastable Solid-Phase High Energy Density Materials	535,000
AFM Investigations of Crystal Growth	290,000
Uranium Casting Program	400,000
Uranium Spin Forming	1,200,000
Plutonium Near Net Shape Casting	2,500,000
Electron Beam Cold Hearth Melting of Uranium	900,000
NIF Capsule Mandrel R&D	800,000
Polyimide Coating Technology for ICF Targets	500,000
Beryllium Ablator Coatings for NIF Targets	600,000

THE WEAPONS RESEARCH, DEVELOPMENT AND TEST PROGRAM

SANDIA NATIONAL LABORATORIES

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

307. **MATERIALS PROCESSING**
$2,999,000
DOE Contact: Bharat Agrawal, (301) 903-2057
SNL Contact: John A. Sayre, (505) 845-9757

The Materials Processes Program focuses on the research required to create laboratory scale materials processes for re-manufacturing weapons components by more rapid, predictable, and affordable methods than those used in the past. Projects emphasize the predictability of microstructure and composition from the processing conditions, and the incorporation of this predictability into scientific models and simulations for use by weapons designers and manufacturing engineers. A new feature of this thrust is a focus on processes which enable fabrication with fewer steps from design to product, with the ultimate goal of one-step fabrication of complex shape parts composed of multiple materials directly from a CAD file.

Keywords: Processing, Fabrication

308. **ATOMIC-SCALE STUDIES OF SURFACE DEFECT CHEMISTRY**
$600,000
DOE Contact: Gerald Green, (202) 586-8377
SNL Contact: Nancy B. Jackson, (505) 272-7619

We propose to use a combination of experimental and theoretical techniques to explore atomic scale defect chemistry on technologically important surfaces, with the goal of determining the salient factors that control defect chemistry. The formation, mobility, reactivity, and dissolution of atomic scale surface defects play an important role in materials areas such as catalysis, corrosion, thin film growth, semiconductor processing, sensors, and magnetic devices. Important defects include single adatoms, surface steps and kinks, dislocations, and vacancies. It is generally believed that a small number of localized surface defects may be particularly reactive and thereby dominate the surface chemistry of many materials. While past studies of this important problem have been limited by an absence of appropriate experimental probes for imaging atomic scale defects, the recent advent of specialized scanning probe microscopies largely overcomes this problem and now allows more detailed studies of defect chemistry than previously possible. The unique Atom Tracking scanning tunneling microscope (STM) recently developed at Sandia is a particularly powerful new technique that allows measurement of atomic-scale kinetic processes on a time scale that is more than three orders of magnitude faster than previous techniques. Similarly, a lack of sufficient computing power has severely limited previous theoretical studies of defect properties. The recent development of massively parallel computational techniques at Sandia, which now allows calculations on systems containing hundreds of atoms per unit cell, will enable studies of surface defects with a level of detail and sophistication far greater than previously possible. By studying well defined, well ordered surfaces, we can greatly simplify the study of defect chemistry and obtain detailed fundamental information on defect formation and reactivity. Coupling experimental results with theoretical studies will allow the development of models that explain, predict, and ultimately help to control surface defect reactivity.

Keywords: Atomic Scale, Chemistry, Defects

309. **EXPLOITING LENS TECHNOLOGY THROUGH NOVEL MATERIALS**
$545,000
DOE Contact: Gerald Green, (202) 586-8377
SNL Contact: Brian Damkroger, (505) 845-3592

LENS (Laser Engineered Net Shaping) is a direct fabrication process in which metal powders are deposited into a laser melted pool, with succeeding layers being deposited to build up complex engineering shapes. In this age of model based designs and requirements the ability to directly transform design information into a manufactured product is extremely desirable. LENS is a rapid, low cost, low footprint direct fabrication process that lends itself to this concept for advanced manufacturing. However, previous work has developed LENS as an advanced manufacturing tool, rather than exploiting its unique attributes. These attributes include: real time microstructural control, tailored material properties at different locations in the same part, the production of graded CTE parts. This project will develop a science based approach to utilize LENS to "process for properties" in a controlled fashion, or for the production of components that cannot be made using other methods. Three materials: a tool steel with an optimized structure/property mix, a graded structure based on stainless steel compositions, and a ceramic-to-metal transition are novel material systems through which LENS will be investigated and exploited.

This goal will be achieved by first developing a thorough understanding of the process in terms of how it impacts solidification and microstructure development. Factors like solidification rate, thermal profiles, cooling rate, powder input, and residual stresses must be understood, as well as their effects on material responses such as dendrite tip velocity and undercooling, microsegregation, precipitation and transformation kinetics. Using pyrometry and thermocouple techniques in conjunction with accurate data regarding powder flow, gas flow, laser power and feed rate, the conditions present in the molten pool will be used to develop models of solidification and microstructural evolution. Additionally, the unique attributes and capabilities of the LENS process will be studied and understood. From this knowledge base, will be designed and produced a suite of experimental materials and structures that optimally exploit the LENS process and demonstrate its unique potential. An understanding of the residual stresses in LENS parts, and what mitigation techniques may be available will be developed.

Keywords: Metals, Processing, Laser, Solidification

310. **ATOMICALLY-ENGINEERED NANO-STRUCTURES: AN INTERDISCIPLINARY APPROACH TO PROPERTIES**
$400,000
DOE Contact: Gerald Green, (202) 586-8377
SNL Contact: Gordon Osbourn, (505) 844-8850

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, but chemically heterogeneous 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. This project is developing theoretical and experimental underpinnings 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 has several subtasks: (1) develop the first "database" of multivariate STM spectral features (i.e., the analogue of satellite "ground truth" spectra); (2) study the effects of different tip states on the STM spectral features and attempt to establish procedures for computationally removing or minimizing variable-tip effects; (3) use pattern recognition of STM spectral imagery, based on the results of tasks (1) and (2), to map out the atomic scale chemical structure of selected cleaved (110) III-V surfaces. The alloy ordering and interfacial structure of III-V structures of current programmatic interest for IR device applications is being studied.

Keywords: Nanostructures, STM

311. **ENABLING SCIENCE & TECHNOLOGY FOR COLD SPRAY DIRECT FABRICATION PROPERTIES**
$330,000
DOE Contact: Gerald Green, (202) 586-8377
SNL Contact: Mark Smith, (505) 845-3256

Direct Fabrication is envisioned as a rapid, agile, economical process technology that additively builds up a net or near-net shaped component made of one or more materials directly from a computer model; such technology would be of enormous benefit to SNL's core National Security Mission and U.S. industry. Cold Spray Processing (CSP) is a recently discovered, poorly understood, Russian technology that can rapidly deposit (mm/sec) metals, polymers, and composites at temperatures < 200°C by accelerating powder particles up to 600-1000 m/s in a supersonic compressed air or gas jet. The Russians have used CSP for high-rate coating deposition, but no one has attempted direct fabrication via CSP. One can envision a radical new fabrication technology in which a highly focused CSP particle "beam" is combined with a multi-axis robotic motion system in order to spray-fabricate a single- or multi-material component directly from a computer model. CSP build rates should be substantially higher than present layer-wise direct fabrication techniques and, since CSP particles are never fully melted, superior surface finishes, microstructures, and properties might be achieved (e.g., finer grain size, no brittle phases, minimal oxidation, less residual stress). With CSP, one might also deposit functionally graded or layered materials at low temperatures, thus eliminating joining operations, simplifying design/fabrication, reducing part counts, and decreasing stress cracking. (For example, aluminum has been CSP-deposited directly onto smooth, unprepared glass with excellent adhesion.) CSP may also be an environmentally friendly alternative to problem technologies, such as copper electroplating and soldering or painting of aircraft and weapons.

This project explores the use of cold spray processing for direct fabrication of simple proof-of-concept shapes.

Keywords: Cold Spray Processing, Direct Fabrication

312. **ATOMIC-LEVEL STUDIES OF SURFACTANT-DIRECTED MATERIALS GROWTH**
$400,000
DOE Contact: Gerald Green, (202) 586-8377
SNL Contact: Terry Michalske, (505) 844-5829

This project is investigating converting surface impurities from a nuisance to a systematically applicable nano-fabrication tool. Combining Sandia's special facilities, including the "atom-tracker" Scanning Tunneling Microscope (AT-STM), Low Energy Electron Microscopy (LEEM), and Massively Parallel Computation (MPC), the objective is to learn how common adsorbed atoms ("surfactants") can be used to manipulate and direct thin-film growth, and to develop a "surfactant toolkit" that enables production of either atomically flat or 3-dimensionally nano-structured surfaces. The approach is to start with model systems, studying surfactant-modified diffusion on and near metal and semiconductor surfaces, and integrating real- time experimental and advanced computational modeling capabilities. The AT-STM is being used to study H-assisted Si adatom diffusion on Si(001), and the LEEM to investigate both H-assisted step fluctuations on the same surface and O-assisted island growth on Pt(111). Ge segregation versus adsorbate overlayer coverage is being investigated in Si-Ge alloys via novel surface stress measurements. Theoretical efforts are closely coupled to experiments—MPC is indispensable in developing reliable, atomic-scale, mechanistic models.

Keywords: AT-STM, LEEM, MPC

313. **FREEFORMING OF CERAMICS AND COMPOSITES FROM COLLOIDAL SLURRIES**
$450,000
DOE Contact: Gerald Green, (202) 586-8377
SNL Contact: Michael Cieslak, (505) 845-9144

This project is developing a model-based direct freeform fabrication technique for ceramic, metal, or graded composite components. These components are fabricated without molds or tooling by building two-dimensional layers into three-dimensional shapes by dispensing colloidal suspensions through an orifice. Any conceivable two-dimensional pattern may be "written" layer by layer into a three-dimensional shape. Initial experiments have demonstrated technique feasibility for simple aluminum oxide shapes. The goal is to develop model-based processing rules that will aid in the development of slurries with the appropriate rheology, density, and drying kinetics to insure process success for a variety of ceramics and composites. Software and equipment development is also essential for precise control of layer thickness and feature resolution.

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

This work directly impacts the production of neutron tubes (MC4277, MC4300 and RP2) and ceramic fixtures for switch tubes (MC3859).

Keywords: Ceramics, Composites, Freeforming

314. **LASER-ASSISTED ARC WELDING FOR ALUMINUM ALLOYS**
$200,000
DOE Contact: Gerald Green, (202) 586-8377
SNL Contact: Brian Damkroger, (505) 845-3592

At this time, there exists a strong need in the defense programs, automotive, aerospace and transportation industries for a rapid, robust, high quality process for welding aluminum alloys, especially for relatively thin gauge product. While laser beam welding is widely applied in these industries it has not proved valuable for aluminum because of problems with reflectivity and weld joint variability. Gas metal arc welding (GMAW) is widely used for thick section aluminum welding because the process can compensate for part fit-up and metallurgical deficiencies. Under this project a new welding process is being developed by combining together a fiber optic-delivered pulsed Nd:YAG laser with a miniaturized GMAW system. The new laser-assisted arc welding (LAAW) process couples the process advantages of these two unique heat sources and will also enable process capabilities never before envisioned in arc welding. These two heat sources are being combined in a compact (likely patentable) device that can be manipulated on the end of a robotic arm. The focused pulsed Nd:YAG laser beam assures deep weld penetration and ablative removal of the tenacious aluminum oxide. The arc is focused and located by the metal vapor and gas ions generated by the high intensity laser beam. Increased arc stability is anticipated since the gas metal arc is known to be stabilized by thermal ionization of the shielding gas. The project is a System of Laboratories (SOL) collaboration among ORNL, INEEL and SNL. These three laboratories have distinguished themselves for their contributions to the science and technology of materials joining. The team established through this SOL interaction should allow the U.S. to successfully compete with international entities, such as Germany's Fraunhofer Institute, in developing (and hence owning) advanced joining technologies for commercially critical markets.

Keywords: Laser-Assisted Arc Welding

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

315. **AGING AND RELIABILITY**
$1,997,000
DOE Contact: Bharat Agrawal, (301) 903-2057
SNL Contact: Richard J. Salzbrenner, (505) 844-9408

The Materials Aging and Reliability Project advances the understanding of the microstructural mechanisms which control the aging, reliability, and performance of materials. The selection of subprojects is based on the risk (likelihood vs. consequence) of the failure of a specific material to weapon performance or surety. All subprojects seek to develop fundamentally-based prediction capability to determine the effects of aging on the performance and reliability of non-nuclear materials used in nuclear weapons. This project supports materials science work that is collaborative with other research programs to develop predictive capability that can be applied to the enduring stockpile.

Keywords: Aging, Reliability

316. **FROM ATOM-PICOSECONDS TO CENTIMETER-YEARS IN SIMULATION AND EXPERIMENT**
$700,000
DOE Contact: Gerald Green, (202) 586-8377
SNL Contact: Michael I. Baskes, (925) 294-3226

Stockpile stewardship is perhaps Sandia's most important mission in the coming millennium. The understanding of aging phenomena is a critical aspect of stockpile stewardship. Accelerated aging tests and examinations of stockpile components play an important role, but both have their limitations. Accelerated aging tests at elevated temperatures skew the relative probabilities of various reactions. Examination of stockpile components provides a limited database and tends to leave us in a reactive rather than proactive position, i.e., we may learn about a problem only when it is almost too late to do anything about it. Consequently, it is a vital part of stockpile stewardship to develop simulation techniques that are accurate and valid over much greater time and length scales than those presently available. Most importantly, the simulation techniques should be tested by experiment at various length and time scales so that they can be validated and improved.

The state of the art in computer simulation allows precise studies of the atomic electronic structure, detailed calculations of atomic trajectories, modeling of long time scales OR modeling of large length scales. These capabilities tend to be mutually exclusive at present due to limits in communication between disciplines, limits in algorithm development, and limits in computer power. This project will use a coordinated multidisciplinary research effort to incorporate the accuracy presently available in atomistic molecular dynamics and electronic structure calculations into simulations at much longer time and length scales.

Four novel complementary computational techniques will be developed and/or employed: hyper molecular dynamics, chain of states method, transition state theory, and stochastic lattice dynamics. The simulations will be coupled with experiments on three specific materials problems critical to Sandia missions:

- The relationship between hardening, strain, and length scale in microcomponents. The response of submicron solid structures to torsion and planar simple shear will be measured.
- Permeation through microporous media (polymers and zeolites).
- Semiconductor deposition. The atom tracker will be used to examine the motion of silicon atoms which occurs during growth of silicon films.

Keywords: Aging, Simulation, Atomic Scale, Molecular Dynamics

317. **SCALE STRUCTURES AND PHENOMENA**
$1,070,000
DOE Contact: Bharat Agrawal, (301) 903-2057
SNL Contact: Michael I. Baskes, (925) 294-3226

The Nanoscale Structures and Phenomena Project encompasses research on all classes of materials whose properties depend on phenomena unique to small (<1 micron) size. Properties are studied in order of decreasing interest and include mechanical, electrical, magnetic, and optical. Synthesis of both materials and structures, materials characterization, and performance are linked using appropriate theory and modeling of model systems. Emphasis is placed on obtaining an understanding of controlling mechanisms in these model systems and extending this understanding to predictions of complex materials and devices.

Keywords: Nanoscale Structures, Nanoscale Phenomena

318. **HARDENING AND TRIBOLOGICAL IMPROVEMENT OF MEMS Ni ALLOYS BY ION IMPLANTATION**
$300,000
DOE Contact: Bharat Agrawal, (301) 903-2057
SNL Contact: Wil Gauster, (505) 284-3504

The performance and lifetime of micro-electromechanical systems (MEMS) constructed from electroformed nickel alloys would be greatly enhanced by surface hardening and reductions in unlubricated friction and wear. Processing to achieve these benefits must minimize dimensional changes and heating, and must avoid the introduction of surfaces layers susceptible to debris-forming exfoliation or aging degradation. Ion implantation satisfies these constraints, and the technique has been shown to allow controlled modification of near-surface composition and microstructure leading to strengthening and reduced friction and wear. We are therefore exploring the use of ion implantation to harden the surfaces and reduce the friction and wear of Ni-based alloys used in MEMS. A scientific objective is to understand and quantify the relationship of mechanical properties to implantation-modified microstructure. Dual ion implantation of titanium and carbon has been demonstrated to produce an amorphous layer with superior mechanical properties in annealed bulk Ni and in the electroformed Ni and $Ni_{75}Fe_{25}$ of MEMS. The intrinsic yield strength of the amorphous Fe-Ti-C layer was determined from nanoindentation and finite-element modeling to be 5 GPa. This exceeds by a factor of two the strength of maximally hardened martensitic bearing steel, and it is also about twice the strength of conventional, metalloid-stabilized amorphous Ni-Fe alloys. Such exceptional resistance to plastic flow is ascribed to the absence of dislocation glide combined with strong atomic-pairing reactions between Ti and C. The near-surface strengthening resulting from implantation is found to suppress the destructive adhesion-and-fracture wear characteristic of untreated Ni surfaces in sliding contact. Scientifically, the present investigation is the first to quantify and mechanistically account for the intrinsic mechanical properties of an implantation-amorphized alloy.

Keywords: Micromachines, Hardening, Friction and Wear

319. **CORROSION BEHAVIOR OF PLASMA-PASSIVATED COPPER**
$400,000
DOE Contact: Bharat Agrawal, (301) 903-2057
SNL Contact: Jeff Nelson, (505) 844-4395

Predictive understanding of corrosion is needed to ensure reliability in both electronics and micro-electronics components. To date, modeling has been hindered by limited knowledge of primary corrosion mechanisms and the large number of coupled chemical reactions, which depend on complex interactions of materials with the environment. This multidimensional problem requires new approaches for quantitative identification of critical phenomena occurring in corrosion phase space. We are examining combinatorial techniques as a first step toward developing these new experimental approaches and determining mechanisms critical to copper sulfidation. In initial experiments, parallel experimentation was used in which the thickness of Cu oxide and the level of irradiation-induced defects were varied to efficiently identify mechanisms for Cu sulfidation. A Cu film was deposited on an SiO_2 covered Si wafer and then masked and oxidized in an electron cyclotron resonance (ECR) plasma to form different thicknesses of CuO_x on Cu. The sample was then implanted with 200 keV Cu^+ ions with different fluences to create different levels of point defects in the oxide and Cu. The sample matrix as well as a control sample, which had been exposed to air to form a native oxide, were then exposed to an H_2S environment. The variation in oxide thickness had little effect on the formation of and quantity of Cu_2S, while the level of irradiation affected the Cu_2S formation greatly. The plasma-oxidized Cu yields a surface which is more resistant to sulfidation than an air-oxidized Cu, thus providing a means to treat Cu for minimizing corrosion in sulfidizing environments. The results of this experiment show that the type of Cu-oxide (CuO vs. Cu_2O) and defect levels in the oxide are more important for controlling the sulfidation reaction than is the oxide thickness.

Keywords: Corrosion, Aging, Reliability

320. ***IN-SITU* STRESS RELAXATION DURING ANNEALING OF AMORPHOUS CARBON FILMS**
$300,000
DOE Contact: Bharat Agrawal, (301) 903-2057
SNL Contact: Wil Gauster, (505) 284-3504

Amorphous carbon thin films grown by pulsed laser deposition can have properties approaching those of diamond. In particular, we have measured thin films of this material that are 90 percent as hard and stiff as crystalline diamond, classing them as the second hardest material known to man. In addition, these films are electrically resistive, have low friction coefficient, and have extremely low wear rates, thus earning the name of amorphous diamond. One major limitation of these films is that very large compressive stresses (10 GPa) are generated during growth. This ultimately limits many applications of amorphous diamond (in particular tribological applications) since thicker films are often required. However, it has been demonstrated that simple thermal annealing treatments can *completely* relax the residual stress in these films. Surprisingly, the films retain their diamond-like nature with only minor changes in the bonding structure due to the annealing procedure. A detailed understanding of the stress relaxation in amorphous diamond is emerging from this work. Importantly, this understanding is predictive and is being used to guide applications development for this new material. In particular, stress relief enables the production of arbitrarily thick films and very thin large-area free-standing membranes. These thick films and membranes have applications in tribological coatings, X-ray and/or electron transparent windows and sensors;

and as a material for microelectromechanical (MEMS) devices.

Keywords: Coatings, Stability, MEMS

321. **PHYSICS OF PHOTOSENSITIVITY IN NOVEL THIN FILMS**
$250,000
DOE Contact: Bharat Agrawal, (301) 903-2057
SNL Contact: Gerry Hays, (505) 844-4135

Photosensitive (PS) materials permanently change their refractive index upon exposure to intense light, enabling a wide range of integrated optical device structures to be rapidly patterned via a single, direct-write optical process step. This project is attempting to merge the development of highly photosensitive films with existing efforts to introduce optical subsystems into the enduring stockpile to produce relevant photonic devices with unique functionality. The ability to produce highly photosensitive germanosilicate thin films using a novel sputtering approach has been developed and has enabled the largest reported Δn (-5×10^{-3}) in as-synthesized materials. In addition, control of processing parameters has allowed engineering, at an atomic level, the defect interactions responsible for the PS response of our films. As a result, the unique ability now exists to control not only the magnitude of the optical response of our films, but also the sign of the induced refractive index change. Optical data transmission and signal manipulation offer significant advantages over more conventional, electronic approaches. Commercial telecommunications and remote sensing technologies rely on the ultrafast data transfer rates, insensitivity to signal interference, and robust physical design that characterize photonic systems based on both optical fibers and waveguides. These characteristics can also provide enhanced nuclear weapons safety in DOE/DP applications as efforts continue at Sandia to integrate optical systems into the enduring stockpile.

Keywords: Optical Materials, Photosensitivity

322. **THE SHOCK PROPERTIES OF PZT 95/5**
$300,000
DOE Contact: Bharat Agrawal, (301) 903-2057
SNL Contact: George Samara, (505) 844-6653

Although pulsed power devices utilizing shock-induced depoling of the ferroelectric ceramic PZT 95/5 have been in use for many years, an important responsibility currently being addressed is the design and certification of several new devices. A strong desire to progress beyond the historical "build and test" approach has resulted in a substantial effort to achieve accurate numerical simulations of device operation. A major challenge at the start of this effort, however, was the fact that very few studies of the complex dynamic behavior of poled PZT 95/5 had been conducted during the past twenty years. Consequently, an extensive experimental program was started two years ago to provide insight and well-characterized data for the development of improved models for PZT 95/5. During the first year, this study addressed the mechanical behavior of unpoled PZT 95/5 over the range of axial stresses of interest (5 to 50 kbar). Planar impact techniques were used with both PVDF film gauges and laser interferometry (VISAR) to characterize wave evolution under conditions that examined the FE to AFE phase transition and dynamic pore collapse. In the second year, emphasis was placed on shock-induced depoling of samples that were either normally or axially poled (poled perpendicular or parallel to the intended shock motion, respectively). Twenty experiments examined the depoling process and corresponding wave evolution over the full range of impact stresses. The database now available represents a substantial challenge to the ongoing development of improved models for PZT 95/5. However, successful simulation of these planar experiments, together with a number of multi-dimensional experiments planned for the coming year, will signify the achievement of an essential goal in the effort to accurately simulate the operation of pulsed power devices.

Keywords: Ferroelectrics, Shock Physics, Power Supplies

323. **THE PROPERTIES AND PHYSICS OF THE SLIM-LOOP FERROELECTRIC PBZT-Bi**
$250,000
DOE Contact: Bharat Agrawal, (301) 903-2057
SNL Contact: George Samara, (505) 844-6653

Complex mixed oxides based on Pb $(Zr_{1-x}Ti_x)O_3$, or PZT, find several applications in nuclear weapons components. One such material based on Pb $(Zr_{.70}Ti_{.30})O_3$, is PBZT-Bi which is used in explosively-driven pulsed power sources. The substitution of Ba^{2+} for Pb^{2+} ions and the addition of a small amount of Bi impart unto this material slim loop ferroelectric (SFE) character and properties qualitatively different from those of PZTs and other normal ferroelectrics. These properties had not been studied in any detail and the physics was not understood before this work. The combined effects of temperature, hydrostatic pressure, frequency, and dc biasing fields on the electrical properties were investigated along with the complementary differential scanning calorimetry, X-ray diffraction and TEM measurements. The results of the work make it clear that the properties and physics of PBZT-Bi are very different from those of normal ferroelectrics. Thus, models developed to describe the response of ferroelectrics such as the PZTs will be inappropriate for PBZT-Bi. The present results provide the basis for an appropriate model.

Keywords: Ferroelectrics, Performance Modeling, PBZT-Bi

324. **CATALYTIC MEMBRANE SENSORS**
$361,600
DOE Contact: Gerald Green, (202) 586-8377
SNL Contact: William Hammetter, (505) 272-7603

The goal of this project is to develop a fundamentally new catalytic membrane-based sensor (CMS) with enhanced sensitivity and specificity through modification of an SNL-developed Pd/Ni-based hydrogen sensor. This will be accomplished through overlays of size selective gas separation membrane and ion exchangeable titanate catalyst. The goal is to process these CMS elements into an array that utilizes different catalysts and membranes. This will enable significant improvement of both the selectivity and specificity via pattern recognition methodologies. The following work has been accomplished: (1) synthesis and characterization of double alkoxides, (2) membrane modified sensor (H_2 sensor), (3) catalytically active HTO or HTO-like layer on a membrane, (4) catalytic adjustability by ion exchange, and (5) catalyst layer on the sensor.

Keywords: Catalysis, Membranes, Sensors

325. **PHOTONIC BAND GAP STRUCTURES AS A GATEWAY TO NANO-PHOTONICS**
$375,000
DOE Contact: Gerald Green, (202) 586-8377
SNL Contact: Adelbert Owyoung, (505) 844-5481

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

Keywords: Photonics, Bandgap, Epitaxy

326. **MOLECULAR-SCALE LUBRICANTS FOR MICROMACHINE APPLICATIONS**
$475,000
DOE Contact: Gerald Green, (202) 586-8377
SNL Contact: Terry Michalske, (505) 844-5829

The nature of this work is to develop the physics and chemistry base for designing molecular-scale lubricants for the reduction of friction- and stiction-induced failure in silicon micromachines. The approach is 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 micromachine test structures specifically designed for friction and stiction studies.

Model lubricants under investigation are the silane coupling agents that form self-assembling monolayer (SAM) films on native oxide silicon surfaces. With atomic force microscopy (AFM) and interfacial force microscopy (IFM), the role of chain length, chemical end group, and chain structures on the frictional and adhesive properties of the SAM films is being examined.

Using a recently-completed scanning near-field optical microscope (SNOM), the goal is to provide the first-ever simultaneous correlation between SAM film structure and dynamic mechanical response. Emission from dilute concentrations of "guest" chromophores, whose orientation(s) are sensitive to lateral- and normal-force-induced changes in the lubricating film structure will be monitored. These AFM, IFM, and SNOM measurements will form a very important link for molecular dynamics simulations, that, in turn, should be able to predict micromachine performance under all conditions.

Keywords: Lubricants, Micromachines

327. **THE INITIATION AND PROPAGATION OF NANO- SCALE CRACKS AT AN ADHESIVE/SOLID INTERFACE**
$400,000
DOE Contact: Gerald Green, (202) 586-8377
SNL Contact: Wendy Cieslak, (505) 844-8633

This project is investigating submicron debonding processes at polymer/solid interfaces with a combination of continuum stress analysis, molecular dynamics (MD) simulations, and a new experimental approach. Each component of this program is designed to provide complementary information with the goal of bridging the gap between molecular and continuum descriptions. The objective is a validated, molecular-to- continuum fracture theory. Despite significant progress made in recent years in the fields of fracture mechanics and adhesion science, it is still not possible to predict the lifetime of a polymer/solid interface from first principles. On the continuum level, considerable headway has been made in an interfacial fracture mechanics approach for preexisting macroscopic cracks between linear elastic materials.

Little is known, however, about modeling cracks on a micron or submicron level, how microcracks develop into macroscopic cracks, or about length scale limitations on the use of a continuum analysis. Furthermore, there is an interphase region with property gradients between the two bulk materials. The effect of interface structure and molecular properties on fracture mechanics parameters is unknown. On the molecular scale, much is known about polymer dynamics, the origin of viscoelastic behavior and relaxation phenomena, and the behavior of polymers near surfaces. Yet it is not clear how stress concentrations develop on a molecular scale in an imperfect thermoset polymer, or how nanoscale inhomogeneities grow into microcracks under stress. An understanding of the link between the molecular and the continuum levels is required before the goal of a truly comprehensive model of fracture can be approached. Such a theory would allow the prediction of lifetimes given the detailed interface structure, material properties, and the thermal history, and would aid greatly in the design of interfaces that are more resistant to aging.

Keywords: Nanoscale, Interface, Adhesive

328. **FUNDAMENTAL ASPECTS OF MICROMACHINE RELIABILITY**
$350,000
DOE Contact: Gerald Green, (202) 586-8377
SNL Contact: Terry Michalske, (505) 844-5829

A fundamental basis for designing micromechanical devices with high yield, reliable performance and long life is lacking. Mechanical design tools for macro-scale machines relate reliability to inertial forces. However, the performance of micron-scale structures of high aspect ratio is dominated by surface forces. The technical goal of this project is to use experimental reliability results obtained directly from micromachined test structures to develop and verify mechanics models containing interaction terms appropriate to the micron scale (e.g., capillarity, van der Waals forces, electro statics). Issues to be addressed include auto-adhesion (stiction), friction and wear. Microbridge structures with varying geometry and surface properties (e.g., roughness, chemical coatings) are being designed and built. Deformations are being monitored by interferometry in an environmental chamber. Finite element models incorporating new surface elements are being developed, verified and refined by comparing against experimental results. An additional objective is to investigate friction and wear using smart micro machined structures that enable self-diagnosis by electrical monitoring of capacitance and Q factor changes. Optical detection technique is being explored. Dynamical response models incorporating internal friction terms as well as damping are being verified and refined using experimental results. Friction due to energy loss at rubbing surfaces can then be extracted.

This project is developing a new tool set based on an experimental and theoretical foundations. The tool set can be used to calculate and characterize reliability of micromachines for integrated microsystem applications.

Keywords: Micromachine, Reliability

329. **INTELLIGENT POLYMERS FOR NANODEVICE PERFORMANCE CONTROL**
$439,000
DOE Contact: Gerald Green, (202) 586-8377
SNL Contact: Clifford Renschler (505) 844-0324

This project is developing a revolutionary enabling technology for the accurate, predictable manipulation of the fundamental optical, electrical and rheological properties of a new class of intelligent polymers. Their potential for write-once memories and nanoscale "device on command" capability could find application in reduced size parts (WPP) and intelligent manufacturing technologies, and compartmentalized activities at Sandia and in other government agencies (use control, tamper detection). The autonomous response polymers will remain passive prior to stimulation from specific light or heat sources, when they will undergo changes in morphology, conductivity or refractive index in response to the stimuli. Existing materials are limited to laboratory-scale manipulation of polymer conductivity with ill-defined thermally- or photochemically-initiated changes to the polymer's chemical structure. The approach of this project provides enhanced, well- defined control of polymer properties through molecular scale design of polymer structure. Materials are synthesized to covalently incorporate energetic chemical functionalities within the polymers' molecular structures. Appropriate energetic groups are then selected as monomers from molecular modeling of the energetic group's kinetic and thermodynamic response to heat and light, and the compatibility of the groups to co-monomers bearing latent reactivity. The energetic groups are incorporated as terminal groups or as blocks of repeat units within the polymer backbone by employing living polymerization techniques including Ring Opening Metathesis Polymerization (ROMP). Energetic group decomposition, stimulated from a specific source, indirectly activates the reactive repeat units, resulting in dramatic changes in macroscopic properties including refractive index, electrical conductivity or material bulk morphology.

Keywords: Polymers, Nanodevices

330. **QUANTUM DOT ARRAYS**
$400,000
DOE Contact: Gerald Green, (202) 586-8377
SNL Contact: George Samara, (505) 844-6653

This project integrates two areas of Sandia research to fabricate new molecularly engineered, cluster-based, nanocomposite materials. First, Sandia has patented the inverse micellar synthesis of highly monodisperse metal and semiconductor nanoclusters, or "quantum dots." These 10-100 Å nanoclusters have many interesting properties, including large catalytic activity, room temperature luminescence, size dependent bandgaps, etc., and are sufficiently monodisperse that size-dependent cluster properties can be easily resolved. However, these clusters are currently stable only in the reaction bath. Second, Sandia has developed an expertise in synthesizing bulk periodic mesoporous materials by templating silica around liquid crystalline surfactant assemblies. These surfactant- templated porous materials (STPMs) are similar to zeolites, but the unit cell size is 40Å versus the 4-8Å typical for zeolites. These are the first periodic materials whose uniform pore size is commensurate with the typical dimensions of quantum dots. These new materials should be an ideal matrix for quantum dots; moreover, the quantum dots should form a highly periodic array, which may give rise to a host of new coherent phenomena. The goal of this project is to synthesize a new class of materials, "Quantum Dot Arrays" (QDAs), that consists of metal or semiconductor clusters periodically arrayed in an isolating silica matrix. Such cluster-based materials will have unique optical, catalytic, and dielectric properties: gold clusters in silica would give a high dielectric material for super capacitors; low work function clusters could make a good field emitter; luminescent silicon clusters could make optical arrays; supported nanocluster catalysts could be made as thin films.

Keywords: Quantum Dot, Nanocluster

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

331. **WIDE-BANDGAP COMPOUND SEMI-CONDUCTORS TO ENABLE NOVEL SEMICONDUCTOR DEVICES PROJECT**
$290,000
DOE Contact: Gerald Green, (202) 586-8377
SNL Contact: Jeffrey Nelson, (505) 844-4395

This project is 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. This work focuses on two important areas in the development of these materials. A portion of the effort concentrates on understanding the growth of III-N materials by gas-source molecular beam epitaxy (GSMBE), specifically the effects of substrate preparation, substrate temperature, V/III ratio, and growth rate on the nucleation and growth of AlGaInN on 6H-SiC (0001) 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, the physical properties of the AlGaInN material system are being investigated. Analytical investigations include calculations to determine band structure 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 is used 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 determine energy dispersion and effective masses and these results are directly compared with band structure calculations. Another aspect of the work 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: MBE, HEED, REMS, STM

332. **SCANNING PROBE-BASED PROCESSES FOR NANOMETER-SCALE DEVICE FABRICATION**
$442,600
DOE Contact: Gerald Green, (202) 586-8377
SNL Contact: Terry Michalske, (505) 844-5829

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. This program integrates and expands Sandia's expertise in scanning-probe based fabrication and characterization of nanostructures with capabilities in microelectronic fabrication to produce fully accessible nanostructures for electronic evaluation. The objective is an order of magnitude decrease in feature size compared to conventional fabrication technology. Approaches to nanostructure fabrication using scanning probe-based (STM, AFM) processes in combination with extensive device fabrication are being explored. For prototype device structures critical nanoscale components are being integrated with conventional test structures to allow full electrical accessibility. Two approaches to nanostructure fabrication are being explored: investigation of molecular layer resists based on simple adsorbed atoms and molecules which can be patterned by electron-induced desorption or reaction, and development of a more general AFM-based nanolithographic capability, based on anodic oxidation under an AFM tip. In parallel with these fabrication approaches, low temperature electrical measurements are being performed, and selected nanoelectronic devices are being fabricated and characterized.

Keywords: Nanoscale, Device Fabrication

333. **SURFACE MICROMACHINED FLEXURAL PLATE WAVE DEVICE INTEGRATED ON SILICON**
$525,000
DOE Contact: Gerald Green, (202) 586-8377
SNL Contact: Stephen Martin, (505) 844-9723

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

Keywords: Micromachines, Silicon

INSTRUMENTATION AND FACILITIES

334. **ADVANCED ANALYTICAL TECHNIQUES**
$998,000
DOE Contact: Bharat Agrawal, (301) 903-2057
SNL Contact: Julia M. Phillips, (505) 844-1071

The Advanced Analytical Techniques Project supports the development of advanced methods of characterizing materials structure and providing chemical analysis. Each of the relatively independent subprojects is directed towards advancing the state-of-the-art in materials characterization by developing new capabilities for extracting information about materials through the development of new hardware or data analysis techniques. Each project must offer at least one of the following: (1) improvement in Sandia's ability to monitor the nuclear stockpile or nuclear weapon production or maintenance processes, or (2) the capability to perform failure analysis on weapons components, materials, or subsystems.

Keywords: Chemical Analysis, Characterization

335. **MONOLITHIC STRUCTURES FOR NANOSEPARATION PROPERTIES**
$339,000
DOE Contact: Gerald Green, (202) 586-8377
SNL Contact: James Wang, (925) 294-2786

Miniaturization in detection and separation technologies requires easily built, rugged devices based on materials that have well understood interactions with analytes at the molecular level. The goal of this project is to design such materials for state-of-the-art separation science, understand their structure/function relationships, and fabricate them into useful devices. Sandia expertise in the synthesis of micro- and nanoporous materials is being utilized to develop contiguous, high surface area polymers as nanoporous supports for ultra-efficient separations. These materials are being evaluated using capillary electrochromatography (CEC) as a test bed. The interaction of functionalized surfaces of these supports with analytes, propelled by the electroosmotic flow (EOF), is being quantified in terms of separation efficiency and selectivity. Dramatic gains enabling miniaturization are anticipated with increased efficiency and selectivity of CEC. The goal is to engineer an open and interconnected network where every nanopore functions as a CEC column. These enhancements are not possible in conventional chromatographic methods. These new solid supports, which are cast as fluid solutions and cured to monolithic polymer structures, are being integrated into micro-machined grooves as pre-prototype devices for ultra-efficient separations. Unfilled microgrooves are also being evaluated for their inherent separation efficiencies.

Keywords: Nanoseparation, Polymers

LOS ALAMOS NATIONAL LABORATORY

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

336. **RAPID SOLIDIFICATION PROCESSING**
$500,000
DOE Contact: R. Jones, (301) 903-6688
LANL Contact: D. J. Thoma, (505) 665-3645

The project incorporates process development and product comparisons resulting from rapid solidification processing techniques including melt spinning and gas atomization. Alloy homogeneity, phase stability, mechanical and physical properties are used for comparison.

Keywords: Rapid Solidification, Melt Spinning, Atomization, Phase Stability, Alloy Homogeneity

337. **NEUTRON DIFFRACTION**
$1,500,000
DOE Contact: B. B. Agrawal, (301) 903-2057
LANL Contact: E. M. Farnum, (505) 665-5523

Neutron scattering is being applied to the characterization of weapons materials in the realms of electronic structure, crystallography, chemical reaction dynamics and residual strain distribution. The primary materials of interest are high explosives, plutonium, uranium, beryllium and organic salts.

The local structure of Pu and its alloys is being studied using neutron pair-distribution-function (PDF) techniques. Neutron resonance Doppler broadening experiments are being performed to understand the phonon behavior of Pu alloys and phonon densities of states (PDOS) measurements will be made across the phase boundaries of Pu. The ability to measure crystallographic texture in plutonium has been demonstrated. The intent is to correlate texture measurements with elastic properties.

Keywords: Neutron Scattering, Pair-Distribution-Function, Phonon Densities, High Explosives, Plutonium, Uranium, Beryllium and Organic Salts

338. **DYNAMIC MECHANICAL PROPERTIES OF WEAPONS MATERIALS**
$2,000,000
DOE Contact: B. B. Agrawal, (301) 903-2057
LANL Contact: G. T. Gray III, (505) 667-5452

This program is focused on experimental measurements and computer modeling of dynamic stress-strain and fracture behavior of polymers, high explosives, actinides, beryllium, and common structural materials.

Development of constitutive relationships and fracture models for the prediction of material performance.

Keywords: Dynamic Properties, Fracture, Microstructure

339. **MATERIALS AGING**
$11,000,000
DOE Contact: D. V. Feather, (301) 903-5815
LANL Contact: L. Salazar, (505) 667-7485

The materials aging program is developing tools, techniques, and procedures to advance our capability to measure, analyze, and predict the aging of materials within nuclear weapons. Experimental work is proceeding in high explosives, polymers, plutonium, uranium, salts, and beryllium. Experimental investigations are proceeding at the atomistic level to examine radiolytic-induced structural changes, molecular levels for polymer degradation, microstructure and bulk levels for mechanical property changes or corrosion.

Keywords: High Explosives, Polymers, Plutonium, Uranium, Salts, Beryllium, Atomistic Bonding, Molecular Dynamics, Mechanical Properties, Corrosion

340. **POWDER CHARACTERIZATION**
$300,000
DOE Contact: B. B. Agrawal, (301) 903-2057
LANL Contact: J. K. Bremser, (505) 667-1179

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

341. **MANUFACTURING PROCESS DEVELOPMENT**
$8,000,000
DOE Contact: G. S. Hearron, (505) 845-5311
LANL Contact: T. R. Neal, (505) 665-5568

The Advanced Design and Process Technology program, ADAPT, has taken the role of catalyst for manufacturing-related goals and for integrating the weapons complex manufacturing activities. This program includes the development of manufacturing process improvements, agile manufacturing techniques, enterprise integration focusing on material resource modeling, and hedge planning for the rapid reconstitution of large-scale production. Investments in the later three categories have been modest because of the intensity of needs in process development. ADAPT is directly integrated with core R&D for specific studies of materials performance, models-based engineering, and manufacturing specifications.

Keywords: Manufacturing Process Improvement, Agile Manufacturing Techniques, Material Resource Modeling, Hedge Planning

342. **COMPONENT FABRICATION**
$10,000,000
DOE Contact: R. Jones (301) 903-6688
LANL Contact: R. Mah, (505) 667-3238

Component fabrication includes the development and modeling of process technologies coupled with extensive materials characterization for the manufacture of demonstration and test components. Processing capabilities cover casting, forming, atomization, rapid solidification processing, powder consolidation, plasma spray, heat treatment, sintering, welding and joining. Characterization includes X-ray diffraction, microscopy, mechanical properties and physical properties determinations. Materials fabricated include uranium, beryllium, stainless steels, refractory metals, palladium, and special alloys.

Keywords: Casting, Forming, Atomization, Rapid Solidification Processing, Powder Consolidation, Plasma Spray, Heat Treatment, Sintering, Welding, Joining, X-ray Diffraction, Microscopy, Mechanical Properties, Physical Properties, Uranium, Beryllium, Stainless Steels, Refractory Metals, Palladium, Special Alloys

LAWRENCE LIVERMORE NATIONAL LABORATORY

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

343. **ENGINEERED NANOSTRUCTURE LAMINATES**
$2,000,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LLNL Contact: Troy W. Barbee, Jr., (925) 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 (0.2nm) to hundreds of monolayers (>100nm). 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

344. **KDP AND DKDP CRYSTAL DEVELOPMENT AND PRODUCTION**
$4,000,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LLNL Contact: J. J. DeYoreo, (925) 423-4240

Potassium dihydrogen phosphate (KDP) and its deuterated analog (DKDP) are important nonlinear crystals which will be used both for frequency conversion as well as for a large Pockels cell on the National Ignition Facility (NIF). 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. This project has developed an alternative growth technique that dramatically increases the growth rate of these crystals.

Using this method both KDP and DKDP are being grown at 10 times the rates achieved with conventional methods. High quality crystals up to almost 57cm on a side have been grown by this method. Crystals at the 10-15cm scale are being grown in order to determine optimum hydrodynamic and regeneration conditions, and to understand the effects of impurities and stresses on the stability of the growing crystal face and the performance of the crystals.

Keywords: KDP, Nonlinear Crystals, Crystallization

345. **ENERGETIC MATERIALS STRATEGIC CHEMISTRY**
$350,000
DOE Contact: Bharat Agrawal, (301) 903-6688
LLNL Contact: R. L. Simpson, (925) 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

346. **CHEETAH THERMOCHEMICAL CODE**
$190,000
DOE Contact: Bharat Agrawal, (301) 903-6688
LLNL Contact: R. L. Simpson, (925) 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

347. **EXPLOSIVES DEVELOPMENT**
$900,000
DOE Contact: Bharat Agrawal, (301) 903-6688
LLNL Contact: R. L. Simpson, (925) 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

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

348. **INTERFACES, ADHESION, AND BONDING**
$265,000
DOE Contact: Iran L. Thomas, (301) 903-6688
LLNL Contact: Wayne E. King, (925) 423-6547

The experimental effort is producing results that are directly comparable with theoretical calculations. Planar metal/metal interfaces and metal/ceramic interfaces (in anticipation of improvements in the theory) of well defined misorientations are being investigated. In order to span the entire range of length scales, macroscopic bicrystals a few millimeters thick, with interfacial areas on the order of a square centimeter, are required. In order to obtain such bicrystals, diffusion bonding is used. An ultra-high-vacuum diffusion bonding machine has been developed in parallel with this research project.

Keywords: Interfaces, Bonding, Electronic Structure

349. **LASER DAMAGE: MODELING AND CHARACTERIZATION**
$400,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LLNL Contact: M. R. Kozlowski, (925) 424-5637

The objective of this project is to understand the mechanisms for laser-induced damage in optical materials used in high-peak-power laser systems such as the National Ignition Facility (NIF). The material system of primary interest is polished fused silica surfaces. The primary characterization tools used in the studies include luminescence spectroscopy and microscopy, total internal reflection microscopy (TIRM), near-field scanning optical microscopy (NSOM), and photothermal microscopy (PTM). Efforts are focused on the understanding of damage growth due to successive pulses and the mitigation of the growth through removal of the damaged material. The damage growth rate determines the functional lifetime of the optic in the laser system. The dependence of the damage growth rate on laser wavelength, pulse length, and pulse repetition rate is being determined. Also of interest is the influence of optic environment (air vs. vacuum) on the damage processes.

Keywords: Silica, Luminescence, Laser Damage

350. **KDP CHARACTERIZATION**
$1,000,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LLNL Contact: J. J. DeYoreo, (925) 423-4240

Very large, high quality crystals of potassium dihydrogen phosphate (KDP) and its deuterated analogue (DKDP) are required for present and advanced high power lasers in the ICF Program. The performance of these crystals is limited by impurities and strain, which induces anomalous birefringence and wavefront distortion and by defects, which result in laser-induced damage at low laser fluence. The level of impurities, internal strain and the laser damage threshold are the most important factors in determining the yield of useable plates from an as-grown boule. The goal of this project is 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.

Techniques used include 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. Strain and damage have been related to specific defects using these methods and the process of laser damage as well as laser and thermal annealing is now under investigation *in situ*.

Keywords: KDP, Strain, Crystal

INSTRUMENTATION AND FACILITIES

351. SCANNING TUNNELING MICROSCOPY (STM), ATOMIC FORCE MICROSCOPY (AFM), NEAR FIELD SCANNING OPTICAL MICROSCOPY (NSOM)
$250,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LLNL Contact: W. Siekhaus, (925) 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. An additional large-stage and a small stage scanning probe microbe have been added and modified to perform near field scanning probe microscopy.

Properties of Nano-scale Particles, Nanometer-scale clusters of various materials, deposited by laser ablation and by evaporation in a noble gas atmosphere onto various substrates are analyzed by AFM and STM to determine their size distribution and by optical spectroscopy and electron spectroscopy to determine their size-dependent optical properties and electronic Structure.

Optical properties of materials on the nanometer scale are being investigated by NSOM. NSOM analysis is restricted to the near field of the scanning probe, and hence is ideally suited to probe the evanescent field on the surface of optical material. NSOM is used to determine local field enhancement by surface irregularities and thus to establish the relationship between surface features and laser damage threshold.

Combined Scanning Probe Microscopy/Nano-Indentation is 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, and also to identify aging-induced changes in local properties of materials in stockpile.

Keywords: NDE, Chemical Reaction, Stockpile Stewardship, Etching, Cluster, Nano-Indentation, Near Field Scanning Probe Microscopy, Optical Properties, Mechanical Properties, Biomaterials, Tooth, Artery, Bone

352. ATOMIC LEVEL EXPLOSIVE CALCULATIONS
$325,000
DOE Contact: Maurice Katz, (202) 586-5799
LLNL Contacts: Larry Fried, (925) 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. Several new target molecules were found with the system in FY98.

Keywords: Energetic Materials, High Explosives, Molecular Design, Detonation

353. METASTABLE SOLID-PHASE HIGH ENERGY DENSITY MATERIALS
$535,000
DOE Contact: Maurice Katz, (202) 586-5799
LLNL Contacts: H. Lorenzana, (925) 422-8982 and M. Finger, (925) 422-6370

Conventional energetic materials such as propellants, explosives and fuel cells store energy within internal bonds of molecules. This work is exploring the predicted 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, experimental capabilities have been developed for synthesizing and characterizing such compounds at megabar pressures.

Keywords: Energetic Materials, High Energy Density Materials

354. **AFM INVESTIGATIONS OF CRYSTAL GROWTH**
$290,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LLNL Contact: J. J. DeYoreo, (925) 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. This project is 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.

This method has been applied to inorganic, organic and macromolecular crystals each of which serve as important model systems. These include KH_2PO_4, $CaCO_3$ doped with amino acids, molecular tapes of diketopipeizine derivatives, the protein canavalin and the satellite tobacco mosaic virus. The results of these investigations are providing an understanding of the fundamental physical controls during solvent mediated crystallization.

Keywords: Morphology, Crystal Surfaces, Atomic Force Microscopy

355. **URANIUM CASTING PROGRAM**
$400,000
DOE Contact: Marshall Sluyter, (301) 903-5491
LLNL Contact: Jeff Kass, (925) 422-4831

The uranium casting program is addressing 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

356. **URANIUM SPIN FORMING**
$1,200,000
DOE Contact: Marshall Sluyter, (301) 903-5491
LLNL Contact: Jeff Kass, (925) 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

357. **PLUTONIUM NEAR NET SHAPE CASTING**
$2,500,000
DOE Contact: Marshall Sluyter, (301) 903-5491
LLNL Contact: Jeff Kass, (925) 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

358. **ELECTRON BEAM COLD HEARTH MELTING OF URANIUM**
$900,000
DOE Contact: Marshall Sluyter, (301) 903-5491
LLNL Contact: Jeff Kass, (925) 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

359. **NIF CAPSULE MANDREL R&D**
$800,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LLNL Contact: R. Cook, (925) 422-3117

This program has as its objective the development of 2mm 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 (<1μm out of round), have wall thickness uniformity better than 1μm, and have a surface finish of less than 10nm (rms over modes >9).

Keywords: Polymers, Laser Fusion Targets, Microencapsulation, Microshells

360. **POLYIMIDE COATING TECHNOLOGY FOR ICF TARGETS**
$500,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LLNL Contacts: R. Cook, (925) 422-3117 and Steve Letts, (925) 422-0937

This program has as its objective the development of a vapor based, high strength polyimide coating technology that will allow production of a smooth, 150 to 200μm polyimide ablator coating on a 2mm 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

361. **BERYLLIUM ABLATOR COATINGS FOR NIF TARGETS**
$600,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LLNL Contacts: R. McEachern, (925) 423-4734, R. Cook, (925) 422-3117, R. Wallace, (925) 423-7864 and A. Jankowski, (925) 423-2519

This program has as its objective the development of materials and processes that will allow sputter-deposition of up to 200μm of a uniform, smooth, high-Z doped Be-based ablator on a spherical hollow mandrel. Capsules made with this type of ablator have been shown by calculation to offer some important advantages as ignition targets for the National Ignition Facility (NIF). Emphasis in the past year has been on improving coating homogeneity and smoothness. Both new materials (glassy boron-beryllium alloys) and process modifications are being studied.

Keywords: Beryllium, Laser Fusion Targets, Ablator, Sputter Deposition

OFFICE OF FOSSIL ENERGY

	FY 1998
Office of Fossil Energy - Grand Total	$8,771,000
Office of Advanced Research	$8,771,000
Fossil Energy AR&TD Materials Program	$5,031,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$2,049,000
Development of Iron Aluminides	95,000
Ultrahigh-Temperature Cr-X Alloys	104,000
Low-Aluminum-Content Iron-Aluminum Alloys	96,000
Mo-Si Alloy Development	150,000
Development of Improved and Corrosion Resistant Surfaces for Fossil Power System Components	4,000
Commercial-Scale Melting and Processing of Low-Aluminum Content Alloys	PYF[1]
Development of Modified Austenitic Alloys	141,000
Application of Advanced Austenitic Alloys to Fossil Power System Components	PYF[1]
Development of Recuperator Materials	45,000
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	50,000
Fabrication of Fiber-Reinforced Composites by Chemical Vapor Infiltration and Deposition	174,000
Compliant Oxide Coating Development	49,000
Development of Oxidation/Corrosion-Resistant Composite Materials and Interfaces	124,000
Transport Properties of Ceramic Composites	65,000
Modeling of Fibrous Preforms for CVD Infiltration	65,000
Development of a Commercial Process for the Production of Silicon Carbide Fibrils	100,000
Processing and Characterization of Fiber-Reinforced Composites	25,000
Corrosion Protection of SiC-Based Ceramics with CVD Mullite Coatings	50,000
Feasibility of Synthesizing Oxide Films on Ceramic and Metal Substrates	65,000
Ceramic Coating and Native Oxide Scales Evaluation	35,000
Development of Novel Activated Carbon Composites	238,000
Activation of Carbon Fiber Composite Molecular Sieves	55,000
Carbon Fiber Composite Molecular Sieves Technology Transfer	44,000
Materials Properties, Behavior, Characterization or Testing	$1,172,000
Oxide Dispersion Strengthened (ODS) Alloys	224,000
Investigation of the Weldability of Polycrystalline Iron Aluminides	70,000
Friction Welding of ODS Alloys	13,000
Evaluation of the Intrinsic and Extrinsic Fracture Behavior of Iron Aluminides	30,000
Investigation of Iron Aluminide Weld Overlays	45,000
In-Plant Corrosion Probe Tests of Advanced Austenitic Alloys	120,000

[1]PYF denotes that funding for this project, active in FY 1998, was provided from prior year allocations.

OFFICE OF FOSSIL ENERGY (continued)

	FY 1998
Office of Advanced Research (continued)	
Fossil Energy AR&TD Materials Program (continued)	
Materials Properties, Behavior, Characterization or Testing (continued)	
Fatigue and Fracture Behavior of Cr-Nb Alloys	PYF[1]
Corrosion and Mechanical Properties of Alloys in FBC and Mixed-Gas Environments	180,000
Optimization of Corrosion-Resistant Iron Aluminide Coatings and Claddings	121,000
Reduction of Defect Content in ODS Alloys	45,000
Corrosion Protection of Ultrahigh Temperature Intermetallic Alloys	99,000
Metal Dusting Initiative	16,000
Support Services for Ceramic Fiber-Ceramic Matrix Composites	29,000
Development of Nondestructive Evaluation Methods and Effects of Flaws on the Fracture Behavior of Structural Ceramics	180,000
Device or Component Fabrication, Behavior or Testing	$1,388,000
Materials and Components in Fossil Energy Applications Newsletter	60,000
Development of Ceramic Membranes for Hydrogen Separation	370,000
Major Equipment	30,000
Investigation of the Mechanical Properties and Performance of Ceramic Composite Components	40,000
Solid State Electrolyte Systems for Fuel Cells and Gas Separation	603,000
Improved Fuel Cell Materials	45,000
Bismuth Oxide Solid Electrolyte Oxygen Separation Membranes	60,000
Oxide-Dispersion-Strengthened Fe_3Al-Based Alloy Tubes	80,000
Iron Aluminide Filters for IGCCs	PYF[1]
Iron Aluminide Filters for PFBCs	PYF[1]
Ceramic Composites for Solid Oxide Fuel Cells	100,000
Instrumentation and Facilities	$422,000
Management of the Fossil Energy AR&TD Materials Program	400,000
General Technology Transfer Activities	17,000
Gordon Research Conference Support	5,000
Advanced Metallurgical Processes Program	$3,740,000
Advanced Refractory Research	340,000
Advanced Casting Technologies	1,160,000
Advanced Coating Techniques	340,000
Advanced Titanium Processing	700,000
Service Life Prediction	1,200,000

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 the Advanced Research and Technology Development (AR&TD) Materials Program. The goal of the Fossil Energy AR&TD Materials Program is to provide a materials technology base to assure the success of coal fuels and advanced power generation systems being pursued by DOE-FE. The purpose of the Program is to develop the materials of construction, including processing and fabrication methods, and functional materials necessary for those systems. The scope of the Program addresses materials requirements for all fossil energy systems, including materials for coal fuels technologies and for advanced power generation technologies such as coal gasification, heat engines, combustion systems, and fuel cells. The Program is aligned with the development of those technologies that are potential elements of the DOE-FE Vision 21 concept, which aims to address and solve environmental issues and thus remove them as a constraint to coal's continued status as a strategic resource.

The principal development efforts of the Program are directed at ceramic composites for high-temperature (~1200°C) heat exchanger applications; new corrosion- and erosion-resistant alloys with unique mechanical properties for advanced fossil energy systems; functional materials, particularly metal and ceramic hot-gas filters and gas separation materials based on ceramic membranes (porous and ion transport) and activated carbon materials; and corrosion research to understand the behavior of materials in coal-processing environments. Included as part of the responsibilities of Oak Ridge National Laboratory (ORNL) on the Fossil Energy AR&TD Materials Program is, with DOE-ORO, the technical management and implementation of all activities on the DOE Fossil Energy Advanced Research and Technology Development (AR&TD) Materials Program. DOE-FE administration of the Program is through the Federal Energy Technology Center (FETC) and the Advanced Research Product Team.

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

362. **DEVELOPMENT OF IRON ALUMINIDES**
$95,000
DOE Contacts: F. M. Glaser, (301) 903-2784,
V. U. S. Rao, (412) 892-4743 and
M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact:
M. L. Santella, (423) 574-4805

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

363. **ULTRAHIGH-TEMPERATURE Cr-X ALLOYS**
$104,000
DOE Contacts: F. M. Glaser, (301) 903-2784,
V. U. S. Rao, (412) 892-4743 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, oxidation- and corrosion-resistant intermetallic alloys for use as hot components in advanced fossil energy conversion and combustion systems to help meet the 65 percent efficiency goal of the Vision 21 Concept. The successful development of these alloys is expected to improve thermal efficiency through increased operating temperatures and decreased cooling requirements. The development effort will be devoted to in-situ composite alloys based on $Cr-Cr_2Nb$ and similar $Cr-Cr_2X$ (X = refractory elements) systems.

Keywords: Alloys, Chromium-Niobium, Corrosion, Intermetallic Compounds

364. **LOW-ALUMINUM-CONTENT IRON-ALUMINUM ALLOYS**
$96,000
DOE Contacts: F. M. Glaser, (301) 903-2784,
V. U. S. Rao, (412) 892-4743 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

365. **Mo-Si ALLOY DEVELOPMENT**
$150,000
DOE Contacts: F. M. Glaser, (301) 903-2784,
V. U. S. Rao, (412) 892-4743 and
M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact:
J. H. Schneibel, (423) 574-4644

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 combustion systems. The successful development of Mo-Si alloys is expected to improve the thermal efficiency and performance of fossil energy conversion systems through increased operating temperatures, and to increase the service life of hot components exposed to corrosive environments at temperatures as high as 1600°C. This effort thus contributes directly to Vision 21, one goal of which is to significantly reduce greenhouse emissions. The effort focuses presently on Mo-Si-B alloys containing high volume fractions of molybdenum silicides and borosilicides.

Keywords: Alloys, Molybdenum, Silicon

366. **DEVELOPMENT OF IMPROVED AND CORROSION RESISTANT SURFACES FOR FOSSIL POWER SYSTEM COMPONENTS**
$4,000
DOE Contacts: F. M. Glaser, (301) 903-2784,
V. U. S. Rao, (412) 892-4743 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

367. **COMMERCIAL-SCALE MELTING AND PROCESSING OF LOW-ALUMINUM CONTENT ALLOYS**
$0 - PYF[1]
DOE Contacts: F. M. Glaser, (301) 903-2784, V. U. S. Rao, (412) 892-4743 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

368. **DEVELOPMENT OF MODIFIED AUSTENITIC ALLOYS**
$141,000
DOE Contacts: F. M. Glaser, (301) 903-2784, V. U. S. Rao, (412) 892-4743 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

[1]PYF denotes that funding for this project, active in FY 1998, was provided from prior year allocations.

369. **APPLICATION OF ADVANCED AUSTENITIC ALLOYS TO FOSSIL POWER SYSTEM COMPONENTS**
$0 - PYF[1]
DOE Contacts: F. M. Glaser, (301) 903-2784, V. U. S. Rao, (412) 892-4743 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

370. **DEVELOPMENT OF RECUPERATOR MATERIALS**
$45,000
DOE Contacts: F. M. Glaser, (301) 903-2784, V. U. S. Rao, (412) 892-4743 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: R. W. Swindeman, (423) 574-5108

The purpose of this task is provide stainless steel technology that will assist Solar Turbines to design and construct an advanced recuperator for a simple cycle gas turbine.

Keywords: Alloys, Austenitics, Technology Transfer

371. **INFLUENCE OF PROCESSING ON MICROSTRUCTURE AND PROPERTIES OF ALUMINIDES**
$175,000
DOE Contacts: F. M. Glaser, (301) 903-2784, V. U. S. Rao, (412) 892-4743 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: I. G. Wright, (423) 574-4451
Idaho National Engineering and Environmental Laboratory Contact: R. N. Wright, (208) 526-6127

This program will determine the influence of processing on improved properties of alloys based on the intermetallic compound Fe_3Al. Thermomechanical processing of these alloys will be pursued to improve their ambient and elevated temperature properties. The response of the microstructure to elevated temperature deformation and subsequent annealing will be characterized in terms of the establishment of equilibrium phases, equilibrium degree of long-range order, and secondary recrystallization. Oxide dispersion strengthened (ODS) alloys fabricated by reaction synthesis will be developed for improved high-temperature strength. Tensile properties of the ODS materials will be determined at room and elevated temperature and related to the microstructure. Creep properties of these alloys will be studied in detail and compared to current theories for creep strengthening by oxide dispersions. The processing/properties relationships determined using reaction-synthesized materials will be applied to more conventional high energy ball milled ODS alloys being developed at Oak Ridge National Laboratory (ORNL). Compositions of the dispersion strengthened Fe_3Al alloys will be determined in collaboration with the program at ORNL.

Keywords: Aluminides, Processing, Microstructure

372. **INVESTIGATION OF ELECTROSPARK-DEPOSITED COATINGS FOR PROTECTION OF MATERIALS IN SULFIDIZING ATMOSPHERES**
$100,000
DOE Contacts: F. M. Glaser, (301) 903-2784,
V. U. S. Rao, (412) 892-4743 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 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

373. **TECHNOLOGY TRANSFER OF ELECTROSPARK-DEPOSITED COATINGS FOR PROTECTION OF MATERIALS IN SULFIDIZING ATMOSPHERES**
$50,000
DOE Contacts: F. M. Glaser, (301) 903-2784,
V. U. S. Rao, (412) 892-4743 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

374. **FABRICATION OF FIBER-REINFORCED COMPOSITES BY CHEMICAL VAPOR INFILTRATION AND DEPOSITION**
$174,000
DOE Contacts: F. M. Glaser, (301) 903-2784,
V. U. S. Rao, (412) 892-4743 and
M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact:
T. M. Besmann, (423) 574-6852

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. In addition, isothermal chemical vapor infiltration will be used to develop oxide-based composite systems for structural and thermochemical (solid oxide fuel cell) applications.

Keywords: Composites, Fiber-Reinforced, Ceramics

375. **COMPLIANT OXIDE COATING DEVELOPMENT**
$49,000
DOE Contacts: F. M. Glaser, (301) 903-2784,
V. U. S. Rao, (412) 892-4743 and
M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact:
D. P. Stinton, (423) 574-4556

SiC-based materials in the form of sintered SiC, siliconized SiC, or SiC-matrix composites are being developed for use as heat exchangers in industrial waste incinerators and advanced fossil- or biomass-fueled power systems. Unfortunately, these SiC-based heat exchangers and filters are susceptible to corrosion by alkali metal salts at elevated temperatures. Protective oxide coatings typically crack and spall when applied to SiC substrates because of the large thermal expansion mismatch. The purpose of this task is to develop low-expansion, low-modulus corrosion-resistant coatings for Si-based ceramics and evaluate candidate materials in facilities at the DOE Federal Energy Technology Center.

Keywords: Ceramics, Oxides, Coatings

376. **DEVELOPMENT OF OXIDATION/ CORROSION-RESISTANT COMPOSITE MATERIALS AND INTERFACES**
$124,000
DOE Contacts: F. M. Glaser, (301) 903-2784, V. U. S. Rao, (412) 892-4743 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: R. A. Lowden, (423) 576-2769

The performance and life of ceramic fiber-reinforced ceramic composites are diminished when they are exposed to fossil energy environments because of the corrosion of the composite constituents, especially the fiber and interface coating. Corrosives such as oxygen or steam can penetrate cracks formed in the ceramic matrix and react with the interface coating and fiber. Corrosion of the interface coating and attack of the fiber cause the mechanical properties to deteriorate and the composite to eventually fail. The purpose of this task is to develop fiber-matrix interface coatings that optimize the mechanical behavior of the ceramic composites at room temperature and at elevated temperatures, and protect the fibers from processing and corrosive environments typical of applications of interest to Fossil Energy programs.

Keywords: Composites, Ceramics, Fiber-Reinforced, Interfaces

377. **TRANSPORT PROPERTIES OF CERAMIC COMPOSITES**
$65,000
DOE Contacts: F. M. Glaser, (301) 903-2784, V. U. S. Rao, (412) 892-4743 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

378. **MODELING OF FIBROUS PREFORMS FOR CVD INFILTRATION**
$65,000
DOE Contacts: F. M. Glaser, (301) 903-2784, V. U. S. Rao, (412) 892-4743 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

379. **DEVELOPMENT OF A COMMERCIAL PROCESS FOR THE PRODUCTION OF SILICON CARBIDE FIBRILS**
$100,000
DOE Contacts: F. M. Glaser, (301) 903-2784, V. U. S. Rao, (412) 892-4743 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: D. P. Stinton, (423) 574-4556
ReMaxCo Technologies, Inc. Contact: R. D. Nixdorf, (423) 483-5060

The DOE Fossil Energy Program has an interest in silicon carbide fibrils as a material for high-temperature heat exchanger and recuperation components in advanced coal combustion plants. The purpose of this project is to develop a commercial process for the production of silicon carbide fibrils. The slow growth of the fibrils and excessive waste of raw materials have been the major impediments. This work is an effort to bring new technology solutions to the future volume production of silicon carbide fibrils.

Keywords: Ceramics, Composites, Fibrils, Modeling

380. **PROCESSING AND CHARACTERIZATION OF FIBER-REINFORCED COMPOSITES**
$25,000
DOE Contacts: F. M. Glaser, (301) 903-2784, V. U. S. Rao, (412) 892-4743 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: D. P. Stinton, (423) 574-4556
University of Tennessee. Contact: P. K. Liaw, ((423) 974-6356

The objective of this effort is to investigate the effects of interface coating composition, processing, and properties on the mechanical behavior of continuous fiber ceramic composites. Specifically, silicon carbide matrix composites reinforced with ceramic fibers of varying composition, and with different coatings, will be fabricated, tested, and characterized.

Keywords: Ceramics, Composites, Fibrils, Modeling

381. **CORROSION PROTECTION OF SiC-BASED CERAMICS WITH CVD MULLITE COATINGS**
$50,000
DOE Contacts: F. M. Glaser, (301) 903-2784, V. U. S. Rao, (412) 892-4743 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

382. **FEASIBILITY OF SYNTHESIZING OXIDE FILMS ON CERAMIC AND METAL SUBSTRATES**
$65,000
DOE Contacts: F. M. Glaser, (301) 903-2784, V. U. S. Rao, (412) 892-4743 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: D. P. Stinton, (423) 574-4556
Lawrence Berkeley National 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

383. **CERAMIC COATING AND NATIVE OXIDE SCALES EVALUATION**
$35,000
DOE Contacts: F. M. Glaser, (301) 903-2784, V. U. S. Rao, (412) 892-4743and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: 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: (1) 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, (3) identify and evaluate compositions and synthesis routes for producing materials with damage-tolerant scales and coatings and (4) apply the approaches developed for surface oxide characterization to other ceramic coatings.

Keywords: Coatings, Corrosion

384. **DEVELOPMENT OF NOVEL ACTIVATED CARBON COMPOSITES**
$238,000
DOE Contacts: F. M. Glaser, (301) 903-2784, V. U. S. Rao, (412) 892-4743 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 (PSA) units for the efficient recovery of hydrogen from refinery purge gases, and for other gas separation operations associated with petroleum refining. Moreover, natural gas frequently contains large fractions of diluents and contaminants such as CO_2 and H_2S. CFCMS materials will be developed to effect the separation of diluents and contaminants from natural gas. Additionally, H_2O must be removed from natural gas to minimize pipeline corrosion. Novel separation techniques, that exploit the unique combination of properties of CFCMS, will be developed to effect the above-mentioned separations. The separation of air (O_2/N_2) is gaining importance because of the need for a compact separation system for vehicles powered by fuel cells. The combination of a suitably modified version of CFCMS and our electrical swing adsorption technology offers considerable potential for this application. Hence, research is being directed toward the tailoring of CFCMS for the separation of O_2/N_2.

Keywords: Carbon Fibers, Sieves, Composites

385. **ACTIVATION OF CARBON FIBER COMPOSITE MOLECULAR SIEVES**
$55,000
DOE Contacts: F. M. Glaser, (301) 903-2784, V. U. S. Rao, (412) 892-4743and 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

386. **CARBON FIBER COMPOSITE MOLECULAR SIEVES TECHNOLOGY TRANSFER**
$44,000
DOE Contacts: F. M. Glaser, (301) 903-2784, V. U. S. Rao, (412) 892-4743 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) 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.

Keywords: Carbon Products

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

387. **OXIDE DISPERSION STRENGTHENED (ODS) ALLOYS**
$224,000
DOE Contacts: F. M. Glaser, (301) 903-2784, V. U. S. Rao, (412) 892-4743 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 address the materials-related barriers to expediting the use of oxide dispersion-strengthened (ODS) alloys in components which are required in DOE's Office of Fossil Energy Vision 21 processes to operate at temperatures higher than are possible with conventionally-strengthened alloys. Specific goals are to develop a detailed understanding of ODS alloy behavior in all phases of their use, including fabrication, service performance, life prediction, mode of failure, repair, and refurbishment. The scope of the effort includes the development of

ODS iron-aluminum alloys that combine strength levels of the same order as commercially-available ODS-FeCrAl alloys, but with the superior resistance to high-temperature sulfidation and carburization attack demonstrated by the best iron aluminides. The data generated will form a resource for designers wishing to incorporate ODS alloys into components which may require modification of alloy processing to maximize strength or environmental resistance of particular forms of the alloys.

Keywords: Aluminides

388. **INVESTIGATION OF THE WELDABILITY OF POLYCRYSTALLINE IRON ALUMINIDES**
$70,000
DOE Contacts: F. M. Glaser, (301) 903-2784,
V. U. S. Rao, (412) 892-4743 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

389. **FRICTION WELDING OF ODS ALLOYS**
$13,000
DOE Contacts: F. M. Glaser, (301) 903-2784,
V. U. S. Rao, (412) 892-4743 and
M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact:
I. G. Wright, (423) 574-4451
The Welding Institute Contact:
P. L. Threadgill, 011-44-1223-891162

The purpose of this project is to establish that friction welding is a feasible method for joining iron aluminide tubes to other iron aluminide tubes, and to austenitic alloys. A companion objective is to establish optimized procedures for making welds, based on ambient temperature properties.

Keywords: Joining, Welding

390. **EVALUATION OF THE INTRINSIC AND EXTRINSIC FRACTURE BEHAVIOR OF IRON ALUMINIDES**
$30,000
DOE Contacts: F. M. Glaser, (301) 903-2784,
V. U. S. Rao, (412) 892-4743 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

391. **INVESTIGATION OF IRON ALUMINIDE WELD OVERLAYS**
$45,000
DOE Contacts: F. M. Glaser, (301) 903-2784,
V. U. S. Rao, (412) 892-4743 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

392. **IN-PLANT CORROSION PROBE TESTS OF ADVANCED AUSTENITIC ALLOYS**
$120,000
DOE Contacts: F. M. Glaser, (301) 903-2784,
V. U. S. Rao, (412) 892-4743 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

393. **FATIGUE AND FRACTURE BEHAVIOR OF Cr-Nb ALLOYS**
$0 - PYF[1]
DOE Contacts: F. M. Glaser, (301) 903-2784, V. U. S. Rao, (412) 892-4743 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 is 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

394. **CORROSION AND MECHANICAL PROPERTIES OF ALLOYS IN FBC AND MIXED-GAS ENVIRONMENTS**
$180,000
DOE Contacts: F. M. Glaser, (301) 903-2784, V. U. S. Rao, (412) 892-4743 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 mechanisms of oxidation, sulfidation, and breakaway corrosion in mixed gas atmospheres typical of both combustion and gasification systems, (2) develop an understanding of corrosion processes that occur in ceramic materials and surface modified alloys, (3) characterize the physical, chemical, and mechanical properties of surface scales that are resistant to sulfidation attack, (4) evaluate the role of deposits containing sulfur and/or chlorine and ash constituents in the corrosion behavior of metallic alloys, selected coatings, and monolithic/composite ceramics, and (5) evaluate the residual mechanical properties of materials after exposure in corrosive environments and quantify the effects of corrosion on the properties to enable life prediction of components.

Keywords: Corrosion, Gasification, Creep Rupture, Fluidized-Bed Combustion

395. **OPTIMIZATION OF CORROSION-RESISTANT IRON ALUMINIDE COATINGS AND CLADDINGS**
$121,000
DOE Contacts: F. M. Glaser, (301) 903-2784, V. U. S. Rao, (412) 892-4743 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 consistent with the Office of Fossil Energy's Vision 21. One 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, including the determination of the influence of sulfur and other reactive gaseous species on corrosion kinetics and oxide scale microstructures and of long-term durability (including lifetime). A second objective is to maximize the high-temperature corrosion resistance of iron aluminides by examining the influence of alloying additions and oxide dispersoids on protective alumina scale formation and integrity.

Keywords: Corrosion, Aluminides, Mixed-Gas, Scales

[1]PYF denotes that funding for this project, active in FY 1998, was provided from prior year allocations.

396. **REDUCTION OF DEFECT CONTENT IN ODS ALLOYS**
$45,000
DOE Contacts: F. M. Glaser, (301) 903-2784, V. U. S. Rao, (412) 892-4743 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: I. G. Wright, (423) 574-4451
The University of Liverpool Contact: A. R. Jones, 151-794-8026

The purpose of this work is to assess the sources of defects in oxide-dispersion-strengthened (ODS) alloys. Experiments to confirm key features of defects in ODS alloys shall be devised and performed, and recommendations shall be made for the reduction of defects in these alloys.

Keywords: Aluminides, Defects

397. **CORROSION PROTECTION OF ULTRAHIGH TEMPERATURE INTERMETALLIC ALLOYS**
$99,000
DOE Contacts: F. M. Glaser, (301) 903-2784, V. U. S. Rao, (412) 892-4743 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, oxidation- and corrosion-resistant intermetallic alloys for use as hot components in advanced fossil energy conversion and combustion systems to help meet the 65 percent efficiency goal of the Vision 21 Concept. The successful development of these alloys is expected to improve thermal efficiency through increased operating temperatures and decreased cooling requirements. The development effort will be devoted to in-situ composite alloys based on Cr-Cr_2Nb and similar Cr-Cr_2X (X=refractory elements) systems.

Keywords: Corrosion, Chromium-Niobium, Mixed-Gas, Scales

398. **METAL DUSTING INITIATIVE**
$16,000
DOE Contacts: F. M. Glaser, (301) 903-2784, V. U. S. Rao, (412) 892-4743 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: P. F. Tortorelli, (423) 574-5119

The purpose of this work element is to examine whether aluminides and/or advanced austenitic alloys can offer substantially improved resistance to materials degradation in carbon-bearing environments associated with systems in advanced high-efficiency coal-fired power plants.

Keywords: Corrosion, Scales

399. **SUPPORT SERVICES FOR CERAMIC FIBER-CERAMIC MATRIX COMPOSITES**
$29,000
DOE Contacts: F. M. Glaser, (301) 903-2784, V. U. S. Rao, (412) 892-4743 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 (UNDEERC) 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

400. **DEVELOPMENT OF NONDESTRUCTIVE EVALUATION METHODS AND EFFECTS OF FLAWS ON THE FRACTURE BEHAVIOR OF STRUCTURAL CERAMICS**
$180,000
DOE Contacts: F. M. Glaser, (301) 903-2784, V. U. S. Rao, (412) 892-4743 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; 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

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

401. ***MATERIALS AND COMPONENTS IN FOSSIL ENERGY APPLICATIONS* NEWSLETTER**
$60,000[1]
DOE Contacts: F. M. Glaser, (301) 903-2784,
V. U. S. Rao, (412) 892-4743 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 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

402. **DEVELOPMENT OF CERAMIC MEMBRANES FOR HYDROGEN SEPARATION**
$370,000
DOE Contacts: F. M. Glaser, (301) 903-2784,
V. U. S. Rao, (412) 892-4743 and
M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact:
R. R. Judkins, (423) 574-4572
East Tennessee Technology Park 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

[1]Matching funding provided by EPRI.

403. **MAJOR EQUIPMENT**
$30,000
DOE Contacts: F. M. Glaser, (301) 903-2784,
V. U. S. Rao, (412) 892-4743 and
M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact:
R. R. Judkins, (423) 574-4572
East Tennessee Technology Park 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

404. **INVESTIGATION OF THE MECHANICAL PROPERTIES AND PERFORMANCE OF CERAMIC COMPOSITE COMPONENTS**
$40,000
DOE Contacts: F. M. Glaser, (301) 903-2784,
V. U. S. Rao, (412) 892-4743 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

405. **SOLID STATE ELECTROLYTE SYSTEMS FOR FUEL CELLS AND GAS SEPARATION**
$603,000
DOE Contacts: F. M. Glaser, (301) 903-2784,
V. U. S. Rao, (412) 892-4743 and
M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact:
R. R. Judkins, (423) 574-4572
Pacific Northwest National Laboratory Contact:
L. R. Pederson, (509) 375-2579

This project seeks to develop functional ceramic materials for applications in fossil energy conversion and gas separation. This project is composed of the following activities: (1) Stability of Solid Oxide Fuel Cell (SOFC) Materials - Aging of fuel cell materials and interfaces under high dc current loads is the principal focus of this task. Aging processes are accelerated through the use of dc currents higher than typical of an operating solid oxide fuel cell. Alternative electrolyte and electrode materials are being developed that would enable operation at reduced temperature and/or at higher efficiencies. (2) Gas Separation Using Mixed-Conducting Ceramic Membranes - Mixed ion and electron-conducting metal oxide ceramics are being developed that can be used to passively separate oxygen of high purity from air. Other uses include application as the cathode in an SOFC operating at reduced temperatures, as the membrane in a reactor to produce synthesis gas, and in the partial oxidation of hydrocarbons to produce more valuable products. This task seeks to develop promising ceramic membrane compositions and forms, to characterize the electrical, physical, and chemical properties of these ceramics, and to demonstrate applications on a laboratory scale. (3) Bismuth Oxide-Based Gas Separation Membranes - In collaboration with Oak Ridge National Laboratory (ORNL), this task will develop bismuth oxide-based solid electrolytes for use in driven oxygen separation membranes. Such compositions offer exceptionally high ionic conductivities, at least a factor of ten higher than zirconia at moderate temperatures. Research at ORNL will focus on the synthesis of alkaline earth-doped bismuth oxide electrolytes, structural characterization, and the development of processing techniques. Research at PNNL will focus on the evaluation of electrical and mechanical properties, on processing methodology, and on compatible electrode development.

Keywords: Fuel Cells, SOFC, Membranes Testing

406. **IMPROVED FUEL CELL MATERIALS**
$45,000
DOE Contacts: F. M. Glaser, (301) 903-2784,
V. U. S. Rao, (412) 892-4743 and
M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact:
R. R. Judkins, (423) 574-4572
East Tennessee Technology Park Contact:
D. E. Fain, (423) 574-9932

The purpose of this project is to develop and demonstrate the capability of porous materials technology existing at the East Tennessee Technology Park as a low-cost fabrication process for the production of air electrodes for the Westinghouse Electric Company's tubular solid oxide fuel cell.

Keywords: Fuel Cells, SOFC

407. **BISMUTH OXIDE SOLID ELECTROLYTE OXYGEN SEPARATION MEMBRANES**
$60,000
DOE Contacts: F. M. Glaser, (301) 903-278,
V. U. S. Rao, (412) 892-4743 and
M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact:
S. D. Nunn, (423) 576-1668

The purpose of this task is to develop bismuth oxide-based ionic conducting solid electrolytes for use as oxygen separation membranes. To produce efficient materials which will be competitive with existing materials and processes will require experimental studies in the following areas: optimization of the crystal chemistry of the solid solutions of bismuth oxide to maximize the oxygen ion transport at moderate operating temperatures; development of processing techniques which will enhance the orientation texture of the ceramic for increased ionic transport; and characterization and evaluation of the performance of selected compositions for comparison with competing materials and technologies.

Keywords: Membranes

408. **OXIDE-DISPERSION-STRENGTHENED Fe_3Al-BASED ALLOY TUBES**
$80,000
DOE Contacts: F. M. Glaser, (301) 903-2784,
V. U. S. Rao, (412) 892-4743 and
M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact:
I. G. Wright, (423) 574-4451
University of California at San Diego Contact:
B. K. Kad, (619) 534-7059

The goal of the work is to explore experimental and computational means by which inherent material and processing-induced anisotropies of ODS Fe_3Al-base alloys can be exploited to meet in-service mechanical and creep-life requirements of the power generation industry. The research shall examine microscopic and microstructural issues with a view to addressing optimum material design for macroscopic components under well prescribed in-service loading criteria. The economic incentive is the low cost of Fe_3Al-based alloys and their superior sulfidation resistance, in comparison to the competing Fe-Cr-Al base alloys and the Ni-base superalloys currently in service.

Keywords: Aluminide, Tubes

409. **IRON ALUMINIDE FILTERS FOR IGCCs**
$0 - PYF[1]
DOE Contacts: F. M. Glaser, (301) 903-2784,
V. U. S. Rao, (412) 892-4743 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

410. **IRON ALUMINIDE FILTERS FOR PFBCs**
$0 - PYF[2]
DOE Contacts: F. M. Glaser, (301) 903-2784,
V. U. S. Rao, (412) 892-4743 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

411. **CERAMIC COMPOSITES FOR SOLID OXIDE FUEL CELLS**
$100,000
DOE Contacts: F. M. Glaser, (301) 903-2784,
V. U. S. Rao, (412) 892-4743 and
M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact:
T. M. Besmann, (423) 574-6852

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. Potential 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 burner 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

412. **MANAGEMENT OF THE FOSSIL ENERGY AR&TD MATERIALS PROGRAM**
$400,000
DOE Contacts: F. M. Glaser, (301) 903-2784,
V. U. S. Rao, (412) 892-4743 and
M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact:
R. R. Judkins, (423) 574-4572

The goal of the Fossil Energy AR&TD Materials Program is to provide a materials technology base to assure the success of coal fuels and advanced power generation systems being pursued by DOE-FE. The purpose of the Program is to develop the materials of construction, including processing and fabrication methods, and functional materials necessary for those systems. The scope of the Program addresses materials requirements for all fossil energy systems, including materials for coal fuels technologies and for advanced power generation technologies such as coal gasification, heat engines, combustion systems, and fuel cells. The Program is aligned with the development of those technologies that are potential elements of the DOE-FE Vision 21 concept, which aims to address and solve environmental issues and thus remove them as a constraint to coal's continued status as a strategic resource.

The principal development efforts of the Program are directed at ceramic composites for high-temperature (~1200°C) heat exchanger applications; new corrosion- and erosion-resistant alloys with unique mechanical properties for advanced fossil energy systems; functional materials, particularly metal and ceramic hot-gas filters and gas separation materials based on ceramic membranes (porous and ion transport) and activated carbon materials; and corrosion research to understand the behavior of materials in coal-processing environments. Included as part of the responsibilities of Oak Ridge National Laboratory (ORNL) on the Fossil Energy AR&TD Materials Program is, with DOE-ORO, the technical management and implementation of all activities on the DOE Fossil Energy Advanced Research and Technology Development (AR&TD) Materials Program. DOE-FE administration of the Program is

[1]PYF denotes that funding for this project, active in FY 1998, was provided from prior year allocations.

through the Federal Energy Technology Center (FETC) and the Advanced Research Product Team.

Keywords: Management, Materials Program

413. **GENERAL TECHNOLOGY TRANSFER ACTIVITIES**
$17,000
DOE Contacts: F. M. Glaser, (301) 903-2784,
V. U. S. Rao, (412) 892-4743 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

414. **GORDON RESEARCH CONFERENCE SUPPORT**
$5,000
DOE Contacts: F. M. Glaser, (301) 903-2784,
V. U. S. Rao, (412) 892-4743 and
M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact:
R. R. Judkins, (423) 574-4572

The task provides funds for partial support of the annual Gordon Research Conference.

Keywords: Technology Transfer

ADVANCED METALLURGICAL PROCESSES PROGRAM

The materials program at the Albany Research Center (ARC), formerly with the Bureau of Mines, incorporates Advanced Metallurgical Processes that provide essential life-cycle information for evaluation and development of materials. The research at ARC directly contributes to FE objectives by providing information on the performance characteristics of materials being specified for the current generation of power systems, on the development of cost-effective materials for inclusion in the next generation of fossil fired power systems, and for solving environmental emission problems related to fossil fired energy systems. The program at ARC stresses full participation with industry through partnerships and emphasizes cost sharing to the fullest extent possible.

The materials research in the Program focuses on extending component service lifetimes through the improvement and protection of current materials, by the design of new materials, and by defining the service operating conditions for new materials in order to ensure their safe and effective use. This process involves developing a better understanding of specific failure modes for materials in severe operating environments, addressing factors which limit their current use in these environments, and by designing new materials and materials processing procedures to overcome anticipated usage challenges in severe operating environments, such as those typically found in fossil energy generating plants and in structures and supporting facilities associated with oil and gas production. Emphasis is placed on high-temperature erosion testing and modeling in environments anticipated for Vision 21 plants, on the development of sulfidation/oxidation resistant materials which can also resist thermal cycling for pressurized circulating fluidized bed reactors, the production of low-cost titanium for use as drill strings or coiled tubing in drilling applications, and repair and development of refractory materials for coal gasifiers.

415. **ADVANCED REFRACTORY RESEARCH**
$340,000
DOE Contact: Richard P. Walters,
(541) 967-5873
Albany Research Center Contact:
Arthur V. Petty, Jr., (541) 967-5878

The emphasis of this high temperature material research has been driven by both short range industrial needs and long range issues in gasifiers. Program emphasis is on the following: (1) identifying material failure mechanisms, (2) identifying/ developing materials that will extend the lifetime of primary refractory liners in slagging gasifier systems, (3) developing ways to shorten system downtime caused by refractory maintenance and, (4) developing improved thermocouples/temperature monitoring techniques.

Keywords: Refractories

416. **ADVANCED CASTING TECHNOLOGIES**
$1,160,000
DOE Contact: Richard P. Walters,
(541) 967-5873
Albany Research Center Contacts:
Arthur V. Petty, Jr. (541) 967-5878 and
Jeffrey A. Hawk, (541) 967-5900

To develop modified austenitic stainless steels with performance characteristics necessary for process streams in advanced heat recovery and hot gas cleanup systems employed with advanced power generation systems (IGCC, PFBC and IGFC). The most difficult near term R&D challenges are development of hot gas particulate and sulfur cleanup systems employed with these advanced power generation systems. Primary focus is on the development of TiC-reinforced *cast* austenitic stainless steels with Al and Si additions for oxidation and sulfidation resistance.

Keywords: Alloys, Casting, Cast Austenitic Stainless Steel, Titanium Carbide

417. **ADVANCED COATING TECHNIQUES**
$340,000
DOE Contact: Richard P. Walters, (541) 967-5873
Albany Research Center Contact: Arthur V. Petty, Jr. (541) 967-5878

The goal of the coating research is to develop sulfidation and/or oxidation resistant aluminide-based coating on stainless steels by utilizing an ARC developed foil-lamination process. Conceptionally, the coating process would consist of a mechanical mechanism to bond an Al foil to a steel substrate, such as roll-bonding or extrusion, followed by an elevated temperature heat- treatment to synthesize the brittle aluminide layer. Thus, the bonding mechanisms and the kinetics of the aluminide forming reactions need to be determined.

Keywords: Alumindes, Coatings, Foil-lamination Process

418. **ADVANCED TITANIUM PROCESSING**
$700,000
DOE Contact: Richard P. Walters, (541) 967-5873
Albany Research Center Contact: Paul C. Turner, (541) 967-5863

Nearly 50 percent of the cost of titanium can be attributed to fabrication. Currently, all wrought products are produced from cylindrical ingot which must be broken down in multiple steps of forging and rolling. The process, although more lengthy, is analogous to the same process that was once used to make wrought steel products prior to the advent of continuous casting. A similar continuous and lower cost process to prepare commercially pure titanium and titanium alloys in a variety of shapes including slab, plate, and billet would reduce costs, increase the usage of titanium, and lead to environmental benefits and energy savings. A successful conclusion of this project will result in a continuous melting and ingot making process that directly utilizes titanium sponge or scrap. Development of a melting process to produce a billet or slab surface finish that is suitable for rolling without the necessity of forging or other preparation will significantly increase yields and productivity.

Keywords: Titanium, Continuous Casting

419. **SERVICE LIFE PREDICTION**
$1,200,000
DOE Contact: Richard P. Walters, (541) 967-5873
Albany Research Center Contact: Jeffrey A. Hawk, (541) 967-5900

Abrasion and erosion are significant materials-related problems in the operation of fossil energy plants. Abrasion is a problem in the production of pulverized coal for use in the burners, and erosion is a problem in the daily operation of the plant. Improvements in abrasion and erosion resistance will result in higher efficiency, less maintenance, and less catastrophic failures in fossil energy plants. An understanding of how materials behave as a result of particle impact will be developed through understanding the contact mechanics of the impact process and by investigating and characterizing the damage inflicted on various materials by impact of particles.

Large temperature gradients and heat fluxes occur in turbines, heat exchangers, and walls of fossil energy power plants. The effects of temperature gradient and heat flux on oxidation, sulfidation, and hot corrosion rates and mechanisms are not well understood. This study also examines non- isothermal oxidation and hot corrosion.

Keywords: Abrasion, Erosion, Oxidation, Corrosion, Wear

DIRECTORY

J. D. Achenbach
Department of Civil Engineering
Northwestern University
Evanston, IL 60201
(847) 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
(423) 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
(423) 574-4565

T. W. Arrigoni
U.S. Dept. of Energy
P.O. Box 10940
Pittsburgh, PA 15236
(412) 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

Samuel J. Barish
ER-32/GTN
U.S. Dept. of Energy
19901 Germantown Road
Germantown, MD 20874-1290
(301) 903-3054

W. Barnett
NE-53/GTN
U.S. Dept. of Energy
19901 Germantown Road
Germantown, MD 20874-1290
(301) 903-3097

Harold N. Barr
Hittman Mat. & Med. Components, Inc.
9190 Red Branch Road
Columbia, MD 21045
(301) 730-7800

Bulent Basol
Interni. 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
(423) 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
(423) 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
(650) 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) 384-6496

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
(510) 486-5682

Theodore M. Besmann
Metals and Ceramics Division
Oak Ridge National Laboratory
P.O. Box 2008
Oak Ridge, TN 37831
(423) 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

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
(423) 574-7071

J. A. M. Boulet
University of Tennessee
310 Perkins Hall
Knoxville, TN 37996
(423) 974-8376

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
(423) 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
(423) 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
(925) 422-2051

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

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

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
(510) 486-5028

Juan Carbajo
ORNL
P.O. Box Y
Oak Ridge, TN 37831
(423) 574-3784

R. W. Carling, Div. 8313
Sandia National Laboratories
Livermore, CA 94550
(925) 422-2206

P. T. Carlson
Oak Ridge National Laboratory
P.O. Box 2008
Oak Ridge, TN 37831
(423) 574-5135

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
(423) 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

D. C. Christensen
LANL
Los Alamos, NM 87545
(505) 667-2556

Richard Christensen
LLNL
University of California
P.O. Box 808
Livermore, CA 94550
(925) 422-7136

L. Christophorou
ORNL
P.O. Box 2008
Bldg. 4500S, 122, Rm. H156
Oak Ridge, TN 37831
(423) 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

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

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

Robert Cook
LLNL
University of California
P.O. Box 808
Livermore, CA 94550
(925) 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
(925) 422-2352

Bruce Cranford
EE-21/FORS
U.S. Dept. of Energy
Washington, DC 20585
(202) 586-9496

Frederick A. Creswick
ORNL
P.O. Box 2009
Oak Ridge, TN 37831
(423) 574-2009

James V. Crivello
Department of Chemistry
Rensselaer Polytechnic Institute
Troy, NY 12180-3590
(518) 276-6825

Randy Curlee
ORNL
P.O. Box 2008
Oak Ridge, TN 37831
(423) 576-4864

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
(423) 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
(630) 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

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

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) 586-9837

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
(630) 972-5068

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

Bob Evans
NASA Lewis Research Center
21000 Brookpark Road, MS 77-6
Cleveland, OH 44135
(216) 433-3400

John Fairbanks
EE-33/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
(423) 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
(650) 723-4007

Mattison K. Ferber
ORNL
P.O. Box 2008
Building 4515
Oak Ridge, TN 37831-6064
(423) 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

D. M. Follstaedt
Division 1110
Sandia National Laboratories
Albuquerque, NM 87185
(505) 844-2102

Christopher A. Foster
Cryogenic Applications F, Inc.
450 Bacon Springs Lane
Clinton, TN 37716
(423) 435-5433

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
(925) 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

R. Glass
LLNL
University of California
P.O. Box 808
Livermore, CA 94550
(925) 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

Robert L. Goldsmith
CeraMem Corporation
12 Clematis Avenue
Waltham, MA 02154
(617) 899-0467

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
(925) 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/GTN
U.S. Dept. of Energy
Washington, DC 20585
(301) 903-3427

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
(630) 252-3513

T. R. Guess
Division 1812
Sandia National Laboratories
Albuquerque, NM 87185
(505) 844-5604

Marvin E. Gunn
EE-60/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

Phil Haley
Allison Turbine Operations
P.O. Box 420
Indianapolis, IN 46206-0420
(317) 230-2272

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
(423) 574-5962

Pat Hart
Pacific Northwest Labs
P.O. Box 999
Richland, WA 99352
(504) 375-2906

Debbie Haught
EE-23/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
(423) 574-4352

Kamithi Hemachalam
Intermagnetics General Corp.
1875 Thomaston Avenue
Waterbury, CT 06704
(203) 753-5215

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
(925) 532-0235

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 Laboratory
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
(510) 422-7759

E. E. Hoffman
U.S. Dept. of Energy
P.O. Box 2001
Oak Ridge, TN 37831-8600
(423) 576-0735

Linda L. Horton
Oak Ridge National Laboratory
Box 2008, Bldg. 4500-S
Oak Ridge, TN 37831-6118
(423) 574-5081

E. Philip Horwitz
Chemistry Division
Argonne National Laboratory
9700 South Cass Avenue
Argonne, IL 60439
(630) 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
FETC
P.O. Box 880
Morgantown, WV 26505
(304) 291-4663

Donald R. Huffman
Dept. of Physics
University of Arizona
Tucson, AZ 85721
(520) 621-4804

Robert A. Huggins
Dept. of Mat. Science & Eng.
Peterson 550I
Stanford University
Stanford, CA 94305
(925) 497-4110

Arlon Hunt
Lawrence Berkeley Laboratory
University of California
Berkeley, CA 94720
(925) 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

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

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
(423) 574-4281

J. L. Jellison
Division 1833
Sandia National Laboratories
Albuquerque, NM 87185
(505) 844-6397

M. M. Jenior
EE-41/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
(630) 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
(423) 576-6832

R. J. Johnson
Hanford Eng. Dev. Lab.
P.O. Box 1970
Richland, WA 99352
(509) 376-0715

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

Chris Kang
EE-142/FORS
U.S. Dept. of Energy
Washington, DC 20585
(202) 586-4563

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
(541) 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) 384-6600

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
(423) 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
(925) 422-6669

G. S. Kino
Edward Ginzton Laboratory
Stanford University
Stanford, CA 94305
(925) 497-0205

Thomas Kitchens
ER-31/GTN
U.S. Dept. of Energy
Washington, DC 20585
(301) 903-5152

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
(860) 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

Victor R. Koch
Covalent Associates, Inc.
10 State Street
Woburn, MA 01801
(617) 938-1140

K. G. Kreider
National Institute of Standards
and Technology
Gaithersburg, MD 20899
(301) 975-2619

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
(925) 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

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
(860) 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
(510) 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

J. Lipkin
Sandia National Laboratories
Livermore, CA 94550
(925) 422-2417

C. T. Liu, Mtl. Ceram. Div.
ORNL
P.O. Box 2008
Bldg. 4500-S, 115, Rm. S280
Oak Ridge, TN 37831
(423) 574-5516

K. C. Liu
ORNL
P.O. Box 2008
Bldg. 4500-S, MS 155
Oak Ridge, TN 37831
(423) 574-5116

Earl L. Long, Jr.
ORNL, Metals & Ceramics Div.
P.O. Box 2008
Bldg. 4515, 069, Room 229
Oak Ridge, TN 37831
(423) 574-5127

Richard W. Longsderff
Thermacore, Inc.
780 Eden Road
Lancaster, PA 17601
(717) 569-6551

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
(925) 422-3187

C. D. Lundin
307 Dougherty Eng. Bldg.
University of Tennessee
Knoxville, TN 37996
(423) 974-5310

MAJ Ross E. Lushbough
DP-225.2/FORS
U.S. Dept. of Energy
Washington, DC 20585
(301) 903-3912

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
(203) 792-1460

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

Douglas McAllister
BIODE, Inc.
2 Oakwood Road
Cape Elizabeth, ME 04107
(207) 883-1492

James W. McCauley
U.S. Army Research Laboratory
AMSRL-WM-M
Aberdeen Proving Ground, MD 21005-5069

Robert W. McClung
ORNL
P.O. Box 2008
Bldg. 4500-S, 151, Rm. D63
Oak Ridge, TN 37831-6088
(423) 574-4466

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

David L. McElroy
ORNL
P.O. Box 2008
Bldg. 4508, 092, Rm. 239
Oak Ridge, TN 37831-6088
(423) 574-5976

A. J. McEvily
Metallurgy Dept., U-136
University of Connecticut
Storas, CT 06268
(860) 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
(925) 422-7792

Carl McHargue
University of Tennessee
Materials & Eng. Dept.
434 Doughtery Eng. Bldg.
Knoxville, TN 37996-2200
(423) 974-8013

M. J. McMonigle
EE-234/FORS
U.S. Dept. of Energy
Washington, DC 20585
(202) 586-2082

Arthur S. Mehner
NE-53/GTN
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

A. Meyer
International Fuel Cells
P.O. Box 739
195 Governors Hwy.
South Windsor, CT 06074
(203) 727-2214

JoAnn Milliken
EE-23, 5G-023/FORS
FORS
U.S. Dept. of Energy
Washington, DC 20585
(202) 586-2480

B. E. Mills
Sandia National Laboratories
Livermore, CA 94550
(925) 422-3230

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
(630) 972-8292

M. C. Nichols
Sandia National Laboratories
Livermore, CA 94550
(925) 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
(925) 422-2767

T. A. Nolan
ORNL
P.O. Box 2008
Bldg. 4515, MS 064
Oak Ridge, TN 37831
(423) 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
(925) 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
(423) 974-5326

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
(510).486-5289

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
(650) 723-2564

E. R. Parker
456 Hearst
Univ. of Ca., Berkeley
Berkeley, CA 24720
(510) 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

Ahmad Pesaran
NREL
1617 Cole Blvd.
Golden, CO 80401
(303) 231-7636

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
(630) 972-4450

Melvin A. Piestrup
Adelphi Technology
13800 Skyline Blvd.
Woodside, CA 94062
(925) 851-0633

James E. Plank
Charles Evans and Associates
301 Chesapeake Drive
Redwood City, CA 94063
(925) 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

Peter Pronko
Universal Energy Systems
4401 Dayton-Xenia Road
Dayton, OH 45432
(513) 426-6900

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

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
(510) 642-0863

P. L. Rittenhouse
ORNL
P.O. Box 2008
Bldg. 45005, 138, Rm. A158
Oak Ridge, TN 37831
(423) 574-5103

H. F. Rizzo
Lawrence Livermore Nat. Lab
University of California
P.O. Box 808
Livermore, CA 94550
(925) 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
(925) 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
(925) 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
(510) 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
(423) 576-4864

M. Rubin
Lawrence Berkeley Laboratory
University of California
Berkeley, CA 94720
(510) 486-7124

E. Russell
LLNL
University of California
Livermore, CA 94550
(925) 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

Peter H. Salmon-Cox
Dir. of Office Ind. Processes
EE-23/FORS
U.S. Dept. of Energy
Washington, DC 20585
(202) 586-2380

R. J. Salzbrenner
Division 1832
Sandia National Laboratories
Albuquerque, NM 87185
(505) 844-5041

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
(423) 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

Y. Schienle
Garrett Turbine Engine Co.
111 South 34th Street
P.O. Box 5217
Phoenix, AZ 85034
(602) 231-4666

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

James Schwarz
Dept. Chem. Eng/Mat Science
Syracuse University
320 Hinds Hall
Syracuse, NY 13244
(315) 423-4575

James L. Scott
Metals and Ceramics Div.
ORNL
P.O. Box 2008, Bldg. 4508
Oak Ridge, TN 37831-6091
(423) 624-4834

Timothy C. Scott
Chemical Technology Division
Oak Ridge National Laboratory
P.O. Box 2008
Oak Ridge, TN 37831
(423) 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

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
(423) 574-5112

Richard Silberglitt
FM Technologies, Inc.
Patriot Square
10529-B Braddock Road
Fairfax, VA 22032
(703) 425-5111

T. B. Simpson
FE-34/GTN
U.S. Dept. of Energy
Washington, DC 20585
(301) 903-3913

J. P. Singh
Argonne National Labs
9700 South Cass
Argonne, IL 60439
(630) 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
(925) 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
(412) 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
(925) 422-3307

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

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
(423) 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
(423) 974-2171

G. Stoner
University of Virginia
Charlottesville, VA 22901
(804) 924-3277

Edwin E. Strain
Garrett Corporation
111 S. 34th Street
P.O. Box 5217, MS 301-2N
Phoenix, AZ 85010
(602) 231-2797

Thomas N. Strom
NASA Lewis Research Center
21000 Brookpark Road, MS 77-6
Cleveland, OH 44135
(216) 433-3408

David Sutter
ER-224/GTN
U.S. Dept. of Energy
Washington, DC 20585
(301) 903-5228

Patrick Sutton
EE-32/FORS
U.S. Dept. of Energy
Washington, DC 20585
(202) 586-8058

Richard Swanson
SunPower Corporation
435 Indio Way
Sunnyvale, CA 94086
(408) 991-0900

R. W. Swindeman
ORNL
P.O. Box 2008
Bldg. 4500-S, 155, Rm. 0040
Oak Ridge, TN 37831
(423) 574-5108

W. Tabakoff
Dept. of Aerospace Eng.
M/L 70
University of Cincinnati
Cincinnati, OH 45221
(513) 475-2849

C. A. Thomas
U.S. Dept. of Energy
P.O. Box 10940
Pittsburgh, PA 15236
(412) 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

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
(423) 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
(423) 574-0768

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-46/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-32/GTN
U.S. Dept. of Energy
Washington, DC 20585
(301) 903-7484

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

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
(423) 483-1859

William K. Warburton
X-ray Instrumentation Associates
1300 Mills Street
Menlo Park, CA 94025-3210
(925) 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

Elizabeth G. Weiss
Membrane Technology and Research, Inc.
1360 Willow Road, Suite 103
Menlo Park, CA 94025
(925) 328-2228

James Wert
Dept. of Mat. Science & Eng.
Vanderbilt University
Station B, P.O. Box 1621
Nashville, TN 37235
(423) 322-3583

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-52/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

Frank Wilkins
EE-11/FORS
U.S. Dept. of Energy
Washington, DC 20585
(202) 586-1684

A. D. Wilks
Signal UOP Research Center
50 UOP Plaza
Des Plaines, IL 60016
(312) 492-3179

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
(925) 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
(925) 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

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
(208) 526-6127

David Yarbrough
Department of Chem. Eng.
Tennessee Tech. University
1155 N. Dixie Ave.
Cookville, TN 38505
(423) 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
(925) 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
(423) 574-4812

F. J. Zanner
Division 1833
Sandia National Laboratories
Albuquerque, NM 87185
(505) 844-7073

C. M. Zeh
FETC
P.O. Box 880
Morgantown, WV 26505
(304) 291-4265

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) 384-6441

KEYWORD INDEX

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U.S. Department of Energy
19901 Germantown Road
Germantown, MD 20874

SC-13