DOE/ER-0734

Energy Materials Coordinating Committee (EMaCC)

Fiscal Year 1997

July 31, 1998

Annual Technical Report

U.S. Department of Energy
Office of Energy Research
Office of Basic Energy Sciences
Division of Materials Sciences

DOE/ER-0734

Energy Materials Coordinating Committee (EMaCC)

Fiscal Year 1997

July 31, 1998

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

TABLE OF CONTENTS

PROGRAM DESCRIPTIONS

TABLE OF CONTENTS (continued)

TABLE OF CONTENTS (continued)

INTRODUCTION

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

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

Six meetings were scheduled for 1998. The dates, themes and speakers are as follows:

November 13, 1997 **Subcommittee on Environmental Management**
Speaker: Helen Farrell

The minutes of the September 9, 1997, EMaCC meeting were accepted. Organizational details regarding EMaCC subcommittees were discussed. Helen Farrell made a presentation on the FY 1998 Environmental Management Science Program (EMSP) Solicitation. The announcement of the solicitation was said to be imminent and that there might be as much as $20 million for new awards in FY98. A draft report from the R&D Council subcommittee on Technical Coordinating Committees (TCC) was also discussed.

January 15, 1998 **Subcommittee on Electrochemical Technologies**
Speaker: Professor Philip N. Ross, Lawrence Berkeley National Laboratory

JoAnn Milliken welcomed the speaker and members; Richard Kelley introduced the guest speaker, Professor Philip N. Ross, who spoke on Surface Electrochemistry—Past, Present and Future. Dr. Ross traced the history of studies of the electrochemical interface through the development of electron-based spectroscopic analysis to the current in-situ photon-in photon-out methods such as Surface X-ray Scattering (SXS) and Surface-Enhanced Raman Spectroscopy (SERS). Progress in understanding a number of electrode processes such as potential-dependent reconstruction of Au(hkl) surfaces were discussed as was progress towards a carbon monoxide tolerant electrode for fuel cell. JoAnn Milliken described recent advances in the Automotive Fuel Cell Program. Significant accomplishments include the development of a highly efficient direct-hydrogen fuel cell stack system by International Fuel Cells, Inc., and the demonstration of technical feasibility of gasoline-powered PEM fuel cells. The latter achievement is important for the development of fuel cell systems powered by hydrogen generated by on-board fuel processing of gasoline. Utilizing the existing fuel infrastructure will enable early introduction of automotive fuel cells since a hydrogen fueling infrastructure is currently unavailable. Neil Rossmeissl spoke on materials issues in hydrogen research. The emphasis was on hydrogen storage and also hydrogen production, which is a high temperature (800-1200°C) process. The minutes of the November 13, 1997, EMaCC meeting were accepted.

March 12, 1998 **Subcommittee on Metals**
Speakers: Dr. Michael Kassner, Oregon State University
Dr. Phil Maziasz, Oak Ridge National Laboratory

Sara Dillich welcomed the speakers on behalf of the Metals Subcommittee and gave a brief overview of planned solicitations/activities of the Office of Industrial Technologies. Dr. Michael Kassner spoke on the Metal Forming Project of the DOE Center for Excellence for the Synthesis and Processing of Advanced Materials. The object of the Metal Forming Project (one of eight Center projects) is to develop a scientific understanding of the phenomena relating to forming of aluminum alloys for industrial (especially automotive) applications. Dr. Phil Maziasz spoke on Achieving Perfect Microstructures for dramatically improving creep-strength of stainless steels. This summarized the results of a Cooperative Research and Development Agreement (CRADA) between ORNL utilizing its alloy R&D and process optimization expertise and Solar Turbines, Inc., as the end-user, and Allegheny-Teledyne as the materials (foil) producer. Dr. Kassner and the Metal Forming project are supported by OER/BES/DMS. Dr. Maziasz's research is supported by the FE/ARTD program.

May 21, 1998 **Subcommittee on Superconductivity**
Speakers: Russell Eaton, DOE Golden Field Office
Maribel Soto, Office of Naval Research Superconductivity Programs
X-D Xiang, Lawrence Berkeley National Laboratory
Bill McCallum, Ames Laboratory

JoAnn Milliken called the meeting to order and Chris Platt welcomed our speakers and guests which included Don Gubser from the Naval Research Laboratories. Russell Eaton spoke on the status of the Superconductivity Partnership Initiative which is sponsored by the Superconductivity for Electric Systems Program, Maribel Soto presented a summary of work supported in the Office of Naval Research Superconductivity Programs, X-D Xiang presented work on the Combinatorial Approach to Study of Superconductors and Other Related Oxide Electronic Materials and Bil McCallum described progress toward understanding the Light Rare-Earth Barium Copper Oxide Superconductors.

July 16, 1998 **Subcommittee on Semiconductors/Photovoltaics**

September 10, 1998 **Subcommittee on Environmental Management**

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 1997 and describes the materials research programs of various offices and divisions within the Department.

The Chairman of EMaCC for FY 1997 was Dr. Yok Chen. The compilation of this report was performed by Dr. Tim Fitzsimmons, EMaCC Executive Secretary for FY 1998, with the assistance of FM Technologies, Inc.

Dr. JoAnn Milliken
Office of Transportation Technologies
EmaCC Chair, FY 1998

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	Thomas Sebestyen, EE-32	202/586-9727
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
	Christine Platt, EE-142	202/586-8943
	Chris Kang, EE-142	202/586-4563

ORGANIZATION	REPRESENTATIVE	PHONE NO.
ENERGY RESEARCH		
Basic Energy Sciences		
Materials Sciences	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
	Helen Farrell, ER-131	301/903-5998
Solid State Physics and Materials Chemistry	W. Oosterhuis, ER-132	301/903-3426
	Jerry Smith, ER-132	301/903-3426
	Richard 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	Paula Davidson, ER-15	301/903-5822
	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	Albert Evans, ER-83	301/903-3427
	Michael Teresinski, ER-83	301/903-5155
Fusion Energy		
Fusion Technologies	F. W. (Bill) Wiffen, ER-52	301/903-4963
ENVIRONMENTAL RESTORATION AND WASTE MANAGEMENT		
Waste Operations		
Waste Management Projects	Doug Tonkay, EM-34	301/903-7212
Science and Technology		
Research and Development	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 1997 budget summary for DOE Materials Activities is presented on page 7. 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 1997 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 1997 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 1997 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 1997
OFFICE OF BUILDING TECHNOLOGY, STATE AND COMMUNITY PROGRAMS	$1,090,000
Office of Building Systems	1,090,000
OFFICE OF INDUSTRIAL TECHNOLOGIES	$32,597,505
Office of Industrial Strategies	10,398,309
Aluminum Vision Team	5,071,000
Forest Products Vision Team	1,084,012
Steel Vision Team	455,000
Glass Vision Team	1,228,000
Metal Casting Vision Team	2,560,297
Office of Crosscut Technologies	22,199,196
Advanced Turbine System (ATS) Program	7,350,000
Continuous Fiber Ceramic Composites (CFCC) Program	8,400,000
Advanced Industrial Materials (AIM) Program	5,793,000
Combustion/Heat Exchanger Program	630,000
OFFICE OF TRANSPORTATION TECHNOLOGIES	$24,249,000
Transportation Materials Technology	24,249,000
Automotive Materials Technology	17,483,000
Propulsion Systems Materials	5,483,000
Lightweight Vehicle Materials Technology	12,000,000
Electric Drive Vehicle Technologies	3,397,000
Advanced Battery Programs	2,997,000
Fuel Cell Materials	400,000
Heavy Vehicle Materials Technology	3,369,000
OFFICE OF UTILITY TECHNOLOGIES	$38,810,000
Office of Solar Energy Conversion	18,460,000
Photovoltaic Energy Technology Division	18,460,000
Office of Geothermal Technologies	600,000
Office of Energy Management	19,750,000
Advanced Utility Concepts Division	19,750,000
High Temperature Superconductivity for Electric Systems	19,750,000

FY 1997 BUDGET SUMMARY FOR DOE MATERIALS ACTIVITIES (continued)

	FY 1997
OFFICE OF ENERGY RESEARCH	**$431,936,392**
Office of Basic Energy Sciences	344,107,192
Division of Materials Sciences	332,060,000
Division of Chemical Sciences	5,143,000
Division of Engineering and Geosciences	6,904,192
Engineering Sciences Research	3,946,973
Geosciences Research	2,957,219
Office of Computational and Technology Research	76,651,200
Division of Advanced Energy Projects and Technology Research	76,651,200
Laboratory Technology Research (LTR) Program	8,062,000
Advanced Energy Projects Program	5,640,000
Small Business Innovation Research Program	58,849,611
Small Business Technology Transfer Program	4,099,589
Office of Fusion Energy Sciences	11,178,000
OFFICE OF ENVIRONMENTAL MANAGEMENT	**$6,870,939**
OFFICE OF NUCLEAR ENERGY, SCIENCE AND TECHNOLOGY	**$65,080,000**
Office of Engineering and Technology Development	2,080,000
Space and National Security Programs	2,080,000
Office of Naval Reactors	63,000,000[1]
OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT	**$15,400,000**
OFFICE OF DEFENSE PROGRAMS	
The Weapons Research, Development and Test Program	$96,633,600
Sandia National Laboratories	23,183,600
Lawrence Livermore National Laboratory	20,250,000
Los Alamos National Laboratory	53,200,000
OFFICE OF FOSSIL ENERGY	**$4,914,000**
Office of Advanced Research	4,914,000
Fossil Energy AR&TD Materials Program	4,914,000
TOTAL	**$717,581,436**

[1]This excludes $47 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	$1,090,000	$0	$0	$0	$1,090,000
Office of Industrial Technologies	$13,722,000	$15,617,208	$3,258,297	$0	$32,597,505
Office of Transportation Technologies	$17,925,000	$2,940,000	$3,084,000	$300,000	$24,249,000
Office of Utility Technologies	$29,310,000	$9,500,000	$0	$0	$38,810,000
Office of Energy Research	$331,608,800	$65,199,200	$34,486,863	$641,529	$431,936,392
Office of Environmental Management	$4,965,355	$250,000	$1,448,252	$207,332	$6,870,939
Office of Nuclear Energy, Science and Technology	$65,080,000	$0	$0	$0	$65,080,000
Office of Civilian Radioactive Waste Management	$15,400,000	$0	$0	$0	$15,400,000
Office of Defense Programs	$96,633,600	$0	$0	$0	$96,633,600
Office of Fossil Energy	$3,979,000	$558,000	$357,000	$20,000	$4,914,000
Totals	$579,713,755	$94,064,408	$42,634,412	$1,168,861	$717,581,436

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 1997
OFFICE OF BUILDING TECHNOLOGY, STATE AND COMMUNITY PROGRAMS	$ 1,090,000
Office of Building Systems	1,090,000
OFFICE OF INDUSTRIAL TECHNOLOGIES	$32,597,505
Office of Industrial Strategies	10,398,309
Aluminum Vision Team	5,071,000
Forest Products Vision Team	1,084,012
Steel Vision Team	455,000
Glass Vision Team	1,228,000
Metal Casting Vision Team	2,560,297
Office of Crosscut Technologies	22,199,196
Advanced Turbine System (ATS) Program	7,350,000
Continuous Fiber Ceramic Composites (CFCC) Program	8,400,000
Advanced Industrial Materials (AIM) Program	5,793,000
Combustion/Heat Exchanger Program	656,196
OFFICE OF TRANSPORTATION TECHNOLOGIES	$24,249,000
Transportation Materials Technology	24,249,000
Automotive Materials Technology	17,483,000
Propulsion Systems Materials	5,483,000
Lightweight Vehicle Materials Technology	12,000,000
Electric Drive Vehicle Technologies	3,397,000
Advanced Battery Programs	2,997,000
Fuel Cell Materials	400,000
Heavy Vehicle Materials Technology	3,369,000
OFFICE OF UTILITY TECHNOLOGIES	$38,810,000
Office of Solar Energy Conversion	18,460,000
Photovoltaic Energy Technology Division	18,460,000
Office of Geothermal Technologies	600,000
Office of Energy Management	19,750,000
Advanced Utility Concepts Division	19,750,000
High Temperature Superconductivity for Electric Systems	19,750,000

OFFICE OF BUILDING TECHNOLOGY, STATE AND COMMUNITY PROGRAMS

	FY 1997
Office of Building Technology, State and Community Programs - Grand Total	$1,090,000
Office of Building Systems	$1,090,000
Materials Properties, Behavior, Characterization or Testing	$1,090,000
Development of Non-HCFC Foam Insulations	250,000
Evacuated Panel Insulation	250,000
Existing Materials Performance	110,000
Development of Sustainable Insulations	250,000
Standard Procedures for Measuring Solar Reflectivity of Roofs and Pavements	230,000

OFFICE OF BUILDING TECHNOLOGY, STATE AND COMMUNITY PROGRAMS

OFFICE OF BUILDING SYSTEMS

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

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

1. **DEVELOPMENT OF NON-HCFC FOAM INSULATIONS**
   $250,000
   DOE Contact: Arun Vohra, (202) 586-2193
   ORNL Contact: Ken Wilkes, (423) 574-5931

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

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

2. **EVACUATED PANEL INSULATION**
   $250,000
   DOE Contact: Arun Vohra, (202) 586-2193
   ORNL Contact: Ken Wilkes, (423) 574-5931

This project is for the development of an advanced technology super insulation concept. A 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

3. **EXISTING MATERIALS PERFORMANCE**
   $110,000
   DOE Contact: Arun Vohra, (202) 586-2193
   LBL Contact: Dariush Arasteh, (510) 486-6844

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. **DEVELOPMENT OF SUSTAINABLE INSULATIONS**
   $250,000
   DOE Contact: Arun Vohra, (202) 586-2193
   ORNL Contact: Ken Wilkes, (423) 574-5931

This project is for the identification and development of low-cost sustainable insulation materials and systems for use in the building envelope. A survey and evaluation of information is being conducted to identify potentially applicable materials, known properties, deficiencies in knowledge of properties, level of availability, climatic and geographic range of applicability, environmental benefits and concerns, and costs of materials, transportation and any required treatment or processing. Laboratory evaluations of candidate materials will focus on thermal performance and other characteristics.

Keywords: Insulation, Sustainability, Building Envelope

5. **STANDARD PROCEDURES FOR MEASURING SOLAR REFLECTIVITY OF ROOFS AND PAVEMENTS**
   $230,000
   DOE Contact: Mark Decot, (202) 586-6501
   LBL Contact: Hashem Akbari, (510) 486-4287
   ORNL Contact: Jeff Christian, (423) 574-5207

Reflectivity of exterior building materials used for pavement and roofing has been demonstrated to affect heating and cooling costs in buildings where they are applied. The reflectivity of these surfaces also has an effect on creating urban heat islands where ambient air temperature has an additional indirect effect on heating and cooling costs in buildings. Exterior surface reflectivity also has an effect on urban smog formation and indoor air quality. This research on procedures for measuring reflectivity and characterizing effects or urban heat islands is being conducted in cooperation with ASTM, the Lawrence Berkeley Laboratory, Oak Ridge National Laboratory, Cool Roof Rating Council, Environmental Protection Agency and other Cool Communities partners.

Keywords: Solar Reflectivity, Building Materials, Heat Islands, Smog, Energy Efficiency

OFFICE OF INDUSTRIAL TECHNOLOGIES

	FY 1997
Office of Industrial Technologies - Grand Total	$32,597,505
Office of Industrial Strategies	$10,398,309
Aluminum Vision Team	$ 5,071,000
Device or Component Fabrication, Behavior or Testing	$ 1,935,000
Aluminum Bridge Deck System	360,000
InLine Sensors for Electrolytic Aluminum Cells	254,000
Detection and Removal of Molten Salts from Molten Aluminum	294,000
High-Efficiency, High-Capacity, Low-NO_x Aluminum Melting Using Oxygen-Enhanced Combustion	527,000
Technology for Converting SPL to Useful Glass Fiber Products	500,000
Materials Properties, Behavior, Characterization or Testing	$ 970,000
Molten Aluminum Explosion Prevention	100,000
Innovative Vertical Flotation Melter	300,000
Aluminum Pilot Cell	570,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 2,166,000
Recycling Aluminum Salt Cake	500,000
Wettable Ceramic-Based Drained Cathode Technology for Aluminum Electrolysis Cells	666,000
Aluminum Spray Forming	1,000,000
Forest Products Vision Team	$ 1,084,012
Materials Properties, Behavior, Characterization or Testing	$ 1,084,012
Corrosivity Monitoring of Kraft Recovery Boilers	1,084,012
Steel Vision Team	$ 455,000
Device or Component Fabrication, Behavior or Testing	$ 455,000
Intermetallic Alloy Development Related to the Steel Industry	455,000
Glass Vision Team	$ 1,228,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 364,000
Chemical Vapor Deposition Ceramic Synthesis	364,000
Materials Properties, Behavior, Characterization or Testing	$ 864,000
Development of Improved Refractories	364,000
Synthesis and Design of $MoSi_2$ Intermetallic Materials	500,000

OFFICE OF INDUSTRIAL TECHNOLOGIES (Continued)

	FY 1997
Office of Industrial Strategies (continued)	
Metal Casting Vision Team	$2,560,297
Materials Preparation, Synthesis, Deposition, Growth or Forming	$1,333,502
Assessment of Fast Shot Transition Point on Filling Patterns and Casting Quality for Pressure Die Castings	122,000
Unconventional Methods for Yield Improvement through Directional Solidification in Steel Castings	200,000
Plasma Refining Process Development	176,000
Heat Transfer at the Mold/Metal Interface in Permanent Mold Casting of Aluminum Alloys	155,921
Clean Cast Steel: 1) Flow of Steel in Gating Systems; 2) Control Ladle Temperature	220,000
Thin Section Steel Castings	88,581
Clean Metal Processing (Aluminum)	169,000
Advanced Lost Foam Casting Technology	202,000
Materials Properties, Behavior, Characterization or Testing	$1,053,185
High Speed Milling and Pulsed ECM	126,000
Design Parameters for Lead Free Copper-Based Engineering Alloys in Permanent Molds	88,000
Process Parameters for Lead-Free Copper-Based Engineering Alloys in Permanent Molds	61,000
Impurity Limits in Aluminum Bronzes	57,000
Characterization of and Procedures to Eliminate Macro-Inclusion During Foundry Processing	43,000
Determination of Residual Stress and Softening Effects on the Life of Die Casting Dies	108,000
Development of Database Design Rules for Cast, High Alloy Steel Components	79,000
Semi-solid Metals Processing Consortium	54,000
Mechanical Properties Structure Correlation for Commercial Specifications of Cast Particulate Metal Matrix Components	46,000
Mechanical Properties of Squeeze and Semi-solid Cast A356	46,000
Ferrite Measurements in Duplex Stainless Steel Castings	50,000
Technology for the Production of Clean, Thin Wall, Machinable Gray and Ductile Iron Castings	201,853
Relationship Between Casting Distortion, Mold Filling and Interfacial Heat Transfer in Sand Molds	93,332
Device or Component Fabrication, Behavior or Testing	$ 173,610
Intelligent Control of the Cupola Furnace	173,610

OFFICE OF INDUSTRIAL TECHNOLOGIES (Continued)

	FY 1997
Office of Crosscut Technologies	$22,199,196
Advanced Turbine System (ATS) Program	$ 7,350,000
Device or Component Fabrication, Behavior or Testing	$ 4,000,000
Ceramic Components for Stationary Gas Turbines in Cogeneration Service	4,000,000
Materials Properties, Behavior, Characterization or Testing	$ 350,000
Long-Term Testing of Ceramic Components for Stationary Gas Turbines	350,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 3,000,000
ATS Materials Base Technology Support	3,000,000
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	$ 5,793,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 3,302,000
Intermetallic Alloy Development and Technology Transfer of Intermetallic Alloys	515,000
Development of Weldable, Corrosion Resistant Iron-Aluminide Alloys	290,000
Composites and Coatings Through Reactive Metal Infiltration	443,000
Conducting Polymers: Synthesis and Industrial Applications	250,000
Membrane Systems for Efficient Separation of Light Gases	309,000
Microwave and Plasma Processing	275,000
Uniform Droplet Processing	440,000
Advanced Materials/Processes	780,000
Materials Properties, Behavior, Characterization or Testing	$ 1,375,000
Materials for Recovery Boilers	940,000
Metals Processing Laboratory User (MPLUS) Center	435,000
Device or Component Fabrication, Behavior or Testing	$ 610,000
Gel Casting Technology	110,000
Microwave Joining of SiC	110,000
Selective Inorganic Thin Films	350,000
High Temperature Particle Filtration Technology	40,000

OFFICE OF INDUSTRIAL TECHNOLOGIES (Continued)

	FY 1997
Office of Crosscut Technologies (continued)	
Advanced Industrial Materials (AIM) Program (continued)	
Materials Structure and Composition	$506,000
Metallic and Intermetallic Bonded Ceramic Composites	165,000
Processing of Polymers in a Magnetic Field	341,000
Combustion/Heat Exchanger Program	$656,196
Materials Properties, Behavior, Characterization or Testing	$630,000
Advanced Heat Exchanger Material Technology Development	630,000
Device or Component Fabrication, Behavior or Testing	$ 26,196
High Pressure Heat Exchanger System (HiPHES) Energy Production	0
High Pressure Heat Exchanger System (HiPHES) for Ethylene Production	26,196

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 the Industries of the Future: chemicals, forest products, steel, aluminum, metalcasting and glass. These industries account for over half of all manufacturing energy use and account for 75 to 90 percent of most manufacturing wastes.

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 (specific) 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 Hank Kenchington, (202) 586-1878

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

6. **ALUMINUM BRIDGE DECK SYSTEM**
   $360,000
   DOE Contact: Sara Dillich, (202) 586-7925
   ORNL Contact: Wayne Hayden, (423) 5746936

The project objective is to develop and refine a bridge deck panel system consisting of aluminum multi-void extrusions joined to make panel sections. The desired results are to renovate deficient bridges and build new bridges throughout the U.S. using the aluminum bridge deck system. The project is being cost-shared under a Cooperative Research and Development Agreement between Reynolds Metals Company, Inc. and Oak Ridge National Laboratory (ORNL). The experimental plan has been established and ORNL is conducting work related to panel welding and NDE procedures, alternative welding procedures for onsite repairs, fatigue characterization of mechanically fastened aluminum joints, wear testing of composite paving surfaces, and environmental fatigue characterization of composite paving surfaces.

Keywords: Aluminum, Bridge Decks, Extrusions

7. **INLINE SENSORS FOR ELECTROLYTIC ALUMINUM CELLS**
   $254,000
   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

8. **DETECTION AND REMOVAL OF MOLTEN SALTS FROM MOLTEN ALUMINUM**
   $294,000
   DOE Contact: Sara Dillich, (202) 586-7925

In a one-year effort beginning in September 1997, Selee Corporation and Alcoa Technical Center will conduct a program to detect and reduce chloride salts in molten aluminum. Selee Corporation has invented a simple electrical probe that senses the presence of salts in molten aluminum. Although consistent results have been seen in laboratory and plant tests, this salt detector needs to be calibrated. That is, its response must be correlated to the specific level of salts in the metal so that the response can be accurately interpreted. Selee has also invented a filter which selectively removes liquid salts from the liquid metal. This has been demonstrated in laboratory tests, but tests in real casting conditions must be carried out to determine efficiency and capacity of the filter. Using the experimental casting facility at the Alcoa Technical Center, these two devices will be exposed to various levels of chlorine and metal flow rates using commercial alloys. The response of the probe will be correlated with chlorine levels over a wide range of conditions. At the same time, the efficiency of the salt filter will be assessed. By monitoring the efficiency of the filter as a function of chlorine and time in casting, the adsorptive capacity of filter media can be determined. The goal of this project is to develop and demonstrate the technology at commercial-scale in one year. Commercial implementation by the domestic aluminum industry should be realized soon after, probably within another year.

Keywords: Molten Aluminum, Salts, Filter, Probe

9. **HIGH-EFFICIENCY, HIGH-CAPACITY, LOW-NO_X ALUMINUM MELTING USING OXYGEN-ENHANCED COMBUSTION**
   $527,000
   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. 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. 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.

Keywords: Aluminum Melting, Combustion, Burner

10. **TECHNOLOGY FOR CONVERTING SPL TO USEFUL GLASS FIBER PRODUCTS**
    $500,000
    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:

1. 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
2. Pilot-scale SPL vitrification test to produce glass fibers
3. Testing and analysis of the fibers from the pilot-scale test with respect to commercial quality specifications
4. Testing and analysis of fibers with respect to human health considerations
5. Sampling and analysis of flue gas from the pilot-scale CMS™ during testing
6. Preliminary design of a commercial-scale air pollution system for aluminum fluoride production.

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

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

11. 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 understanding of entrapment of heat transfer over submerged coated and uncoated surfaces. Partners have 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, will be 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. The initial coping assessment and the preliminary testing to verify the project's approach and direction have been completed. In addition, feedback has been provided to industry testing programs. Suppression capability data for various coatings with different curing times and their application criteria has been obtained, as well as the suppression capability data for various coatings based on the evolution of non-condensable gases and wettability.

Keywords: Explosions, Molten Aluminum, Water

12. INNOVATIVE VERTICAL FLOATATION MELTER

$300,000
DOE Contact: Ramesh Jain, (202) 586-2381

The vertical floatation melter (VFM) is being developed by Energy Research Company, Gillespe and Powers, IMCO, and Stein, Atkinson and Stordy with support from the Office of Industrial Technologies. 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.

Keywords: Floatation Melter, Aluminum Scrap

13. ALUMINUM PILOT CELL

$570,000
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

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

14. RECYCLING ALUMINUM SALT CAKE

$500,000
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 NMP is critical for cost-effective salt cake recycling. Impurities constitute about 10 percent of NMP and lower its market value. Research is investigating hydrometallurgical processes to purify NMP, since higher NMP purity results in higher market value for refractory aggregate and other potential alumina markets. Markets which will require lower development costs, such as alternative alumina units for the blast furnace in ironmaking, are also being explored.

Keywords: Aluminum, Salt Cake, Recycling, Electrodialysis

15. **WETTABLE CERAMIC-BASED DRAINED CATHODE TECHNOLOGY FOR ALUMINUM ELECTROLYSIS CELLS**
$666,000
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:

1. Development and evaluation of candidate TiB_2-carbon materials (tiles and coating)
2. Development and evaluation of proprietary carbon materials
3 Development of the drained cathode design
4. Evaluation of the best candidate materials and the drained cathode design in the 12 kA pilot cell
5. Design and construction of a 70 kA prebake cell retrofitted with a drained cathode using TiB_2-based and or the proprietary materials
6. 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

16. **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

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

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION, OR TESTING

17. **CORROSIVITY MONITORING OF KRAFT RECOVERY BOILERS**
$1,084,012
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

STEEL VISION TEAM – The DOE Steel team leader is Scott Richlen, (202) 586 - 2078

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

18. **INTERMETALLIC ALLOY DEVELOPMENT RELATED TO THE STEEL INDUSTRY**
    $455,000
    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 higher strength of intermetallic alloys including nickel aluminides (Ni_3Al) to Steel industry related manufacturing applications. Progress in bringing technologies to development and commercialization in FY 1997 focused on furnace transfer rolls for use in the heat treating of steel slabs: 1) Two types of furnace roll designs have been fabricated and are being tested at Bethlehem Steel; both types utilize a welded connection between a trunnian and a roll body, 2) Technology for joining thick sections of Ni_3Al to dissimilar metals was developed, and two rolls are being tested utilizing HK or HP steel trunnians welded to Ni_3Al roll bodies, 3) After working with various companies on materials and process development of Ni_3Al two companies have been licensed, including Alloy Engineering and Casting Company, Sandusky International to produce Ni_3Al materials and components.

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

19. **CHEMICAL VAPOR DEPOSITION CERAMIC SYNTHESIS**
    $364,000 (funded by the OIT Glass Vision team)
    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. The objective of this project is to use the unique diagnostic and modeling capabilities at the Sandia National Laboratories - California to understand and develop new techniques for chemical vapor deposition (CVD). A research reactor, originally constructed with DOE-OIT funding, is being used to determine identities and amounts of gaseous phase species present during CVD. Research efforts are focused on development of CVD processes for oxide fiber-preforms and plate glass surfaces for the improvement of properties. In FY1997 a CRADA was developed with Libby- Owens-Ford Co. on developing new CVD techniques for depositing coatings on glass. With respect to this project: (1) a database was developed of thermodynamic properties for the deposition of coatings on glass, (2) experimental techniques were developed for identifying reactions of the glass-coating precursors, and (3) the kinetics of several reactions were measured. In the task on composite and the fiber coating efforts: (1) an analytical model was completed to predict deposition of coatings on ceramic fiber preforms, and (2) a model to quantitatively predict boron nitride coating rates in chemical reactors was optimized.

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

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

20. **DEVELOPMENT OF IMPROVED REFRACTORIES**
$364,000
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, and steel or aluminum smelting and melting vessels are lined with refractories. The goal of this project is to develop improved refractories and to determine critical mechanical and thermophysical and mechanical properties. In FY 1997, work was focused on determining high temperature creep and corrosion behavior of refractories for use in oxifuel fired glass making furnaces. 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 Thermophysical, Properties, Corrosion

21. **SYNTHESIS AND DESIGN OF $MOSI_2$ INTERMETALLIC MATERIALS**
$500,000
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 $MoSi_2$-based composites that will combine good room temperature fracture toughness with excellent oxidation resistance and high-temperature strength for industrial applications. Activities in FY 1997 included various major tasks. A CRADA with Johns Manville Corporation on the use of $MoSi_2$ for glass industry applications is continuing. The corrosion behavior of $MoSi_2$ materials in molten fiberglass has been initially evaluated, and is similar to AZS refractory. Maximum corrosion rates occur at the glass-air interface. Efforts have been initiated with IGT to test $MoSi_2$ materials in a gas radiant tube environment. This will be a 500 hour test at 1800°F under gas combustion conditions.

Keywords: Composites, Intermetallics, Molydisilicides, Coatings

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

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

22. **ASSESSMENT OF FAST SHOT TRANSITION POINT ON FILLING PATTERNS AND CASTING QUALITY FOR PRESSURE DIE CASTINGS**
$122,000
DOE Contact: Toni Maréchaux, (202) 586-8501
Principal Investigator: Jerald Brevick, Ohio State University (614) 292-0177

The objective of this project is to evaluate common approaches to cavity filling, compare the results of current software metal flow models with fluid flow observed on high-speed video, and compare the location, size and total volume of contained gas porosity.

Keywords: Metalcasting, Metal Flow

23. **UNCONVENTIONAL METHODS FOR YIELD IMPROVEMENT THROUGH DIRECTIONAL SOLIDIFICATION IN STEEL CASTINGS**
$200,000
DOE Contact: Toni Maréchaux, (202) 586-8501
Principal Investigator: Christoph Beckermann, University of Iowa, (319) 335-5681

This project is designed to increase yield through the use of solidification software to simulate imposed thermal gradients and evaluate their effect on yield.

Keywords: Metalcasting, Metal Flow

24. **PLASMA REFINING PROCESS DEVELOPMENT**
$176,000
DOE Contact: Toni Maréchaux, (202) 586-8501
Principal Investigator: Carl Lundin, University of Tennessee, (423) 974-5310

The objective of this project is to improve the weldability and corrosion resistance of high alloy castings; to demonstrate reductive alloying in a plasma furnace to minimize oxidation losses of chromium and other elements; and to decarburize stainless steels efficiently.

Keywords: Metalcasting, Corrosion, Welding, Stainless Steel

25. **HEAT TRANSFER AT THE MOLD/METAL INTERFACE IN PERMANENT MOLD CASTING OF ALUMINUM ALLOYS**
$155,921
DOE Contact: Toni Maréchaux, (202) 586-8501
Principal Investigator: Robert Pehlke, University of Michigan, (313) 764-7489

The objective of this project is to achieve enhanced dimensional control in permanent mold castings, decreased cycle time and accurate control of heat transfer. It is designed to increase die life and enable thinner section sizes.

Keywords: Metalcasting, Aluminum, Permanent Mold Casting

26. **CLEAN CAST STEEL: 1) FLOW OF STEEL IN GATING SYSTEMS; 2) CONTROL LADLE TEMPERATURE**
$220,000
DOE Contact: Toni Maréchaux, (202) 586-8501
Principal Investigator: Charles Bates, University of Alabama - Birmingham, (205) 975-8011

The objective of this project is: (1) to evaluate the effect of the flow of steel in gatings systems on steel casting quality; (2) to evaluate the effect of ladle temperature homogenization on steel casting quality.

Keywords: Metalcasting, Steel, Gatings

27. **THIN SECTION STEEL CASTINGS**
$88,581
DOE Contact: Toni Maréchaux, (202) 586-8501
Principal Investigator: Robert C. Voigt, Pennsylvania State University, (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.

Keywords: Metalcasting, Steel

28. **CLEAN METAL PROCESSING (ALUMINUM)**
$169,000
DOE Contact: Toni Maréchaux, (202) 586-8501
Principal Investigator: Diran Apelian, Worcester Polytechnic Institute, (508) 831-5992

The objective of this project is to investigate and develop implementable metal cleanliness assessment methods, melt contamination avoidance, and augmentation of the fundamental knowledge base of phase separation technology.

Keywords: Metalcasting, Aluminum, Phase Separation

29. **ADVANCED LOST FOAM CASTING TECHNOLOGY**
$202,000
Principal Investigator: Charles Bates, University of Alabama - Birmingham, (205) 975-8011

The objective of this project is to perform research to advance the theory and application of lost foam casting including: making castings under vacuum; to extend the technology to allow bronze and steel alloy casting; coating improvements; and flow, fill and solidification experiments.

Keywords: Metalcasting, Lost Foam Casting

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION, OR TESTING

30. **HIGH SPEED MILLING AND PULSED ECM**
$126,000
DOE Contact: Toni Maréchaux, (202) 586-8501
Principal Investigator: Taylan Altan, Ohio State University

The objective of this project is to determine the influence of HSM and PECM on residual stresses in the die surface and its resistance to thermal fatigue and to develop guidelines for machining H-13 at a fully heat treated state. This will test the findings and determine time and cost savings.

Keywords: Metalcasting, Residual Stress, Machining

31. **DESIGN PARAMETERS FOR LEAD FREE COPPER-BASED ENGINEERING ALLOYS IN PERMANENT MOLDS**
$88,000
DOE Contact: Toni Maréchaux, (202) 586-8501
Principal Investigator: Yemi Fasoyinu, Materials Technology Laboratory, (613) 996-0325

The three year project objectives are to: determine the tensile, fracture toughness, impact and fatigue properties of 12 copper-base alloys for use in more demanding engineering applications; determine the dry and lubricating sliding wear and slurry wear resistance; carry out corrosion studies (salt spray, atmospheric and marine); and determine pattern makers shrinkage and metal core taper allowance in permanent mold.

Keywords: Metalcasting, Copper Alloys, Corrosion

32. **PROCESS PARAMETERS FOR LEAD-FREE COPPER-BASED ENGINEERING ALLOYS IN PERMANENT MOLDS**
$61,000
DOE Contact: Toni Maréchaux, (202) 586-8501
Principal Investigator: Kumar Sadayappan, Materials Technology Laboratory, (613) 992-0741

The objective of this project is to develop process parameters such as evaluation of mold materials, improvement in casting fluidity, and grain refinement; to perform water and computer modeling to explain mold filling and to evaluate high phosphorous lead-free brass for plumbing applications.

Keywords: Metalcasting, Copper Alloys, Metal Flow

33. **IMPURITY LIMITS IN ALUMINUM BRONZES**
$57,000
DOE Contact: Toni Maréchaux, (202) 586-8501
Principal Investigator: Yemi Fasoyinu, Materials Technology Laboratory, (613) 992-5475

The objective of this project is to study the effect of impurity elements on the mechanical properties, weldability and heat treatment of two common aluminum bronze alloys C95800 and C95400. The impurity elements are Pb, Zn, Sn, Bi, Se, Si,Cr and Be. These will be added as single elements, and in two element and three element combinations.

Keywords: Metalcasting, Bronze, Mechanical Properties

34. **CHARACTERIZATION OF AND PROCEDURES TO ELIMINATE MACRO-INCLUSION DURING FOUNDRY PROCESSING**
$43,000
DOE Contact: Toni Maréchaux, (202) 586-8501
Principal Investigator: Alan Cramb, Carnegie Mellon University, (412) 268-3517

An inclusions atlas has been developed along with a set of standards to evaluate the cleanliness of steel castings. The atlas has been made available on the world wide web.

Keywords: Metalcasting, Steel, Macro-inclusions

35. **DETERMINATION OF RESIDUAL STRESS AND SOFTENING EFFECTS ON THE LIFE OF DIE CASTING DIES**
$108,000
DOE Contact: Toni Maréchaux, (202) 586-8501
Principal Investigator: Jack Wallace, Case Western Reserve University, (216) 368-4222

The objective of this project is to evaluate measurement methods and develop ways of reducing losses in die life caused by softening of the steel and build-up of residual stress.

Keywords: Metalcasting, Residual Stress, Die Casting

36. **DEVELOPMENT OF DATABASE DESIGN RULES FOR CAST, HIGH ALLOY STEEL COMPONENTS**
$79,000
DOE Contact: Toni Maréchaux, (202) 586-8501\
Principal Investigator: Martin Prager, Materials Properties Council, (215) 705-7694

The objective of this project is to develop design data, screening tests and an atlas of micrographs.

Keywords: Metalcasting, Steel, Design Rules

37. **SEMI-SOLID METALS PROCESSING CONSORTIUM**
$54,000
DOE Contact: Toni Maréchaux, (202) 586-8501
Principal Investigator: Diran Apelian, Worcester Polytechnic Institute, (508) 831-5992

The objective of this project is to characterize semi-solid materials from a microstructure and rheology point of view, to better understand thixotropic flow behavior, and to develop new and enhanced alloys.

Keywords: Metalcasting, Semi-Solid, Rheology

38. **MECHANICAL PROPERTIES STRUCTURE CORRELATION FOR COMMERCIAL SPECIFICATION OF CAST PARTICULATE METAL MATRIX COMPONENTS**
$46,000
DOE Contact: Toni Maréchaux, (202) 586-8501
Principal Investigator: Pradeep Rohadgi, University of Wisconsin - Milwaukee, (414) 229-4987

The objective of this project is to establish procedures for mechanical testing and structural characterization and to provide comparative data and composites for quality assurance.

Keywords: Metalcasting, Metal Matrix Composite, Mechanical Testing

39. **MECHANICAL PROPERTIES OF SQUEEZE AND SEMI-SOLID CAST A356**
$46,000
DOE Contact: Toni Maréchaux, (202) 586-8501
Principal Investigator: Robert Aikin, Case Western Reserve University, (216) 368-4221

The objective of this project is to develop a mechanical properties database for A356 castings produced by the processes of squeeze casting and semi-solid casting.

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

40. **FERRITE MEASUREMENTS IN DUPLEX STAINLESS STEEL CASTINGS**
$50,000
DOE Contact: Toni Maréchaux, (202) 586-8501
Principal Investigator: Carl Lundin, University of Tennessee, (423) 974-5310

The objective of this project is to develop suitable methods for non-destructively measuring ferrite amounts for the surface of castings.

Keywords: Metalcasting, Non-destructive Evaluation, Stainless Steel

41. **TECHNOLOGY FOR THE PRODUCTION OF CLEAN, THIN WALL, MACHINABLE GRAY AND DUCTILE IRON CASTINGS**
$201,853
DOE Contact: Toni Maréchaux, (202) 586-8501
Principal Investigator: Charles Bates, University of Alabama - Birmingham, (205) 975-8011

This project will focus on identifying the phases and compounds which degrade properties and machinability. It will then determine methods for eliminating objectionable inclusions.

Keywords: Metalcasting, Gray Iron, Cast Iron, Inclusions

42. **RELATIONSHIP BETWEEN CASTING DISTORTION, MOLD FILLING AND INTERFACIAL HEAT TRANSFER IN SAND MOLDS**
$93,332
DOE Contact: Toni Maréchaux, (202) 586-8501
Principal Investigator: Thomas Piwonka, University of Alabama - Tuscaloosa, (205) 348-1589

The objective of this project is to determine the effect of interfacial heat transfer coefficients and gap formation in iron and aluminum sand mold castings on casting dimensional accuracy.

Keywords: Metalcasting, Iron, Aluminum, Sand Mold

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

43. **INTELLIGENT CONTROL OF THE CUPOLA FURNACE**
$173,610
DOE Contact: Toni Maréchaux, (202) 586-8501
Principal Investigator: Kevin Moore, Idaho State University, (208) 236-4188

The objective of this project is to develop a controller for the cupola process using intelligent and conventional control methods.

Keywords: Metalcasting, Cupola, Intelligent Control

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 Program (ATS), Continuous Fiber Ceramic Composites (CFCC) Program, Advanced Industrial Materials (AIM) Program and the Combustion (Heat Exchanger) 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% increase) and environmental performance (80% reduction in emissions) of gas turbines while reducing the cost of electricity by 10%. The DOE program manager is Patricia Hoffman, (202) 586-6074.

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

44. **CERAMIC COMPONENTS FOR STATIONARY GAS TURBINES IN COGENERATION SERVICE**
    $4,000,000
    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 ceramic blades, first stage ceramic nozzles and ceramic composite combustor liners. This project will design and test these components for a stationary 4.0 Mw gas turbine for cogeneration service. The project will culminate in a 4000-hour field demonstration of the engine.

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

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

45. **LONG-TERM TESTING OF CERAMIC COMPONENTS FOR STATIONARY GAS TURBINES**
    $350,000
    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

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

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

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

Keywords: Gas Turbines, Castings, Thermal Barrier Coatings

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 six industrial teams developing more than 20 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

47. 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 Dow Corning, Du Pont Lanxide Composites, Amercom, General Electric, McDermott Technologies, and Textron.

Keywords: Ceramic Composites, Continuous Fiber

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

48. 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 initiative and of crosscutting industries including carbon products, forging, heat treating, and welding. Efforts in FY 1996 were focused on partnerships between industry and the National Laboratories for commercialization of new materials and processes. The program manager is Charles A. Sorrell, (202) 586-1514.

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

49. INTERMETALLIC ALLOY DEVELOPMENT AND TECHNOLOGY TRANSFER OF INTERMETALLIC ALLOYS
$515,000
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 1997 included: (1) research on Ni_3Al welding technology applicable to, for example, furnace transfer rolls, obtaining materials properties of intermetallic and metallic alloys, modeling of stresses in structural components, continuation of exposure of furnace fixtures in continuous carburization heat treating furnaces (continue to show exceptional corrosion resistance), (2) evaluating technology for joining thick sections of Ni_3Al to dissimilar metals, (3) testing components in various chemical industry processes, (4) completion of the CRADA with GM Saginaw on the development of Ni_3Al for heat treating fixtures, and (5) licensed two companies, including Alloy Engineering and Casting Company, Sandusky International, to produce Ni_3Al materials and components.

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

50. DEVELOPMENT OF WELDABLE, CORROSION RESISTANT IRON-ALUMINIDE ALLOYS
$290,000
DOE Contact: Charles A. Sorrell, (202) 586-1514
ORNL Contact: P. J. Maziasz, (423) 574-5082
Univ. of Cincinnati Contacts: A. Jordan and O. N. C. Uwakweh (513) 556-3108

The objectives of this project are to develop FeAl alloys with improved weldability and mechanical and corrosion properties for use in structural applications; and to develop the potential for weldable FeAl alloys for use in weld-overlay cladding applications. Several developments were made in FY 1997. New industrial tests of cast FeAl alloys showed superior oxidation resistance in air + 5% water vapor at 1100 C up to 500 h, surprising caburization resistance in both oxidizing (H_2 5.5% CH_4 - 4.5% CO_2) and reducing (H_2 - 1% CH_4) atmospheres, and the expected outstanding sulfidation resistance at

816°C. Testing of the material in various applications is continuing (neutral salt heat treating baths for steels, and molten carbonate salt environments for fuel cells). Cast grate bars and pallet tips used in an industrial calcination furnace continue to show oxidation/sulfidation resistance. Crack-free welds were successfully made on hot-extrusion (fine grained ingot)-produced FeAl alloys with no pre heat or post heat. For the first time, crack free autogenous welds were also made on cast FeAl alloys with pre and post-heat.

Keywords: Iron Aluminides, Coatings, Claddings, Thermophysical Properties

51. **COMPOSITES AND COATINGS THROUGH REACTIVE METAL INFILTRATION**
$443,000
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 1997 a detailed mechanistic model was developed for composite formation that explains the observed microstructure and kinetics as a function of time and temperature. This new model has led to a process diagram showing the conditions where reactive metal penetration (RMP) is a practical process. The process has also been used to optimize composites of AL_2O_3-$MoSi_2$, Al_2O_3-$Mo(Si_{0.93}Al_{1.43})$, and Al_2O_3-$Mo(Si_{0.93}Al_{1.43})$-Mo_3Al_8 families, and then evaluating their properties.

The effort on coating technology at Stanford University emphasized Al coatings on steel. Coupon specimens exhibited excellent corrosion resistance in 1000 hr salt spray.

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

52. **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 1997, 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 1997, operation of a chlor-alkai cell at target cell operating conditions was demonstrated. The system used an oxygen cathode and a commercial chlor-alkali membrane of high current efficiency (>95%).

Keywords: Electrically Conducting Polymers, Gas Separation, Capacitors

53. **MEMBRANE SYSTEMS FOR EFFICIENT SEPARATION OF LIGHT GASES**
$309,000
DOE Contact: Charles A. Sorrell, (202) 586-1514
Los Alamos National Laboratory Contact:
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 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, a method for developing carbon pores for capillary condensation of hydrocarbons was devised. The use of oblique angle sputter techniques to develop thin films with controlled pore size has been demonstrated. Separation of butane gases form streams containing methane, argon, and hydrogen has been demonstrated. The effort will continue in FY 1998 as a CRADA with Amoco.

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

54. **MICROWAVE AND PLASMA PROCESSING**
$275,000
DOE Contact: Charles A. Sorrell, (202) 586-1514
Los Alamos National Laboratory Contact:
M. Trkula, (505) 667-0591

The project focuses on developing coating technologies to obtain erosion, and corrosion resistant, thermodynamically 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 1997, initial thin film AlN, and amorphous B_4C were successfully deposited on steel. Characterization included coating thickness, composition, mechanical and tribological properties.

Keywords: Coatings, Chemical Vapor Deposition, Ion Processing, Erosion, Corrosion

55. **UNIFORM DROPLET PROCESSING**
$440,000
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 1997, (1) a system able to operate at temperatures up to 1500 C was assembled and initial testing begun, (2) additional materials wee produced on the intermediate temperature system (1250°C) (including copper and bronze), and 3) a license of the technology was taken by Uniform Metals Technology for production of copper and bronze uniform droplet materials for filter applications in chemical systems.

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

56. **ADVANCED MATERIALS/PROCESSES**
$780,000
DOE Contact: Charles A. Sorrell, (202) 586-1514
ORNL Contact: P. Angelini, (423) 574-4459,
P. S. Sklad, (423) 574-5069, and C. T Liu, (423) 574-4459

The goals of this project are to develop new and improved materials. Many metallic and ordered intermetallic alloys possess unique properties and have the potential to be developed as new materials for energy related applications. In FY 1997, (1) evaluated the parallelization of a casting program in order to provide capability for increased throughput and more realistic analyses, (2) developed infra-red technology for depositing coatings, surfacing and heating substrate materials, (3) developed initial corrosion resistant Iron-Chromium-Silicon alloys which are applicable in various glass industry applications, (4) determined the initial weldability of Ni_3Si and made significant compositional changes to the alloy.

Keywords: Intermetallics, Ordered Alloys, TiAl, Ni_3Al, Ni_3Si, Metalcasting, Glass, Alloys

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

57. **MATERIALS FOR RECOVERY BOILERS**
$940,000
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 from pulp and paper companies, boiler manufacturers and composite tube manufacturers, (2) to determine residual stresses in new and used composite tubes and microstructural characteristics of tubes as related to stresses and failure mechanisms, and (3) to develop new materials and/or fabrication methods for improvements in boiler efficiency, service life, and safety. Participants include Oak Ridge National Laboratory, Institute of Paper Science and Technology, and 11 industrial collaborators. In FY 1997: (1) analyses of tube specimens from many mills showed cracks have common characteristics, (2) temperature and strain gauges installed in the floor of a recovery boiler indicate that occasional temperature excursions do occur (10 to 200°C above normal operating temperature), (3) extended and verified a model showing stress in tubes versus materials properties and boiler operating conditions (developed a response surface indicating that alloy 825 and 625 may be more optimum alloys for use as cladding), (4) laboratory stress corrosion results (focusing on boiler conditions during start-up or cool-down) identified various conditions under which currently used cladding of 304L would crack, and (5) the research received the Best Paper Award for 1996 from the Technical Association of the Pulp and Paper Industry (TAPPI).

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

58. **METALS PROCESSING LABORATORY USER (MPLUS) CENTER**
    $435,000 (includes $50K from OIT Glass Vision team)
    DOE Contact: Charles A. Sorrell, (202) 586-1514
    Oak Ridge National Laboratory Contact:
    M. Mackiewicz-Ludtka, (423) 576-4652 and
    H. W. Hayden, (423) 574-6936

The Metals Processing Laboratory User (MPLUS) Center was officially designated as a DOE User Facility in February, 1996. Its primary purpose is to assist U.S. industry and academia in improving energy efficiency and enhancing U.S. competitiveness. MPLUS is designed to provide U.S. Industries with access to the specialized technical expertise and capabilities to solve metals-processing issues that limit the development and implementation of emerging materials and materials processing technologies. MPLUS includes the following primary user centers: Metals Processing, Metal Joining, Metals Characterization and Metals Process Modeling. As of September 30, 1997, a total of 76 MPLUS Proposals were received from 60 companies and universities representing 26 states. Twelve organizations submitted 2 or more proposals for different projects. Of the 76 proposals, 53 were reviewed, and 31 of these 53 User projects were initiated. Ten (10) MPLUS projects were completed, and the 23 proposals were either (a) accepted contingent on legal approval, (b) under development, or c) being modified. A total of 546 user days were logged during FY 1997. Projects crosscut all of the seven industries in the Industries of the Future initiative; other crosscutting industries including forging, heat treating, and welding; and crosscutting programs.

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

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

59. **GEL CASTING TECHNOLOGY**
    $110,000
    DOE Contact: Charles A. Sorrell, (202) 586-1514
    ORNL Contact: M. A. Janney, (423) 576-5183

Gelcasting is an advanced powder forming process. It can be used to form ceramic or metal powders into simple or complex, near net shapes. The sol-gel process is being developed in order to produce aluminum oxide tubes for use in high-intensity industrial lighting, and H13 steel dies. For the lighting application the sol-gel process will produce identical materials at lower temperatures and in far less time than do conventional methods which involve prolonged high temperature sintering with sintering aids. In FY 1997, the effort relative to the CRADA with OSRAM demonstrated: (1) ability to make complex shape optical quality Al_2O_3, (2) ability to use meltable cores in gel casting to make complex hollow shapes. In additional FY 1997 efforts the ability to machine gel cast metal parts was also completed. Technology was developed to gel cast various metal alloys including, H13, 174ph, and nickel superalloys.

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

60. **MICROWAVE JOINING OF SIC**
    $110,000
    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 1997 the effort included: (1) joining of continuous fiber-reinforced (CFCC) SiC/SiC composite and sintered SiC specimens with SiC formed *in situ* from pyrolysis of either polysiloxane (silicone resin) or allyhydridopoly-carbosilane (AHPCS) precursors, (2) determining the maximum shear strength of joints (microwave processing resulted in joints of comparable strength to those processed conventionally, and (3) joining and testing (high temperature strength) 8" long by 1" OD sintered SiC specimens (under the HiPHES project).

Keywords: Microwave Processing, Microwave Joining, SiC, Tubes

61. **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 membranes for light gas separation and use this technology to improve separation efficiencies currently available with polymer membranes, particularly for light alkanes. The approach is to nucleate and crystallize zeothlitic phases from sol-gel derived amorphous coatings, using porous filters and gas membranes as supports for these films. In FY1997 efforts included: (1) initiation of a CRADA with Amoco on the feasibility of using shape selective molecular sieve membranes to enrich p-xylene from mixtures, (2) fabrication of cesium phosphate molecular sieve membranes on porous zinc oxide wafers, (3) production of zinc oxide phosphates with larger pores of the $M_3Zn(PO_4)_3$ structure type, and (4) formation of methylammonium zinc oxide phosphate phase that remains microporous after the water template is removed.

Keywords: Coatings, Sol-Gel Processing

62. **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. 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. The current focus is on filtration technology for the k, dimethyldichlorosilane process. In FY 1997, the CRADA with Dow Corning continued. Modification to laboratory furnaces were made for bench scale testing of filter specimens. A large number of filter specimens was obtained and each filter was tested for 24 h under conditions simulating the chemical environment of interest.

Keywords: High Temperature, Filtration, Chemicals, Compatibility

MATERIALS STRUCTURE AND COMPOSITION

63. **METALLIC AND INTERMETALLIC BONDED CERAMIC COMPOSITES**
$165,000
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 1997 various specimens were tested in a number of environments and a data information package was prepared.

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 FY1997 efforts included: (1) determining carbon content effects of resulting TiC composites and the applicability of producing TiB_2 powders, (2) preparation of TiC powder, and (3) fabrication of specimens at numerous sites and subsequent testing of composite specimens.

Keywords: Ceramics, Composites, Nickel Aluminide, Powder

64. **PROCESSING OF POLYMERS IN A MAGNETIC FIELD**
$341,000
DOE Contact: Charles A. Sorrell, (202) 586-1514
Los Alamos National Laboratory Contacts:
M. E. Smith, (505) 665-6858, and
B. C. Benicewicz, (505) 665-0101

The purpose of this project is to demonstrate the utility of magnetic fields, to beneficially modify or control the physical, optical and electrical properties of materials through the application of magnetic fields during polymerization processing and solidification. Researchers at Los Alamos National Laboratory, in collaboration with an industrial partner, have demonstrated that using high (10-20 Tesla) magnetic fields to orient liquid crystal polymers during processing can lead to substantial improvements in mechanical properties. In FY 1997, (1) successfully produced polymer composite plaques (approximately 8" x 8" x 0.125") of excellent uniformity as determined by visual inspection and mechanical property measurements, (2) demonstrated feasibility of using magnetic fields in the 1 to 2 Tesla range as provided with commercially available magnets, and (3) determined the nature of the molecular packing structures as aligned in the magnetic field by the use of nuclear magnetic resonance spectroscopy.

Keywords: Organic Polymers, Magnetic Processing, Mechanical Properties

COMBUSTION/HEAT EXCHANGER PROGRAM

The goal of the Combustion Program activities is to maximize efficiency and minimize emissions at the lowest practical cost. The program is designed to move superior combustion concepts for the laboratory through industry host site demonstration resulting in commercialization. The DOE program manager is Gideon Varga, (202) 586-0082.

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

65. ADVANCED HEAT EXCHANGER MATERIAL TECHNOLOGY DEVELOPMENT
$630,000
DOE Contact: G. Varga, (202) 586-0082
ORNL Contact: M. Karnitz, (423) 574-5150

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

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

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

66. HIGH PRESSURE HEAT EXCHANGER SYSTEM (HIPHES) ENERGY PRODUCTION
$0
DOE Contact: Gideon Varga, (202) 586-0082
Solar Turbines Contact: B. Harkins, (619) 544-5398

The High Pressure Heat Exchanger System (HiPHES) uses exhaust heat from a hazardous waste incinerator to drive a power turbine. Under this concept, a ceramic heat exchanger replaces the combustor in the gas generator section of a combustion turbine. The testing of a prototype high pressure ceramic heat exchanger for more than 800 hours at 1800°F and 100 psi solved critical issues of joining, system assembly, and repair. This included long term exposure in a dust-laden slip stream of a working hazardous waste incinerator. An optimal system comprises both monolithic ceramics and ceramic matrix composites. Uncertainties in various market forces for waste incineration has postponed a 4 Mw demonstration. The technology has been transferred to DOE's Advanced Turbine Systems (ATS) program.

Keywords: Ceramic Composites, Heat Exchangers, Waste Incineration

67. HIGH PRESSURE HEAT EXCHANGER SYSTEM (HiPHES) FOR ETHYLENE PRODUCTION
$26,196
DOE Contact: Gideon Varga, (202) 586-0082
Stone & Webster Engineering Corp. Contact: Joe Gondolfe, (281) 368-4379

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

Keywords: Structural Ceramics, Ethylene, Heat Exchangers

OFFICE OF TRANSPORTATION TECHNOLOGIES

	FY 1997
Office of Transportation Technologies - Grand Total	$24,249,000
Transportation Materials Technology	$24,249,000
Automotive Materials Technology	$17,483,000
Propulsion Systems Materials	$5,483,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$3,027,000
Gelcasting: Scale-up and Commercialization	550,000
Optimization of Silicon Nitride Ceramics	177,000
in situ Toughened Silicon Nitride	350,000
Gas Turbine Engine Components Manufacturing Scale-Up and Demonstration	1,200,000
Advanced Automation Gelcasting Processes for Silicon Nitride Components	750,000
Materials Properties, Behavior, Characterization or Testing	$1,626,000
Characterization and Life Prediction of Ceramic Recuperator Materials	71,000
Component Verification	275,000
High Frequency Fatigue	250,000
Tensile Stress Rupture Testing	270,000
Toughened Ceramics Life Prediction	200,000
Life Prediction Methodology	0
Environmental Effects in Toughened Ceramics	385,000
Nondestructive Evaluation	175,000
Technology Transfer and Management Coordination	$ 425,000
Technical Project Management	425,000
Device or Component Fabrication, Behavior or Testing	$ 405,000
Corrosion-Resistant Coatings	195,000
Ceramic-Metal Joining	110,000
Mechanical Reliability Assessment of Electronic Ceramics and Electronic Ceramic Components	100,000
Lightweight Vehicle Materials Technology	$12,000,000
Device or Component Fabrication, Behavior or Testing	$12,000,000
Low-Cost High Performance Aluminum Alloy Sheet for Automotive Applications	1,250,000
Low-Cost High Performance Cast Light Metals for Automotive Applications	1,300,000
Advanced Materials and Processes for Automotive Applications	375,000
Northwest Alliance for Transportation Technologies (NATT)	2,500,000
Automotive-Related Graduate Fellowships	350,000
Materials and Processes for Propulsion System Applications	650,000
Technology Assessment and Evaluation	450,000
Glass Reinforced Composite Materials Joining, Durability and Enabling Technologies	1,850,000
Composite Material Design, Manufacturing and Demonstration	1,425,000
USAMP Cooperative Agreement	1,000,000
Carbon Fiber Based Composite Materials Technology	850,000

OFFICE OF TRANSPORTATION TECHNOLOGIES (continued)

	FY 1997
Transportation Materials Technology (continued)	
Electric Drive Vehicle Technologies	$3,397,000
Advanced Battery Program	$2,997,000
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	$1,530,000
Carbon Electrochemistry	250,000
Fabrication and Testing of Carbon Electrodes as Lithium Intercalation Anodes	75,000
Reactivity and Safety Aspects of Carbonaceous Anodes in Lithium-Ion Batteries	140,000
Battery Materials: Structure and Characterization	140,000
Polymer Electrolyte for Ambient Temperature Traction Batteries: Molecular Level Modeling for Conductivity Optimization	145,000
Analysis and Simulation of Electrochemical Systems	235,000
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
Device or Component Fabrication, Behavior or Testing	$ 584,000
Development of a Thin-Film Rechargeable Lithium Battery for Electric Vehicles	71,000
Applied Research on Novel Cell Components for Advanced Capacitors	115,000
Sol-Gel Derived Metal Oxides for Electrochemical Capacitors	123,000
Optimization of Metal Hydride Properties in MH/NiOOH Cells for Electric Vehicle Applications	90,000
Preparation of Improved, Low Cost Metal Hydride Electrodes for Automotive Applications	185,000
Fuel Cell Materials	$ 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

OFFICE OF TRANSPORTATION TECHNOLOGIES (continued)

	FY 1997
Transportation Materials Technology (continued)	
Heavy Vehicle Materials Technology	$3,369,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 998,000
Cost-Effective SRBSN/Microwave Annealing of Silicon Nitride	400,000
Continuous Sintering of Silicon Nitride Ceramics	148,000
Cost-Effective, High-Toughness Silicon Nitride	350,000
Characterization/Testing of Low CTE Materials	100,000
Low CTE Materials/Diesel Exhaust Insulation	0
Low Cost NZP Powder	0
Advanced Manufacturing of Diesel Engine Turborotors	0
Advanced Manufacturing of Ceramic Exhaust Valves for Diesel Engines	0
Insulating Structural Ceramics for High Efficiency, Low Emission Engines	0
Thick Thermal Barrier Coatings (TTBCs) for Low Emissions, High Efficiency Diesel Engine Components	0
Materials for Low Emissions, High Efficiency Diesel Engine Components	0
Materials for Low Emissions, High Efficiency Diesel Engine Components	0
High Strength Materials for Diesel Engine Fuel Injectors	0
Materials Properties, Behavior, Characterization or Testing	$ 770,000
Diesel Exhaust Catalyst Characterization	200,000
Life Prediction Verification	200,000
High Temperature Tensile Testing	250,000
Computed Tomography	120,000
On-Machine Inspection	0
Mechanical Properties of CMZP	0
Technology Transfer and Management Coordination	$1,065,000
Technical Project Management	565,000
International Exchange Agreement (IEA)	200,000
Standard Reference Materials	200,000
Mechanical Property Standardization	100,000
Device or Component Fabrication, Behavior or Testing	$ 536,000
Thick Thermal Barrier Seal Coatings	33,000
Characterization of Machined Ceramics	200,000
Advanced Machining/Manufacturing	223,000
Next-Generation Grinding Wheel	0
High Speed Grinding	0
Laser-Based NDE Methods	80,000
Grinding Machine Stiffness	0
Next Generation Grinding Spindle	0
Process Cost Model	0
Intelligent Grinding Wheel	0

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 **Electric Drive Vehicle Technologies** program. The **Transportation Materials Technologies** program develops: (a) ***Automotive Propulsion System Materials*** to enable advanced propulsion systems for hybrid vehicles, and (b) ***Lightweight Vehicle Materials*** to reduce vehicle weight and thereby decrease fuel consumption. The program seeks to develop advanced materials with the required properties and the processes needed to produce them at the costs and volumes needed by the automotive industries. Improved materials for body, chassis, and power train are critical to attaining the challenging performance standards for advanced automotive vehicles. The DOE contacts are Thomas Sebestyen, (202) 586-9727, for automotive propulsion system materials and Joseph Carpenter, (202) 586-1022, for automotive lightweight vehicle materials. The **Electric Drive Vehicle Technologies** program includes the support of **Advanced Battery Materials R&D** for electric and hybrid vehicle applications. The DOE contact is Ray Sutula, (202) 586-8064. The program also supports **Fuel Cell R&D,** which includes materials for proton-exchange membrane (PEM) fuel cells. 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 SYSTEMS MATERIALS

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

68. **GELCASTING: SCALE-UP AND COMMERCIALIZATION**
$550,000
DOE Contact: T. M. Sebestyen, (202) 586-9727
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 with industrial partners. The project goals include improving the gelcasting chemical system to enhance control of processing parameters and molded part characteristics, and improving gelcasting compositions and machining methods to produce high-precision components with features which are machined in the ceramic body. Surface-preparation techniques and mold-release agents which enhance separation of the part from the mold and which yield high-quality surface finish will also be identified.

Keywords: Silicon Nitride, Ceramics, Gelcasting, Forming

69. **OPTIMIZATION OF SILICON NITRIDE CERAMICS**
$177,000
DOE Contact: T. M. Sebestyen, (202) 586-9727
ORNL Contact: D. P. Stinton, (423) 574-4556
University of Michigan Contact: T. Y. Tien, (313) 764-9449

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

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

70. ***In situ* TOUGHENED SILICON NITRIDE**
$350,000
DOE Contact: T. M. Sebestyen, (202) 586-9727
ORNL Contact: T. N. Tiegs, (423) 574-5173
AlliedSignal Ceramic Components Contact: J. M. Wimmer, (310) 512-3183

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

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

71. **GAS TURBINE ENGINE COMPONENTS MANUFACTURING SCALE-UP AND DEMONSTRATION**
$1,200,000
DOE Contact: T. M. Sebestyen, (202) 586-9727
AlliedSignal Engines Contact: M. L. Easley, (602) 231-4242
AlliedSignal Ceramic Components Contact: J. M. Wimmer, (310) 512-3183
Kyocera Industrial Ceramics Contact: W. D. Carruthers, (360) 750-6215

This project facilitates introduction of monolithic ceramic components in turbine engines and gathering essential and substantial field experience with these engines. The objectives are to: (1) improve the manufacturing processes for ceramic turbine engine components (nozzle vanes and turbine blades/bladed disks) and (2) demonstrate these processes in the production environment.

Keywords: Nozzle Vane, Turbine Blade, Turbine Rotor, Silicon Nitride, Ceramics, Forming, Machining

72. **ADVANCED AUTOMATION GELCASTING PROCESSES FOR SILICON NITRIDE COMPONENTS**
$750,000
DOE Contact: T. M. Sebestyen, (202) 586-9727
ONR Contact: S. G. Fishman, (703) 696-0285
AlliedSignal Ceramic Components Contact:
D. D. Foley, (310) 512-5916

This project is Enhancement #2 of a DARPA/ONR Advanced Materials Partnership Program with the Advanced Structural Ceramics Virtual Company (Cooperative Agreement #N00014-95-2-0006). The objectives of Enhancement #2 are to: (1) custom design and build equipment system capable of automating the gelcasting process, (2) demonstrate capability to produce 500 to 1000 turbine wheels per month for a period of two months and (3) integrate the equipment onto the production floor.

Keywords: Silicon Nitride, Ceramics, Gelcasting, Forming, Automation

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

73. **CHARACTERIZATION AND LIFE PREDICTION OF CERAMIC RECUPERATOR MATERIALS**
$71,000
DOE Contact: T. M. Sebestyen, (202) 586-9727
ORNL Contact: M. K. Ferber, (423) 576-0818
Contact: S. F. Duffy, (330) 678-7328

The purpose of this effort is to characterize the thermomechanical response, define and help establish (in conjunction with researchers at ORNL and design engineers at Teledyne Ryan) the requisite material database, as well as perform life-prediction estimates for Teledyne Ryans' ceramic recuperator. This effort supports the Hybrid Electric Vehicle (HEV) Program.

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

74. **COMPONENT VERIFICATION**
$275,000
DOE Contact: T. M. Sebestyen, (202) 586-9727
ORNL Contact: D. P. Stinton, (423) 574-4556
ORNL Contact: P. F. Becher, (423) 574-5157

The objectives of this effort are to: (1) develop test methodology to measure mechanical properties of ceramics from complex-shaped components (e.g., gas turbine blades, nozzles, and rotors) at elevated temperatures; and (2) generate a mechanical properties database for recuperator thin sheet ceramic composites being developed by Du Pont Lanxide Composites (DLC). The database will be used for the finite element analysis and life prediction of the recuperator components.

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

75. **HIGH FREQUENCY FATIGUE**
$250,000
DOE Contact: T. M. Sebestyen, (202) 586-9727
ORNL Contact: D. P. Stinton, (423) 574-4556
ORNL Contact: K. C. Liu, (423) 574-5116

The objective of this task is to develop the baseline information on tensile and cyclic fatigue behavior of structural ceramics at room and elevated temperatures and at frequencies up to 4 kHz. Material behavior models for design and life evaluation analysis of ceramic components are being developed. A benefit of this task will be a baseline database of candidate ceramic materials for use by ceramic materials manufacturers and ceramic components designers, fabricators, and users.

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

76. **TENSILE STRESS RUPTURE TESTING**
$270,000
DOE Contact: T. M. Sebestyen, (202) 586-9727
ORNL Contact: D. P. Stinton, (423) 574-4556
ORNL Contact: K. C. Liu, (423) 574-5116

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

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

77. **TOUGHENED CERAMICS LIFE PREDICTION**
$200,000
DOE Contact: T. M. Sebestyen, (202) 586-9727
ORNL Contact: D. P. Stinton, (423) 574-4556
NASA - Lewis Research Center Contact:
J. A. Salem, (216) 433-3313

The objective of this research is to develop and verify models and test methods for life prediction of brittle materials such as *in situ* toughened ceramics, glasses, and intermetallics. A reliability model for anisotropic brittle materials such as single-crystal intermetallics and semiconductors has been developed and will be verified.

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

78. **LIFE PREDICTION METHODOLOGY**
$0
DOE Contact: T. M. Sebestyen, (202) 586-9727
ORNL Contact: C. R. Brinkman,
(423) 574-5106
AlliedSignal Engines Contact: N. Menon,
(602) 231-1230

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

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

79. **ENVIRONMENTAL EFFECTS IN TOUGHENED CERAMICS**
$385,000
DOE Contact: T. M. Sebestyen, (202) 586-9727
ORNL Contact: M. K. Ferber, (423) 576-0818
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 materials are being evaluated.

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

80. **NONDESTRUCTIVE EVALUATION**
$175,000
DOE Contact: T. M. Sebestyen, (202) 586-9727
ORNL Contact: D. P. Stinton, (423) 574-4556
ORNL Contact: W. A. Simpson, Jr.,
(423) 574-4421

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

Keywords: NDE, Structural Ceramics, Ultrasonics

TECHNOLOGY TRANSFER AND MANAGEMENT COORDINATION

81. **TECHNICAL PROJECT MANAGEMENT**
$425,000
DOE Contact: T. M. Sebestyen, (202) 586-9727
ORNL Contact: D. P. Stinton, (423) 574-4556

The objective of this effort is to help assess the materials and manufacturing technology needs for advanced automotive propulsion systems, formulate technical plans to meet these needs, and prioritize and implement a long-range research and development program.

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

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

82. **CORROSION-RESISTANT COATINGS**
$195,000
DOE Contact: T. M. Sebestyen, (202) 586-9727
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 and SiC ceramic materials in hostile combustion environments and to assess coating manufacturability which will lead to component demonstration and commercialization.

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

83. **CERAMIC-METAL JOINING**
$110,000
DOE Contact: T. M. Sebestyen, (202) 586-9727
ORNL Contact: D.P. Stinton, (423) 574-4556
ORNL Contact: M. L. Santella, (423) 574-4805

The objective of this task is to develop a technology for producing strong, reliable joints between two ceramic subassemblies and between a ceramic and a metallic subassembly. Experiments are being done to identify and understand the effects of chemical reactions that occur during active metal brazing on the mechanical properties of silicon nitride.

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

84. **MECHANICAL RELIABILITY ASSESSMENT OF ELECTRONIC CERAMICS AND ELECTRONIC CERAMIC COMPONENTS**
$100,000
DOE Contact: T. M. Sebestyen, (202) 586-9727
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, Reliability

LIGHTWEIGHT VEHICLE MATERIALS TECHNOLOGY

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

85. **LOW-COST HIGH PERFORMANCE ALUMINUM ALLOY SHEET FOR AUTOMOTIVE APPLICATIONS**
$1,250,000
DOE Contact: Joseph Carpenter, (202) 586-1022
ORNL Contact: Phil Sklad, (423) 574-5069
Laboratory Partners: ORNL, LANL, INEEL, PNNL
Industry Partners: Reynolds Metals Company, American Society of Mechanical Engineers (ASME), Commonwealth Aluminum, ARCO Aluminum, Ravenswood Aluminum

The objectives of this effort are: 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; and todemonstrate advanced aluminum alloys and forming process for the manufacture of sheet aluminum components.

Keywords: Aluminum, Sheet Forming, Extrusion, Automotive

86. **LOW-COST HIGH PERFORMANCE CAST LIGHT METALS FOR AUTOMOTIVE APPLICATIONS**
$1,300,000
DOE Contact: Joseph Carpenter, (202) 586-1022
ORNL Contact: Phil Sklad, (423) 574-5069
Laboratory Partners: LLNL, ORNL, SNL, INEEL, PNNL, ANL
Industry Partners: USAMP (Ford, GM, Chrysler), LEP (Ford, GM, Chrysler)

The objectives of this effort are: to optimize design knowledge and improve product capability for light-weight, high-strength, cast structural components; to develop a 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; and to improve the energy efficiency and cost effectiveness of large-scale automotive aluminum die castings by extending die life and reducing die wear.

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

87. **ADVANCED MATERIALS AND PROCESSES FOR AUTOMOTIVE APPLICATIONS**
$375,000
DOE Contact: Joseph Carpenter, (202) 586-1022
ORNL Contact: Phil Sklad, (423) 574-5069
Laboratory Partners: Ames Laboratory, ORNL
University Partners: University of Wisconsin-Milwaukee
Industry Partners: USAMP (Ford, GM, Chrysler), The Electric Power Research Institute (EPRI)

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; and 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.

Keywords: Metal Matrix Composites, Powder Metallurgy, Aluminum, Particle Reinforced Aluminum

88. **NORTHWEST ALLIANCE FOR TRANSPORTATION TECHNOLOGIES (NATT)**
$2,500,000
DOE Contact: Joseph Carpenter, (202) 586-1022
PNNL Contact: Gary McVay, (509) 375-3762
Laboratory Partners: PNNL, Albany Research Center
Industry Partners: Alcoa, Reynolds, MC-21

NATT is a PNNL initiative comprised of multiple regional industrial sectors brought together to improve U.S. industrial technologies. The principal focus is the development of technologies to achieve the 50 percent weight reduction required to meet PNGV's objectives. NATT partners will use their resources to design new lightweight metals shaping and connecting, and to lower material costs. Some specific objectives of this effort are: to lower the cost of titanium and demonstrate the feasibility of manufacturing a cost-competitive/ performance enhanced product; to develop an alternative molten salt electrolyte to be used in the low-cost electrowinning of primary magnesium metal; to develop and optimize tailored aluminum blank fabrication and forming characteristics for high-volume, low-cost automotive panels and structures; 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 and an efficient and economical machining process for finishing Al-MMC castings; and to develop efficient, cost competitive technologies for sorting shredded aluminum automotive scrap.

Keywords: Titanium, Aluminum, Magnesium, Tailor Welded Blanks, Scrap Sorting, Metal Matrix Composite

89. **AUTOMOTIVE-RELATED GRADUATE FELLOWSHIPS**
$350,000
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: Graduate Fellowship, Lightweight Materials, Automotive Applications, Characterization Technique

90. **MATERIALS AND PROCESSES FOR PROPULSION SYSTEM APPLICATIONS**
$650,000
DOE Contact: Joseph Carpenter, (202) 586-1022
ORNL Contact: Phil Sklad, (423) 574-5069
Laboratory Partners: ORNL, SNL, LBNL
Industry Partners: USAMP (Ford, GM, and Chrysler), National Center for Machining Sciences

The objective of these efforts are: to develop a multi-physics computational model of the induction heating and hardening process in order 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; to develop a model and methodology, based on finite element techniques, that predicts changes in the size and shape of parts that are attributable to heat treatment (heat treat distortion), and thus to provide the ability to optimize designs before heat treatment; and to increase the quality of wear-coated engine blocks by using nondestructive evaluation techniques.

Keywords: Induction Hardening, Heat Treat Distortion, Nondestructive Evaluation, Steel

91. **TECHNOLOGY ASSESSMENT AND EVALUATION**
$450,000
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

92. **GLASS REINFORCED COMPOSITE MATERIALS JOINING, DURABILITY AND ENABLING TECHNOLOGIES**
$1,850,000
DOE Contact: Joseph Carpenter, (202) 586-1022
ORNL Contact: Dave Warren (423)574-9693
Laboratory Partners: ORNL, LBNL
Industry and University Partners: USAMP/ Automotive Composites Consortium, University of Texas, University of Tennessee, Oak Ridge Institute of Science and Technology, Tennessee State University, Goodrich, Baydur Adhesives, University of Tulsa

The objective of this effort is to develop critical enabling technologies necessary for the implementation of advanced structural composite materials. These nclude 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-adherend pairs using three composite adherends 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. The project will develop and demonstrate reliable attachment technologies for use in lightweight composite structures for automotive applications. 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 models. Technology implementation is conducted through Automotive Composites Consortium (ACC) focal projects. An additional objective is to develop NDE technology to evaluate bonded joint integrity of automotive assemblies, such as a body-in-white.

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

93. **COMPOSITE MATERIAL DESIGN, MANUFACTURING AND DEMONSTRATION**
$1,425,000
DOE Contact: Joseph Carpenter, (202) 586-1022
ORNL Contact: Dave Warren, (423) 574-9693
Laboratory Partners: ORNL, LLNL, INEEL
Industry and University Partners: USAMP/ Automotive Composites Consortium, 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 is to develop the design and manufacturing methodologies to allow safe, reliable, repeatable and cost- effective implementation of composite materials in automotive structures. Specific efforts include the following: develop and model slurry preforming processes applicable to the automotive industry. After initial development, optimize the processes for repeatabilty of glass fiber positioning at increased production rates. 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. 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, Crash, Energy Management, Processing, Automotive, Preforming, Molding

94. **USAMP COOPERATIVE AGREEMENT**
$1,000,000
DOE Contact: Joseph Carpenter, (202) 586-1022
ORO Contact: Harold Clark, (423) 576-0823
Industry Partner: US Automotive Materials Partnership (Chrysler, Ford, GM), Aplicator, Budd

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

95. **CARBON FIBER BASED COMPOSITE MATERIALS TECHNOLOGY**
$850,000
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.

Keywords: Polymer, Composites, Carbon Fiber

ELECTRIC DRIVE VEHICLE TECHNOLOGY

ADVANCED BATTERY PROGRAM

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

96. **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. By using lower-density acetylene black, greatly improved utilization of the sulfur active material in the range of 40% and higher was demonstrated.

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

97. **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. A study of the transport properties of PEO-NaTFSI ($TFSI=N(CF_3SO_2)_2$) electrolytes was completed, and thin solid films of $Li_{3x}La_{0.67-x}TiO_3$ were prepared by hydraulically pressing powders under an inert atmosphere.

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

98. **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. Polymer electrolytes containing oxymethylene-linked polyethylene glycol and polypropylene oxide were prepared.

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

99. **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. Cycling studies on $Li_xM_yMnO_2$ (M = Li, Na, K) showed that the highest capacity and longest life was obtained when M = K, which provided the largest interlayer spacing.

Keywords: Intercalation Electrodes, Rechargeable Batteries

100. **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. Electrochemical studies revealed that electrolytes containing imidazole and $AlCl_3$ had a relatively large electrochemical window of 4 V.

Keywords: Intercalation Electrodes, Rechargeable Batteries

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

101. **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. The collaboration with Superior Graphite and LLNL continued with the focus to evaluate alternative graphitized carbons for the negative electrodes in Li-ion cells. The graphitized carbons obtained from Superior Graphite so far have demonstrated that high heat-treatment temperatures (~2800°C) may not be required to obtain acceptable electrode materials for Li-ion cells.

Keywords: Carbon, Li Batteries, Li intercalation

102. **FABRICATION AND TESTING OF CARBON ELECTRODES AS LITHIUM INTERCALATION ANODES**
$75,000
DOE Contact: Ray Sutula, (202) 586-8064
Lawrence Livermore National Laboratory Contact: T. Tran, (510) 422-0915

The objectives of this work are to evaluate the performance of carbonaceous materials as hosts for lithium intercalation negative electrodes, and to develop reversible lithium intercalation negative electrodes for advanced rechargeable lithium batteries. The approach is to fabricate electrodes from various commercial carbons and graphites and evaluate them in small lithium-ion cells. Electrode performance will be correlated with carbon structure and properties in collaboration with LBNL. The Li intercalation capacities of petroleum needle cokes (190LS, Superior Graphite Co.) that were air milled and heat treated to 1800°, 2100° or 2350°C were examined The highest Li intercalation capacity (x = 0.93 in Li_xC_6) was obtained with the sample that was heat treated at 2350°C and then air milled.

Keywords: Carbon, Li Batteries, Intercalation

103. **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. This project was a new initiative in FY 1997. Initial results indicate that a large amount of gaseous species is generated on graphitic carbons when mixed cyclic carbonate and alkyl carbonate-based electrolytes are used.

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

104. **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. The EXAFS study shows that midway through the charge there is considerable disorder in the Li_xNiO_2 material, but it reverts to a more ordered structure towards the end of charge. On the other hand, $LiMn_2O_4$ shows much less changes in the spinel structure during charge than $LiNiO_2$.

Keywords: Electrodes, Batteries, EXAFS

105. **POLYMER ELECTROLYTE FOR AMBIENT TEMPERATURE TRACTION BATTERIES: MOLECULAR LEVEL MODELING FOR CONDUCTIVITY OPTIMIZATION**
$145,000
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. A simple model was developed in which the polyelectrolyte species are semibound, i.e. they cannot diffuse long distances. this model suggests that more flexible polyelectrolytes will have smaller diffusion barriers and higher ionic conduction.

Keywords: Batteries, Electric Vehicles, Polymeric Electrolytes

106. **ANALYSIS AND SIMULATION OF ELECTROCHEMICAL SYSTEMS**
$235,000
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. A mathematical model has been developed which showed good agreement with data obtained by slow charge/discharge potential transients, cyclic voltammetry, and potential-step measurements using a nickel hydroxide-hydrogen thin film cell. These data compare well with output from the numerical model.

Keywords: Electrochemical Phenomena, Galvanostatic Charge/Discharge

107. **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. It was observed that, after short-term normal cycle tests of Li/V_6O_{13} cells, only a small amount of corrosion pits appeared on Al collectors, but serious pitting corrosion occurred after overcharging.

Keywords: Current Collectors, Advanced Batteries

108. **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. Quantitative analysis of the SER spectra of a $Ni/Ni(OH)_2$ electrode showed that the precursor α-$Ni(OH)_2$ phase is only partially converted into β-$Ni(OH)_2$ during cycling. Cyclic voltammetry of TiO_2-modified Ni electrode shows that TiO_2 addition does not significantly shift the O_2-evolution potential.

Keywords: Ion Implantation, Electrodes, Rechargeable Batteries

109. **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 MH/NiOOH secondary cells through microstructural modeling of the NiOOH electrode.

These studies should lead to improved energy densities in MH/NiOOH batteries by determining optimal microstructures for NiOOH substrates. The study is focused on the effects of the microstructure of fibrous composite electrodes on thermal and electrical conductivity, strength, and lifetime. Studies on a variety of fibers, including carbon (7-12 μm diameter) and polypropylene (~10 μm diameter) fibers, both coated with nickel and sinter-bonded, and pure sinter-bonded nickel fibers, were completed. A novel network generation approach has been validated with experimental resistivities in fibrous substrates, and a new mechanics technique has been developed to model the damage progression in the fibrous substrates, and damage simulations have been initiated.

Keywords: MH/NiOOH Batteries Modeling, Microstructural Characterization

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

110. 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. Laboratory-scale solid-state cells with $LiMn_2O_4$ electrodes were fabricated with open circuit voltages (OCVs) between 2.98 and 4.03 V, consistent with the cathode composition with $x = 1$ for $Li_xMn_2O_4$. Studies indicate that the cathode surface has undergone a phase change to the orthorhombic structure for $x > 1$, and the cell resistance increased as a result of the initial discharge.

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

111. APPLIED RESEARCH ON NOVEL CELL COMPONENTS FOR ADVANCED CAPACITORS
$115,000
DOE Contact: Ray Sutula, (202) 586-8064
SAFT Research & Development Center
Contact: Guy Chagnon, (410) 771-3200

The objective of this research is to evaluate the double-layer capacitance of high-surface-area carbons, and to develop low-cost carbon electrodes for electrochemical double-layer capacitors that meet the DOE goal of 1600 W/kg, 10 Wh/kg and $1/kW. Cells with 140°F capacitance and 20 milliohms resistance, corresponding to high-performance capacitors delivering 6.1 Wh/kg and 3.9 Kw/kg were built and tested. An additional 10 cells were fabricated and tested at INEEL; results (typically 1.4-1.8 Wh/kg at about 63 W/kg) are documented in an INEEL report. This project has been completed.

Keywords: Electrochemical Capacitors, Carbon Electrodes

112. SOL-GEL DERIVED METAL OXIDES FOR ELECTROCHEMICAL CAPACITORS
$123,000
DOE Contact: Ray Sutula, (202) 586-8064
University of Wisconsin - Madison Contact:
Marc A. Anderson, (608) 262-2674

The objective of this research is to improve the chemical and materials properties of the NiO/Ni system for electrochemical capacitors (ultracapacitors). Prototypes made from nickel oxide thin-film electrodes have been successfully fabricated with a total thickness of the cell (including outside packaging material) of less than 1 mm. Five cells were tested at INEEL; results are documented in an INEEL report. This project has been completed.

Keywords: Electrochemical Capacitor, NiO Electrodes

113. 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 microencapsulation of hydrogen storage alloys metal hydride electrodes for MH/NiOOH batteries. Microencapsulation of the hydrogen storage alloys with electroless nickel or cobalt-nickel coatings was found to improve the cycle life by forming a conductive passive film on the surface which prevents the oxidation of the active materials.

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

114. PREPARATION OF IMPROVED, LOW COST METAL HYDRIDE ELECTRODES FOR AUTOMOTIVE APPLICATIONS
$185,000
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 presence of cobalt and Al in AB_5 hydride electrodes was found to strongly inhibit corrosion by reducing the lattice expansion and contraction in the electrochemical charge-discharge process and, in the case of Co, from the formation of a corrosion-resistant surface layer.

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

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

Physically meaningful mechanistic models are essential for the interpretation of electrode behavior and are useful in directing the research on new classes of materials for electrochemical energy conversion and storage devices. The objective of this project is to develop an atomic-level understanding of the processes taking place in complex electrochemical reactions at electrode surfaces. Researchers are employing low energy electron diffraction (LEED) to study single crystals; high resolution electron microscopy (HREM) for carbon electrode materials; and X-ray absorption fine structure (EXAFS) for organometallic catalysts. Low Energy Ion Scattering (LEIS) and Auger Electron Spectroscopy (AES) are being utilized to study the composition of sputtered and UHV-annealed polycrystalline Pt-based bulk alloys for hydrogen electrocatalysis. It was found that both the surface and bulk composition of $Pt_{75}Mo_{25}$ alloy for hydrogen oxidation was the same.

Keywords: Spectrographic Analysis, Electrocatalysts, Electrooxidation

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

Platinum is the most active single-component catalyst for CH_3OH electrooxidation in DMFCs; however, poisoning reactions at the surface render the anode ineffective under target operation conditions. The objective of this research is to obtain information on the nature of the poisoning intermediate(s) in CH_3OH electrooxidation on Pt-based electrocatalysts by NMR. 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.

Keywords: NMR, Electrooxidation, Fuel Cells

HEAVY VEHICLE MATERIALS TECHNOLOGY

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

117. **COST-EFFECTIVE SRBSN/MICROWAVE ANNEALING OF SILICON NITRIDE**
$400,000
DOE Contact: Sidney Diamond, (202) 586-8032
ORNL Contact: D. R. Johnson, (423) 576-6832
ORNL Contact: J. O. Kiggans, (423) 574-8863

There are two major objectives of this research element. The first objective is the development of new sintered reaction-bonded silicon nitride (SRBSN) materials that will serve as cost-effective materials for use in suitable heavy-duty-diesel applications. The second is the investigation of microwave heating as a means for the nitridation of silicon for the fabrication of sintered reaction-bonded silicon nitride.

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

118. **CONTINUOUS SINTERING OF SILICON NITRIDE CERAMICS**
$148,000
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 through the development of continuous sintering techniques and the use of lower cost Si_3N_4 powders and sintering aids.

Keywords: Cost-Effective Ceramics, Silicon Nitride, Sintering

119. **COST-EFFECTIVE, HIGH-TOUGHNESS SILICON NITRIDE**
$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

In silicon nitride, acicular or elongated grains can be generated by *in situ* growth and these can provide significant toughening on the same order as the whisker-toughened materials. Microstructural development to promote growth of *in situ* toughened microstructures in silicon nitride is the current emphasis of this project.

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

120. **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 $Ba_{1+x}Zr_4P_{6-2x}Si_{2x}O_{24}$ (BaZPS) and $Ca_{1-x}Sr_xZr_4P_6O_{24}$. ORNL is assisting with the characterization and evaluation of the LoTEC compositions.

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

121. **LOW CTE MATERIALS/DIESEL EXHAUST INSULATION**
$0
DOE Contact: Sidney Diamond, (202) 586-8032
ORNL Contact: D.R. Johnson, (423) 576-6832
LoTEC, Inc. Contact: Santosh Limaye, (801) 277-6940

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

Keywords: Structural Ceramics, Ultra-low Expansion, Zirconia

122. **LOW COST NZP POWDER**
$0
DOE Contact: Sidney Diamond, (202) 586-8032
ORNL Contact: D.R. Johnson, (423) 576-6832
LoTEC, Inc. Contact: Santosh Limaye, (801) 277-6940

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

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

123. **ADVANCED MANUFACTURING OF DIESEL ENGINE TURBOROTORS**
$0
DOE Contact: Sidney Diamond, (202) 586-8032
ORNL Contact: D. R. Johnson, (423) 576-6832
Kyocera Contact: E. Kraft, (206) 750-6147

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

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

124. **ADVANCED MANUFACTURING OF CERAMIC EXHAUST VALVES FOR DIESEL ENGINES**
$0
DOE Contact: Sidney Diamond, (202) 586-8032
ORNL Contact: A. E. Pasto, (423) 574-4956
Norton Contact: Vimal Pujari, (508) 351-7929

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

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

125. **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: Michael Haselkorn, (309) 578-2953

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

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

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

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

127. **MATERIALS FOR LOW EMISSIONS, HIGH EFFICIENCY DIESEL ENGINE COMPONENTS**
$0
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 new program is to develop advanced material applications in diesel engine components to enable the design of cleaner, more efficient engines. Advanced materials may include ceramics, intermetallic alloys, advanced metal alloys, or ceramic or metal coatings. Components may include in-cylinder components, valve-train components, fuel-system components, exhaust system components, and air handling systems.

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

128. **MATERIALS FOR LOW EMISSIONS, HIGH EFFICIENCY DIESEL ENGINE COMPONENTS**
$0
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: Alloys, Ceramics, Coatings and Films, Components, Diesel, Engines, Intermetallics

129. **HIGH STRENGTH MATERIALS FOR DIESEL ENGINE FUEL INJECTORS**
$0
DOE Contact: Sidney Diamond, (202) 586-8032
ORNL Contact: R. L. Beatty, (423) 574-4536
Cummins Contact: Thomas Yonushonis, (812) 377-7078

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

Keywords: Ceramics, Cermets, Components, Diesel

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

130. **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 electron microscopy to characterize the microstructures of emission control catalysts. Emphasis is placed on relating microstructural changes to performance of diesel oxidation catalysts.

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

131. **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 this research program is to generate engineering data from ambient to high-temperature mechanical testing of silicon nitride and SiAlON. The second is to characterize the evolution and role of damage mechanisms using metallography, SEM, and TEM. Lastly, available analytical and numerical models will be utilized to predict the life of complex-shaped components and prototype engine parts (e.g., valves).

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

132. **HIGH TEMPERATURE TENSILE TESTING**
$250,000
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 Si_3N_4 at high temperatures. Microstructural/microchemical analysis of the fracture surfaces using scanning electron microscopy (SEM), transmission electron microscopy (TEM), and energy-dispersive spectral analysis (EDS) is an integral part of this effort.

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

133. **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 has been 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 valve guides as part of an effort with Caterpillar. Current processing technology is via cold isostatic pressing. Other, more-cost-effective processing methods may be assessed and a non-destructive method to establish carbon fiber distribution would be highly desirable.

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

134. **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

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

Keywords: Machining, Nondestructive Evaluation, Structural Ceramics

135. **MECHANICAL PROPERTIES OF CMZP**
$0
DOE Contact: Sidney Diamond, (202) 586-8032
ORNL Contact: D. R. Johnson, (423) 576-6832
Caterpillar Contact: M. K. Haselkorn, (309) 578-6624

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

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

TECHNOLOGY TRANSFER AND MANAGEMENT COORDINATION

136. **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: AGT, Advanced Heat Engines, Coordination, Diesel, Management, Structural Ceramics

137. **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

138. **STANDARD REFERENCE MATERIALS**
$200,000
DOE Contact: Sidney Diamond, (202) 586-8032
ORNL Contact: D. R. Johnson, (423) 576-6832
NIST Contact: G. Onoda, (301) 975-4489

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

139. **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 Heavy Vehicle Propulsion System Materials Program.

Keywords: Mechanical Properties, Test Procedures

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

140. **THICK THERMAL BARRIER SEAL COATINGS**
$33,000
DOE Contact: Sidney Diamond, (202) 586-8032
ORNL Contact: D. R. Johnson, (423) 576-6832
ORNL Contact: D. P. Stinton, (423) 574-4556

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

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

141. **CHARACTERIZATION OF MACHINED CERAMICS**
$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 was to develop, in conjunction with U.S. industry, advanced technologies and the associated scientific and economic concepts necessary to reduce the costs for machining of structural ceramics for energy-efficient, low-emissions transportation systems. This effort was conducted by industry, other national laboratories, and in-house at ORNL. The ORNL research concerned two technical areas: 1) investigating the effects of machining practices on the durability of ceramics for valve and valve-seat applications; and 2) understanding and characterizing the detailed nature of machining-induced surface and subsurface damage and their evolution in advanced ceramic materials using a range of analytical tools.

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

142. **ADVANCED MACHINING/MANUFACTURING**
$223,000
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

143. **NEXT-GENERATION GRINDING WHEEL**
$0
DOE Contact: Sidney Diamond, (202) 586-8032
ORNL Contact: P. J. Blau, (423) 574-5377
Norton Contact: Robert H. Licht, (508) 351-7815

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

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

144. **HIGH SPEED GRINDING**
$0
DOE Contact: Sidney Diamond, (202) 586-8032
ORNL Contact: P. J. Blau, (423) 574-5377
Eaton Contact: Joseph A. Kovach, (216) 523-6766

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

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

145. **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

146. **GRINDING MACHINE STIFFNESS**
$0
DOE Contact: Sidney Diamond, (202) 586-8032
ORNL Contact: P. J. Blau, (423) 574-5377
University of Connecticut Contact: Bi Zhang, (203) 486-3576

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

Keywords: Machining, Silicon Nitride

147. **NEXT GENERATION GRINDING SPINDLE**
$0
DOE Contact: Sidney Diamond, (202) 586-8032
ORNL Contact: P. J. Blau, (423) 574-5377
Eaton Contact: J. A. Kovach, (216) 523-6766

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

Keywords: Machining, Structural Ceramics

148. **PROCESS COST MODEL**
$0
DOE Contact: Sidney Diamond, (202) 586-8032
ORNL Contact: S. G. Winslow, (423) 574-0965
AlliedSignal Ceramic Components Contact: J. M. Wimmer, (312) 512-3183

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

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

149. **INTELLIGENT GRINDING WHEEL**
$0
DOE Contact: Sidney Diamond, (202) 586-8032
ORNL Contact: P. J. Blau, (423) 574-5377
University of Massachusetts Contact: Stephen Malkin, (413) 545-3687

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

Keywords: Cost-Effective Ceramics, Machining, Structural Ceramics

OFFICE OF UTILITY TECHNOLOGIES

	FY 1997
Office of Utility Technologies - Grand Total	$38,810,000
Office of Solar Energy Conversion	$18,460,000
Photovoltaic Energy Technology Division	$18,460,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$12,800,000
Amorphous Silicon for Solar Cells	3,370,000
Polycrystalline Thin Film Materials for Solar Cells	8,110,000
Deposition of III-V Semiconductors for High-Efficiency Solar Cells	1,320,000
Materials Properties, Behavior, Characterization or Testing	$ 3,550,000
Materials and Device Characterization	$ 3,550,000
Device or Component Fabrication, Behavior or Testing	$ 2,110,000
High-Efficiency Crystalline Silicon Solar Cells	2,110,000
Office of Geothermal Technologies	$ 600,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 125,000
Thermally Conductive Composites for Heat Exchangers	125,000
Materials Properties, Behavior, Characterization or Testing	$ 475,000
Advanced High Temperature Geothermal Well Cements	125,000
Corrosion Mitigation at The Geysers	100,000
Advanced Coating Materials	100,000
Thermally Conductive Cementitious Grouts for Geothermal Heat Pumps	150,000
Office of Energy Management	$19,750,000
Advanced Utility Concepts Division	$19,750,000
High Temperature Superconductivity for Electric Systems	$19,750,000
Device or Component Fabrication, Behavior or Testing	$19,750,000
Wire Technology	5,000,000
Systems Technology	5,250,000
Superconductivity Partnership Initiative	9,500,000

OFFICE OF UTILITY TECHNOLOGIES

OFFICE OF SOLAR ENERGY CONVERSION

PHOTOVOLTAIC ENERGY TECHNOLOGY DIVISION

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

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

150. AMORPHOUS SILICON FOR SOLAR CELLS
$3,370,000
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. Achieving that goal will enable amorphous silicon to be a cost-effective utility-scale generator.

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

151. POLYCRYSTALLINE THIN FILM MATERIALS FOR SOLAR CELLS
$8,110,000
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. Achieving this goal will enable polycrystalline thin film material to be a cost-effective utility-scale generator.

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

152. DEPOSITION OF III-V SEMICONDUCTORS FOR HIGH-EFFICIENCY SOLAR CELLS
$1,320,000
DOE Contact: Jeffrey Mazer, (202) 586-2455
NREL Contact: John Benner, (303) 384-6496

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

Achieving these goals will enable systems using these technologies to be cost-effective utility-scale generators.

Keywords: Semiconductors, Chemical Vapor Deposition, Solar Cells

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

153. MATERIALS AND DEVICE CHARACTERIZATION

$3,550,000
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

154. HIGH-EFFICIENCY CRYSTALLINE SILICON SOLAR CELLS

$2,110,000
DOE Contact: Jeffrey Mazer, (202) 586-2455
NREL Contact: John Benner, (303) 384-649
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 Defects 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

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

155. THERMALLY CONDUCTIVE COMPOSITES FOR HEAT EXCHANGERS

$125,000
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.

Fundamental work to elucidate the interactions that take place at the thermally conductive composite/ scale interface was performed. The results of these studies indicated that polymers containing ester, ketone or ether functional groups should not be used as liner materials because of their susceptibility to oxidation reactions with hot brine. This reaction led to formation of carboxylic acid groups which subsequently react with Ba and Ca in geothermal brines. The Ba- and Ca-complexed carboxylate salt derivatives not only acted to promote the rate of scale deposition, but also caused the development of high bond strength at the interfaces between the coating and scale. Based on these findings, the incorporation of antioxidants and the use of polyaryl type polymers were selected for field testing.

Field tests with flowing hypersaline brine under heat exchange conditions in conjunction with NREL are in progress to evaluate the following coatings.

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

Preliminary results indicate a trend for the coats containing antioxidants to have greater fouling resistance. If this behavior is sustained the coatings will represent a significant advancement in overcoming problems of both corrosion and scale resistance. Research is also underway to improve methods of attaching the lined heat exchanger tubes to tube sheets. 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% could be realized.

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

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

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

Lightweight (<1.2 g/cc), environmentally benign, chemically and thermally resistant well cements are needed to reduce the potential for lost circulation problems during well completion operations and to ensure long-term well integrity. Materials designed for temperatures >400°C will be needed as higher temperature resources are developed. Cements resistant to brines containing high concentrations of CO_2 at temperatures >150°C are also needed. Emphasis is being placed on high temperature rheology, phase chemistry, and the mechanical, physical, and chemical resistance properties of the cured materials. Retarding admixtures required to maintain pumpability during placement operations are also being identified.

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 and permeability after exposure to CO_2 solutions at 300°C were completed. As a result, a formulation was tentatively selected for use in a full-scale test performed in FY 1997. The basic cement formulation consists of 23.7 wt% fly ash; 15.8 wt% calcium aluminate cements, 12.6 wt% sodium polyphosphate, 29.1 wt% Al_2O_3-shelled microspheres, and 18.8 wt% water. This formulation has a slurry density of approximately 1.2 g/cc, and after hydrothermal curing forms a strong, CO_2-resistant cement. As an example, autoclave exposure for 120 days to a 4 wt% Na_2CO_3 solution at 300°C produced no evidence of carbonation or strength retrogression. In contrast, Class G cement that is conventionally used for geothermal well completions was severely deteriorated. A production well in Indonesia was recently successfully completed with the developed calcium phosphate cement and use of this material in two more wells in 1998 is planned.

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

157. **CORROSION MITIGATION AT THE GEYSERS**
$100,000
DOE Contact: R. LaSala, (202) 586-4198
BNL Contact: M. L. Allan, (516) 344-3060

Increased HCl gas concentrations in the steam produced from geothermal wells at The Geysers in Northern California have resulted in severe corrosion problems in casings in the upper regions of wells where condensation may occur, in the well-head, transmission piping, turbines, and cooling towers. The objective of the program is to optimize and field test polymers, polymer matrix composites, and ceramic matrix composites for utilization as corrosion resistive liners on components exposed to low pH steam condensates at temperatures up to ~200°C. The identification of need, performance of prototype and full-scale field evaluations, and subsequent economic studies are performed as cost-shared activities with firms active at The Geysers.

In FY 1997, a number of potential coating systems were developed by BNL and were investigated in laboratory-scale work. These included: (a) refractory oxides (ZrO_2, Al_2O_3, and Y_2O_3), (b) ceramic-sealed NiAl alloy composites, (c) fly ash-derived glass ceramics and (d) PPS-sealed NiAl alloy composites. These materials were evaluated for use as corrosion/oxidation/abrasion-resistant coatings for mild carbon steel, stainless steel, Ni-Cr steel and Ti-based alloys.

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

158. **ADVANCED COATING MATERIALS**
$100,000
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 metal composites, developed in other parts of the Geothermal Materials Development Program, as corrosion protective systems for use in brine dominated geothermal electric generation processes and for the biochemical treatment of plant wastes. Successful evaluations and subsequent technology transfer will result in reduced plant construction and operation costs, increased generation efficiencies and utilization factors, and enhanced environmental acceptance.

Thermal sprayed WC-12%Co and Cr_3C_2-NiCr coatings were evaluated for corrosion and erosion protection of vent gas blowers. These coatings are currently undergoing field tests. Thermal sprayed ethylene tetrafluoroethylene and ethylene methacrylic acid polymers, spray-and-bake fluoropolymers and brushable ceramic-filled epoxy were investigated as coatings to protect mild steel and 316L stainless steel from geothermal sludge, synthetic hypersaline brine and *Thiolacillus ferrooxidans* at 55°C in laboratory scale tests. All thermal spraying was performed at the State University of New York at Stony Brook. The coatings were selected on the basis of their predicted resistance to chemical attack and biodegradation, ease of large-scale application, and economics. Long-term exposure tests in simulated environments were conducted and the coatings performance assessed. Residual adhesion after exposure was measured. Cathodic disbondment tests were also conducted to determine the possibility of using the coatings in conjunction with cathodic protection.

It was found that the tested coatings were resistant to chemical attack and biodegradation at the test temperature of 55°C. The thermal sprayed ethylene methacrylic acid coatings protected 316L stainless steel from corrosion in coupon tests. However, corrosion of mild steel substrates coated with ethylene methacrylic acid and ethylene tetrafluoroethylene occurred in Atlas cell tests that simulated a lined reactor operating environment, and this resulted in decreased adhesive strength. The ceramic-filled epoxy performed well with only slight substrate corrosion occurring after 18 weeks of exposure. This coating also displayed excellent abrasion resistance and is recommended for further testing in pilot-scale biochemical processing equipment.

Keywords: Corrosion Protection, Polymers, Composites, Biochemical Processes, Thermal Spraying, Adhesion, Cathode Protection

159. **THERMALLY CONDUCTIVE CEMENTITIOUS GROUTS FOR GEOTHERMAL HEAT PUMPS**
$150,000
DOE Contact: R. LaSala, (202) 586-4198
BNL Contact: M. L. Allan, (516) 344-3060

Ground head 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.

In FY 1997 Brookhaven National Laboratory initiated research to develop high thermal conductivity cementitious grouts for geothermal heat pumps. This research is focused on cement-silica sand grouts. 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 between 2.4 and 2.8 W/mK have been achieved, depending on sand type, content and water/cement ratio. This compares with 0.84 and 0.80 W/mK for neat cement grouts with water/cement ratios of 0.6 and 0.8, respectively. Conventional high solids bentonite grout has a thermal conductivity around 0.75-0.8 W/mK and bentonite-sand grout can be expected to have a value around 1.46 W/mK. Cost analysis and the impact of the developed thermally conductive grouts on heat exchanger length design have been conducted in collaboration with the University of Alabama.

It is intended to conduct a field trial in FY98 to evaluate the developed grout under realistic working conditions, further examine bonding between grout, U-tube and surrounding formation, measure freeze-thaw resistance of the grouts and investigate non-destructive methods for detecting loss of bonding in any grouting material.

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

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

160. **WIRE TECHNOLOGY**
$5,000,000
DOE Contact: Jim Daley, (202) 586-1165
Argonne National Laboratory Contact:
U. Balachandran, (708) 252-4250
Brookhaven National Laboratory Contact:
David Welch, (516) 282-3517
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: Peter Roth, (505) 845-9301
American Superconductor Contact: G. N. Riley, (508) 836-4200
Intermagnetics General Corp. Contact:
Paradeep Haldar, (518) 782-1122

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

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

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

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

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

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

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

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

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

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

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

161. **SYSTEMS TECHNOLOGY**
$5,250,000
DOE Contact: Jim Daley, (202) 586-1165
Argonne National Laboratory Contact: U. Balachandran, (708) 252-4250
Brookhaven National Laboratory Contact: David Welch, (516) 282-3517
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: Thomas Bickel, (505) 845-9301
American Superconductor Contact: G. N. Riley, (508) 836-4200
Intermagnetics General Corp. Contact: Paradeep Haldar, (518) 782-1122
Oxford Instruments, Inc. Contact: K. R. Marken, (908) 541-1300

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

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

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

b. Practical conductor development for electrical power systems utilizing high T_c oxides: characterization of electrical and magnetic properties - The purpose of this project is: to make detailed characterization of electrical and magnetic properties, such as ac losses and critical currents, of cuprate conductors in order to make critical assessments of the conductors, as well as to provide pertinent data for the design of various electrical devices.

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

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

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

f. HTS transmission cable - The purpose of this project is to develop the technology necessary to proceed to commercialization of high temperature superconducting transmission cable. The objectives are to design and construct a low-cost, 2000 A AC, bare 1 m HTS cable prototype, and test its performance.

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

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

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

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

162. **SUPERCONDUCTIVITY PARTNERSHIP INITIATIVE**
$9,500,000
DOE Contact: Chris Platt, (202) 586-4563

The Superconductivity Partnership Initiative (SPI) is an industry-led venture between the Department of Energy and four industrial consortia intended to accelerate the use of high temperature superconductivity in energy applications. Each SPI team includes a vertical integration of non-competing companies that represent the entire spectrum of the R&D cycle. That is, the teams include the ultimate user of the technology—the electric utilities—as well as a major manufacturing company and a small company supplier of superconducting components. Each team also includes one or more national laboratories who perform specific tasks defined by the team. The SPI goal is to design cost-effective HTS systems for electricity generation, delivery and use. The funding amount below includes the Department's share of the SPI design activities, as well as parallel HTS technology development that directly supports the SPI teams. In FY 1997, projects are underway for a superconducting fault-current limiter (Lockheed-Martin) , and 100 HP motor (Rockwell Automation) . In addition, a transmission cable project, led by the Electric Power Research Institute and Pirelli Cable, was funded. All of these projects will incorporate high-temperature superconducting wire. Four Department of Energy National Laboratories are currently directly supporting the Superconductivity Partnership Projects: Argonne, Los Alamos, Oak Ridge, and Sandia.

Project subtasks are as follows:

a. Fault Current Limiter - The fault current limiter project undertook conceptual studies of various device designs, provided a market survey for current limiter applications, completed an energy benefit assessment, conducted a network interface assessment, determined conductor requirements, and analyzed the economic potential of fault current limiters. Fault current limiters can be used on transmission and distribution systems to improve system flexibility, reliability and performance.

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

b. Motor - Electrical and mechanical design and thermal analysis was completed. In addition, the construction of the components for a motor prototype will be nearly completed, with assembly and testing. Superconducting motors can have a large impact on electrical energy utilization through reduced losses and size compared to conventional iron core motors. 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. High Temperature Superconducting Power Cable - The first phase of the contract calls for the development and fabrication of a 30-meter prototype 115KV HTS underground power transmission cable which will be tested at a utility test site. Additionally, the project will conclude with design of a 3-phase, 100 meter cable system.

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

Keywords: Motor, Fault Current Limiter, Transmission Cable

OFFICE OF ENERGY RESEARCH

	FY 1997
Office of Energy Research - Grand Total	$431,936,392
Office of Basic Energy Sciences	$344,107,192
Division of Materials Sciences	$332,060,000
Division of Chemical Sciences	$ 5,143,000
Division of Engineering and Geosciences	$ 6,904,192
Engineering Sciences Research	$ 3,946,973
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 1,009,868
Fundamentals of Thermal Plasma Processing	478,000
Multivariable Control of the Gas-Metal Arc Welding Process	153,000
Metal Transfer in Gas-Metal Arc Welding	124,000
Thermal Plasma Chemical Vapor Deposition of Advanced Materials	157,975
Research on Combustion-Driven HVOF Thermal Sprays	96,893
Effect of Forced and Natural Convection on Solidification of Binary Mixtures	0
Materials Properties, Behavior, Characterization or Testing	$ 2,579,682
Continuum Damage Mechanics - Critical States	0
An Investigation of History-Dependent Damage in Time-Dependent Fracture Mechanics	99,729
Intelligent Control of Thermal Processes	517,000
Elastic-Plastic Fracture Analysis Emphasis on Surface Flaws	132,000
Nondestructive Evaluation of Superconductors	205,000
Origins of Asymmetric Stress-Strain Response in Phase Transformations	80,535
Modeling and Analysis of Surface Cracks	192,000
Development of Measurement Capabilities for the Thermophysical Properties of Energy-Related Fluids	425,000
High-T_c Superconductor-Semiconductor Integration and Contact Technology	116,800
Thin Film Characterization and Flaw Detection	0
Transport Properties of Disordered Porous Media From the Microstructure	116,959
Inelastic Constitutive Equation: Deformation Induced Anistropy and the Behavior at High Homologous Temperature	149,828
Stress and Stability Analysis of Surface Morphology of Elastic and Piezoelectric Materials	137,700
Optical Techniques for Characterization of High Temperature Superconductors	231,000
3-D Experimental Fracture Analysis at High Temperatures	76,721
Simulation and Analysis of Dynamic Failure in Ductile Materials	99,410

OFFICE OF ENERGY RESEARCH (continued)

	FY 1996
Office of Basic Energy Sciences (continued)	
Division of Engineering and Geosciences (continued)	
Engineering Sciences Research (continued)	
Device or Component Fabrication, Behavior or Testing	$ 357,423
An Analytical-Numerical Alternating Method for 3-D Inelastic Fracture and Integrity Analysis of Pressure-Vessels and Piping at Elevated Temperatures	85,000
Pulse Propagation in Inhomogeneous Optical Waveguides	200,493
Flux Flow, Pinning and Resistive Behavior in Superconducting Networks	71,930
Geosciences Research	$2,957,219
Materials Preparation, Synthesis , Deposition, Growth or Forming	$ 620,789
Organic Anion-Mineral Surface Interactions During Diagenesis	200,000
Solution-reprecipitation of Calcite and Partitioning of Divalent Metals	129,999
Transition Metal Catalysis in the Generation of Petroleum and Natural Gas	109,313
Mineral Dissolution and Precipitation Kinetics: A Combined Atomic-Scale and Macro-Scale Investigation	181,477
Materials Structure and Composition	$ 519,258
Reaction Mechanisms of Clay Minerals and Organic Diagenesis: An HRTEM/AEM Study	139,065
Infrared Spectroscopy and Hydrogen Isotope Geochemistry of Hydrous Silicate Glasses	141,634
Biomineralization: Systematics of Organic-directed Controls on Carbonate Growth Morphologies and Kinetics Determined By *in situ* Atomic Force Microscopy	38,559
Reactions and Transport of Toxic Metals in Rock-Forming Silicates at 25°C	200,000
The Crystal Chemistry and Structural Analysis of Uranium Oxide Hydrates	0
Materials Properties, Behavior, Characterization or Testing	$1,817,172
Oxygen and Cation Diffusion in Oxide Materials	180,000
Structure and Reactivity of Ferric Oxide and Oxyhydroxide Surfaces: Quantum Chemistry and Molecular Dynamics	200,000
Cation Diffusion Rates in Selected Silicate Minerals	150,000
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	133,661
Theoretical Studies of Metal Species in Solution and on Mineral Surfaces	55,817
Micromechanics of Failure in Brittle Geomaterials	223,820
Three-Dimensional Imaging of Drill Core Samples Using Synchrotron-Computed Microtomography	225,000
Shear Strain Localization and Fracture Evolution in Rocks	144,987
Dissolution rates and surface chemistry of feldspar glass and crystal	107,026
Transport Phenomena in Fluid-Bearing Rocks	0
Cation Chemisorption at Oxide Surfaces and Oxide-Water Interfaces: X-Ray Spectroscopic Studies and Modeling	246,861

OFFICE OF ENERGY RESEARCH (continued)

	FY 1996
Office of Computational and Technology Research	$13,702,000
Division of Advanced Energy Projects and Technology Research	$13,702,000
Laboratory Technology Research (LTR) Program	$ 8,062,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 2,887,000
Lumeloid, A New Solar Energy Conversion Material (ANL94-42)	200,000
Cold Cathode Electron Emission from Diamond and Diamond-Like Carbon Thin Films for Flat Panel Computer Displays (ANL95-02)	140,000
Giant Magnetoresistance Wire Sensor (ANL95-07)	75,000
High Performance Tailored Materials for Levitation and Permanent Magnetic Technologies (ANL97-02)	125,000
Synthesis and Crystal Chemistry of Technologically Important Ceramic Membranes (ANL97-06)	125,000
Composite Metal-Hydrogen Electrodes for Metal-Hydrogen Batteries (BNL94-06)	115,000
Development of CdTe/CdZnTe Materials for Radiation Detectors (BNL94-09)	115,000
Corrosion Resistance of New Alloys for Biomedical Applications (BNL94-20)	140,000
Catalytic Production of Organic Chemicals Based on New Homogeneously Catalyzed Ionic Hydrogenation Technology (BNL97-05)	118,000
Novel Biocompatible "Smart" Contact Lens Material (LBL94-28)	211,000
Alloy Design of Neodymium ($Nd_2 Fe_{14} B$) Permanent Magnets (ORL94-15)	155,000
Development of Aluminum Bridge Deck System (ORL94-56)	105,000
Manufacturing of Ni-Base Superalloys with Improved High-Temperature Performance (ORL95-05)	137,000
New Thermoelectric Materials for Solid State Refrigeration (ORL95-10)	150,000
Polymer Multilayer (PML) Film Applications of Optics, Electrolytes, and Glazings (PNL94-06)	200,000
Development of Mixed Metal Oxides (PNL94-28)	25,000
Development of Tape Calendaring Technology for Separation Membranes (PNL95-04)	257,000
Innovative Multilayer Thermal Barrier Coatings for Gas Turbine Engines (PNL95-07)	245,000
Interfacial Interactions of Biological Polymers with Model Surfaces (PNL97-21)	124,000
Highly Dispersed Solid Acid Catalysts on Mesoporous Silica (PNL97-28)	125,000
Device or Component Fabrication, Behavior or Testing	$ 3,074,000
Application of High Performance Computing of Automotive Design and Manufacturing (ANL94-54)	175,000
Development of Rapid Prototyping Technology for Bioceramic Applications (ANL95-08)	276,000
Smooth Diamond Films for Friction and Wear Applications and Chemically Protective Coatings (ANL97-05)	150,000
Microfabrication of a Multi-Axis Micro-Accelerometer Using High Aspect Ratio Microfabrication (HARM) and Silicon Micromachining (BNL94-02)	100,000
Nondestructive X-Ray Scattering Characterization of High Temperature Superconducting Wires (BNL95-10)	160,000
Thin Film Lithium Batteries (BNL95-11)	80,000
New Catalysts for Direct Methanol Oxidation Fuel Cells (BNL95-14)	80,000
Development of Multi-Channel ASICs for CdZnTe Gamma Detectors Arrays (BNL97-06)	82,000
Microcircuits and Sensors for Portable, Low-Power Data Collection and Transmission (BNL97-07)	125,000

OFFICE OF ENERGY RESEARCH (continued)

	FY 1997
Office of Computational and Technology Research (continued)	
Division of Advanced Energy Projects and Technology Research (continued)	
Laboratory Technology Research Program (continued)	
Device or Component Fabrication, Behavior or Testing (continued)	
Rechargeable Zinc/Air Batteries for Consumer Applications (LBL94-43)	62,000
Micromagnetic Structures (LBL95-12)	378,000
Development of Zinc/Nickel Oxide Batteries for Electric Vehicle Applications (LBL95-27)	42,000
Catalytic Conversion of Chloro-Fluorocarbons Over Palladium-Carbon Catalysts (LBL95-45)	275,000
Ionically Conductive Membranes for Oxygen Separation (LBL97-03)	125,000
Light Emission Processes and Dopants in Sold State Light Sources (LBL97-13)	125,000
Combinatorial Discovery and Optimization of Novel Materials for Advanced Electro-Optical Devices (LBL97-18)	125,000
Development of a Thin-Film Battery Powered Hazard Card and Other Microelectronic Devices (ORL94-39)	74,000
Ion Implantation Processing Technologies (ORL94-72)	136,000
Rapid Prototyping of Ceramics (ORL94-95)	153,000
Development of a Thin Film Battery Powered Transdermal Medical Device (ORL95-11)	187,000
Rapid Prototyping of Bioceramics for Implants (ORL95-12)	64,000
Development of High-Temperature Superconducting Wire Using RABITS Coated Conductor Technologies (ORL97-02)	100,000
Instrumentation and Facilities	$ 1,079,000
Micro-Spectroscopy Facility for New Infrared Imaging Materials (BNL94-60)	91,000
Development of Environmentally Conscious Machining Fluids (ORL94-91)	204,000
Novel Methods for Fabrication Cost Reduction of Pressure Infiltration Cast Metal Matrix Composite Components (ORL95-01)	192,000
Ultra-Precision Automated Measurement for Manufacturing (ORL95-08)	75,000
Neural Network Model (ORL95-90)	248,000
Microfabricated Instrumentation for Chemical Sensing in Industrial Process Control (ORL97-08)	99,000
Modeling and Simulation of Advanced Sheet Metal Forming (PNL94-38)	170,000
Materials Properties, Behavior, Characterization of Testing	$ 1,022,000
Next Generation Corrosion Inhibitors for Steel in Concrete (BNL95-12)	50,000
Prevention/Elimination of Metal-Water Explosions in Aluminum Casting Pits (ORL92-05)	174,000
In-Line Aluminum Sensors (ORL95-04)	113,000
The Role of Yttrium in Improving the Oxidation Resistance in Advanced Single Crystal Nickel-based Superalloys for Turbine Applications (ORL95-07)	149,000
Atomic Scale Structure of Ultrathin Magnetic Multilayers and Correlation with Resistance, Giant Magnetoresistance, and Spin-Dependent Tunneling (ORL97-03)	100,000
Processing/Property Relationships in Centrifugally Cast Al-Metal Matrix Composites (MMC) (PNL94-02)	245.000
Bioactive and Porous Metal Coatings for Improved Tissue Regeneration (PNL95-23)	191,000

OFFICE OF ENERGY RESEARCH (continued)

	FY 1997
Office of Computational and Technology Research (continued)	
Division of Advanced Energy Projects and Technology Research (continued)	
Advanced Energy Projects Program	$5,640,000
Device or Component Fabrication, Behavior or Testing	$2,553,000
Composite Magnetostrictive Materials for Advanced Automotive Magnetomechanical Sensors	449,000
Energy Related Applications of Selective Line Emitters	266,000
Investigation of High Efficiency Multi Band Gap Multiple Quantum Well Solar Cells	225,000
A Novel Tandem Homojunction Solar Cell: An Advanced Technology for High Efficiency Photovoltaics	255,000
Magnetically Enhanced Thermoelectric Cooling	250,000
Photochemical Solar Cells	150,000
Efficient Energy Up-Conversion of Infrared to Visible Light at Semiconductor Heterojunctions	268,000
Electrically Active Liquid Matrix Composites	300,000
Semiconductor Broadband Light Emitters	390,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$2,178,000
Next Generation High-Temperature Structural Materials for Heat Exchangers and Heating Elements	294,000
Photorefractive Liquid Crystals: New Materials for Energy-Efficiency Imaging Technology	289,000
Tritiated Porous Silicon: A Standalone Power Source	250,000
Supported Molten Metal Catalysts: Development of a New Class of Catalysts	322,000
Combinatorial Synthesis of High T_c Superconductors	250,000
Fabrication and Characterization of Micron Scale Ferromagnetic Features	106,000
Micro-Hollow Cathode Discharge Arrays: High Pressure, Nonthermal Plasma Sources	259,000
Rapid Melt and Resolidification of Surface Layers Using Intense, Pulsed Ion Beams	300,000
Experimental and Theoretical Investigation of Dual-Laser Ablation for Stiochiometric Large-Area Multicomponent Film Growth	108,000
Materials Properties, Behavior, Characterization or Testing	$ 909,000
Shape Memory Alloy Reinforcement of Metals	405,000
Exploitation of Room Temperature Molecule/Polymer Magnets for Magnetic and Electromagnetic Interference Shielding and Electromagnetic Induction Applications	212,000
Molecular Surface Modification as a Means of Corrosion Control	292,000

OFFICE OF ENERGY RESEARCH (continued)

	FY 1997
Office of Computational and Technology Research (continued)	
Division of Advanced Energy Projects and Technology Research (continued)	
Small Business Innovation Research Program	$58,849,611
Materials, Preparation, Synthesis, Deposition, Growth or Forming	$17,920,148
Phase I	$3,368,833
Controlled Permeability Chemically Activated Fly Ash (CAFA) for Reactive Contaminant Barrier	75,000
Advanced Multilayer Braze Foil for Si_3N_4 Joining	74,997
A Novel Reactive Joining Compound for High Temperature Applications	74,993
Fabrication of Active Braze Alloys for High Temperature Service	75,000
Diamond-Like Nanocomposites: Hard, Wear Resistant, Low Friction Coatings for Tribological Applications	74,869
High Growth Rate Cubic Boron Nitride Deposition	74,867
Development of Novel Boron-Based Multilayer Thin-Film	73,420
Nano-Layered Diboride Materials with Enhanced Hardness, Strength, and Toughness for Wear Applications	74,929
Advanced Plasma Surface Modification System	74,669
High-Flux, Low Energy, Ion Source for High Rate Ion-Assisted Deposition of Hard Coatings	75,000
An Ion Source Design Useful for the Production of Tribiological Thin Films	74,996
Semi-Solid Thermal Transformation to Produce Semi-Solid Formable Alloys	75,000
A Simple Process to Manufacture Grain Aligned Permanent Magnets	74,840
A Novel Technique for the Enhancement of Coercivity in High Energy Permanent Magnets	73,130
Controlled Atmosphere Plasma Spraying of NdFeB Magnet Materials	75,000
Stabilization of Nitride Magnet Material Via Sol-Gel Route	75,000
A Novel Process to Produce Nanostructured Permanent Magnetic Materials	75,000
Coke Resistant Catalyst for the Partial Oxidation Reforming of Hydrocarbon Fuels	75,000
CO Tolerant Doped-Metal Oxide Catalysts	74,987
Advanced Electrocatalysts for Direct Methanol Oxidation	74,974
A Combinatorial Approach to the Synthesis and Characterization of Novel Anode Materials for Direct Methanol Fuel Cells	74,582
Novel Multifunctional Direct Methanol Fuel Cell Catalysts	75,000
Low Cost Deposition of Buffer Layers for Manufacturable YBCO HTS Conductors	75,000
Stoichiometric YBCO Epitaxial Coatings on RABITS Using Low Cost CCVD Processing	75,000
Buffer Layers on Textured Nickel Using Commercially Viable CCVD Processing	75,000
Micromachined SiC Sensors For Harsh Environment Applications	75,000
Silicon Carbide Sensors for Harsh Environments	74,840
Development of Efficient and Practical Passive Solar Building Systems with High Recycled Content Using the Preplaced Aggregate Concrete Technology	75,000
Heterogeneous Hydroformylation of Alkanes with Syngas	75,000
Advanced NZP-Ceramic Based Thermal Barrier Coatings with Enhanced Oxidation and Thermal Shock Resistance	74,900

OFFICE OF ENERGY RESEARCH (continued)

	FY 1997
Office of Computational and Technology Research (continued)	
Division of Advanced Energy Projects and Technology Research (continued)	
Small Business Innovation Research Program (continued)	
Materials, Preparation, Synthesis, Deposition, Growth or Forming (continued)	
Phase I (continued)	
Tubular SOFC with Deposited Nano-Scale YSZ Electrolyte	75,000
Integrated Bandpass Filter Contacts for TPV Cells	74,976
In-Situ Ultrahigh-Pressure Waterjet Peening of Nuclear Reactor Internals for the Prevention of Stress Corrosion Cracking	74,879
Thallium-Containing III-V Quaternary Compound Semiconductor for Use in Infrared Detection	75,000
High Speed Long Wavelength Infrared Detector Array/Preamplifier Development	75,000
Development of Cadmium Germanium Arsenide Crystals	74,995
AlInGaN Light Emitting Diodes for Spectroscopic Applications	74,195
An Easily Dispersed Reactive Coating for Surface Decontamination	75,000
High Quantum Efficiency Spin-polarized Photocathodes	74,991
Rapid Quench Nb_3Al for High Field Accelerator Applications	75,000
Ultra-Lightweight Carbon-Carbon Cooling Structure For Pixel and Silicon Strip Detectors	75,000
Epitaxial Growth of SiC on Silicon for Radiation Hard Particle Detectors	74,873
Development of Scintillators and Waveshifters for Detection of Ionizing Radiation	75,000
Low Viscosity Organic Insulation Systems For Improved Processing and Reduced Radiation Induced Gas Evolution	74,994
Radiation Resistant Joining Methods for Structural Applications in Fusion Energy Systems	74,937
Phase II (First 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 1997
Office of Computational and Technology Research (continued)	
Division of Advanced Energy Projects and Technology Research (continued)	
Small Business Innovation Research Program (continued)	
Materials, Preparation, Synthesis, Deposition, Growth or Forming (continued)	
Phase II (Second Year)	
Low Cost, Contamination-Tolerant Electrocatalysts for Low-Temperature Fuel Cells	750,000
A Low Cost, High Temperature Superconductor Wire Manufacturing Technology	750,000
A Low Cost Receiver Plate Manufacturing Process for High Concentration Photovoltaic Systems	680,000
An Intumescent Mat Material for Joining of Ceramics to Metals at High Temperatures	750,000
Development of Modulator Quality Rubidium Titanyl Arsenate Crystals for Remote Sensing Laser Systems	750,000
A Novel Method to Recycle Thin Film Semiconductor Materials	600,000
An Improved Material and Low-Cost Fabrication Options for Candle Filters	750,000
An Integrated Catalyst/Collector Structure for Regenerative Proton-Exchange Membrane Fuel Cells	719,147
Nanostructured Interstitial Alloys as Catalysts for Direct Energy Applications	750,000
Environmentally Responsible Recycling of Thin-Film Cadmium Telluride Modules	750,000
Low-Cost, Large-Area, High-Resistivity Substrates for Gas Microstrip Detectors	749,973
An Economic Sorbent for the Removal of Mercury, Chlorine, and Hydrogen Chloride from Coal Combustion Flue Gases	750,000
Materials Properties, Behavior, Characterization or Testing	$12,202,888
Phase I	$ 971,422
Nondestructive Measurements of Key Mechanical Properties of Alloy 718 Welded Structures Using Novel Stress-Strain Microprobe Technology	75,000
Processing For Surface Hardness: Novel Characterization Techniques for Dynamic Tribological Properties of Thin Films	74,993
A Novel Mass Spectrometer for Characterization of Electrochemical Processes	75,000
New Insulation Techniques for High Voltage, High Frequency Motors	74,985
Development of Carbon Products from the Waste Stream of the Super Critical Deashing Process in Coal Liquefaction	75,000
Sol-Gel Coatings as Corrosion Barriers for Carbonate Fuel Cell Components	75,000
Enhanced Flaw Detection by Time-Reversal Auto-Focusing of an Ultrasonic Array	74,988
High Resolution Cryogenic Calorimeter for Beta and Gamma Ray Detection	74,976
High Current Density High Repetition Rate Ferroelectric Cathode	75,000
High Current Capacity High Temperature Superconducting Film Based Tape for High Field Magnets	75,000
A Polycrystalline Pixel Diamond Film Particle Detector	71,483
Resistance Welding Vanadium Alloys	74,997
Low Cost Technique for Testing Ceramic Insulator Coatings	75,000

OFFICE OF ENERGY RESEARCH (continued)

	FY 1997
Office of Computational and Technology Research (continued)	
Division of Advanced Energy Projects and Technology Research (continued)	
Small Business Innovation Research Program (continued)	
Materials Properties, Behavior, Characterization or Testing (continued)	
Phase II (First Year)	$8,242,295
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
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
Phase II (Second Year)	$2,989,171
Rotating, In-Plane Magnetization and Magneto-Optic Imaging of Cracks Under Coatings on Ferromagnetic Metals	750,000
Development of Laser Materials and Rugged Coatings as Components for Tunable Ultraviolet Laser Systems	739,171
Application of Raman Spectroscopy to Identification and Sorting of Post-Consumer Plastics for Recycling	750,000
A Sensor for Automated Plastics Sorting	750,000
Device or Component Fabrication, Behavior or Testing	$28,726,575
Phase I	$ 2,095,557
Hydrocarbon Gas Sensors Based on Wide Band-Gap Semiconductors	74,195
Shaft Weld Replacement with a Ceramic Locking Assembly Joint	74,986
A Novel Technology for Si_3N_4-To Superalloy Joints With High Use Temperature Capability	75,000
Development of Economical Procedures for Producing and Processing Fine Grained SSM Feedstock via Mechanical Stirring	72,667
A New Semi-Solid Forming Process For Fabrication of High Volume Fraction (>15 vol%) Metal/Metal Carbide Nanocomposites	75,000
Alternative Metal Forming Using Laser Engineered Net Shaping	74,777
Production of High Performance BSCCO-2223 Tapes Using Hydrostatic Pressure	75,000
Development of Long-length Fabrication Technology for High T_c Superconductors Operation in High Magnetic Fields at 77K	74,999

OFFICE OF ENERGY RESEARCH (continued)

	FY 1997
Office of Computational and Technology Research (continued)	
Division of Advanced Energy Projects and Technology Research (continued)	
Small Business Innovation Research Program (continued)	
Device or Component Fabrication, Behavior or Testing (continued)	
Phase I (continued)	
Non-Linear Inductor for Power Electronics Protection	75,000
Novel Fabrication of Low Cost Performance Bipolar Plates	75,000
Corrosion Resistant Bipolar Plates for PEM Fuel Cells	74,989
Reduced Part Count Motor Fabrication	74,900
Removal of Particulate and SO_x/NO_x Precursors in Integrated Gasification Combined Cycle Systems	75,000
Use of Novel, Low-Cost Additives to Improve Sorbent Efficiency for Control of Mercury Emissions in Coal-Fired Power Plant Flue Gases	74,996
Mixed Phase Positive Electrodes for Long Life AMTEC Modules	75,000
High Brightness LEDs Based on the (Al,Ga,In)N Materials System	75,000
Development of High Power RF Windows and Waveguide Components for the Next Linear Collider	75,000
Cost Reduction for Production of Superconducting Niobium Cavities	74,355
Electrical Discharge Machining Application to the Development of mm-wave Accelerating Structures	74,000
Direct Adhesive Technology for Arbitrary Conductors	74,839
Controlled Processing for High-Performance Fine Filament Bi-2223 Conductors	75,000
Development of a High Field NbTi Superconductor Using an Approach Combining Artificial Flux Pinning With Conventional Thermomechanical Processing	74,993
Conventionally Processed NbTi Superconductors with Artificial Ferromagnetic Pinning Centers for High Magnetic Field (>8 T) Application	74,997
Liquid Core Optical Scintillating Fibers	74,973
High Performance Heat Pipe Cooling of Electron Cyclotron Heating Mirrors P12-2426	74,971
Reaction Bonding of Silicon Carbide Composites for Fusion Applications	74,945
Net Shape Gradient W-Cu Plasma Facing Components by Pressure Infiltration	74,975
Joining of Silicon Carbide for Fusion Applications	75,000
A Novel Divertor Design Based on a Tungsten Wire Brush Tile	75,000
Beryllium and Tungsten Brush Armor for Plasma Facing Components	75,000
Fabrication for Reliable Tungsten Brush Structures for Fusion Reactor Applications	75,000
Phase II (First 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

OFFICE OF ENERGY RESEARCH (continued)

FY 1997

Office of Computational and Technology Research (continued)

Division of Advanced Energy Projects and Technology Research (continued)

Small Business Innovation Research Program (continued)

Device or Component Fabrication, Behavior or Testing (continued)

Phase II (First Year) (continued)

Stratospheric Water Vapor Microsensor	750,000
Compact, Airborne Laser Multigas Sensor	600,443
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 $Cd_{1-x}Zn_xT_e$ 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

Phase II (Second Year) $6,540,879

Advanced High Power Silicon Carbide Internally Cooled X-Ray	749,291
Chemical Microsensor Arrays as Integrated Chip Compatible Devices for Chemical Weapons Nonproliferation Inspection	600,787
A High Resolution Multi-hit Time to Digital Converter Integrated Circuit	749,890
A Helium-Cooled Faraday Shield Using Porous Metal Cooling	695,343
Low Cost Fabrication of Large Silicon Carbide/Silicon Carbide Composite Structures	750,000
Bandgap-Engineered Thermophotovoltaic Devices for High Efficiency Radioisotope Power	747,791
Rugged, Tunable Infrared Laser Sources	750,000
An Innovative Membrane and Process for Removal and Recovery of Natural Gas Liquids	750,000
A Lower Cost Molten Carbonate Matrix	747,777

OFFICE OF ENERGY RESEARCH (continued)

	FY 1997
Office of Computational and Technology Research (continued)	
Division of Advanced Energy Projects and Technology Research (continued)	
Small Business Technology Transfer Program	$4,099,589
Materials Preparation, Synthesis, Deposition, Growth or Forming	$2,299,868
Phase I	$ 299,891
Improved Beta-Alumina Fabrication Using Rapid Plasma Sintering	99,896
New High-Performance GaSb-Based Thermophotovoltaic (TPV) Devices	99,995
High Efficiency Magnet Refrigerators as Alternate Environmentally Safe Commercial Refrigeration Devices	100,000
Phase II (First Year)	$ 499,977
Cabled Monofilament Subelements for Improved Multifilament Niobium Tin Performance and Reduced Cost	499,977
Phase II (Second Year)	$1,500,000
Laser Processing of Thermal Sprayed Beryllium Plasma Facing Components	500,000
Amorphous Silicon/Crystalline Silicon Heterojunctions for Nuclear Radiation Detector Applications	500,000
Low Loss Sapphire Windows for High Power Microwave Transmission	500,000
Device or Component Fabrication, Behavior or Testing	$1,799,721
Phase I	$ 299,761
Novel Thin Film Scintillator for Intermediate Energy Photons Detection and Imaging	99,796
Silicon Carbide Heat Exchanger for Advanced Coal-Based Power Systems	99,965
Advanced Ceramic Hot Gas Filters	100,000
Phase II (First Year)	$ 999,960
High Speed Motor Alternators for Hybrid Electric Vehicle Energy Storage	499,960
A Flywheel Motor Alternator for Hybrid Electric Vehicles	500,000
Phase II (Second Year)	$ 500,000
Environmentally Benign Manufacturing of Compact Disk Stampers	500,000

OFFICE OF ENERGY RESEARCH (continued)

	FY 1997
Office of Fusion Energy Sciences	$11,178,000
Materials Properties, Behavior, Characterization or Testing	$11,178,000
Structural Materials Development	670,000
Modeling Irradiation Effects in Solids	50,000
Fusion Systems Materials	3,270,000
Structural Materials for Fusion Systems	960,000
Development of Radiation-hardened Ceramic Composites for Fusion Applications	28,000
Damage Analysis And Fundamental Studies for Fusion Reactor Materials Development	150,000
Development of Lithium-bearing Ceramic Materials for Tritium Breeding in Fusion Reactors	100,000
Post-irradiation Examination of Lithium-bearing Ceramic Materials for Tritium Breeding in Fusion Reactors	20,000
International Thermonuclear Experimental Reactor (Iter) Materials Development for Plasma Facing Components	5,000,000
ITER Materials Evaluation	330,000
ITER Structural Materials Evaluation	200,000
Development of Nb_3sn Superconducting Wire for the ITER Magnet Program	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 Health and Environmental Research - Division of Physical and Technology Research

Office of Fusion Energy - Division of Advanced Physics and Technology

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

OFFICE OF BASIC ENERGY SCIENCES

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

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

DIVISION OF MATERIALS SCIENCES

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

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

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

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

NATIONAL USER FACILITIES UNDER THE OFFICE OF BASIC ENERGY SCIENCES

Basic Energy Sciences (BES) is responsible for the planning, construction, and operation of many of the Nation's most sophisticated research facilities, including third-generation synchrotron light sources and high-flux neutron sources as well as specialized facilities for microcharacterization, materials synthesis and processing, combustion research, and ion beam studies. These facilities are unmatched in the world in their breadth of capabilities and number of scientific users. BES facilities have enormous impact 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 $5,143,000 and was allocated to 23 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, characterizatioon methodologies and systems development and modeling. Although both primary and secondary battery systems are considered, the greatest emphasis is placed on rechargeable (i.e., secondary) battery systems. The program covers a broad spectrum of research including investigations of lithium cells, metal hydrides, fundamental studies of composite electrode structures, failure and degradation of active electrode materials, thin-film electrodes, electrolytes and interfaces. Characterization and methodologies include problems of electrode morphology, corrosion, separator/electrolyte stability, stable microelectrodes and the transport properties of electrode and electrolyte materials and surface films. Investigations in computational chemistry, modeling and simulations, including property predictions, phenomenological studies of reactions and interactions at critical interfaces, film formation, phase change effects on electrodes and characterization of crystalline and amorphous materials are also of interest.

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

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

For information about specific programs the DOE contact is William S. Millman, (301) 903-3285. The reader also is referred to the Worldwide Web for the publication Summaries of FY 1997 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

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

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

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

Keywords: Plasma Processing, Functionally Gradient Materials

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

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

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

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

Keywords: Gas-Metal Arc, Welding

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

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

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

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

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

Keywords: Gas-Metal Arc, Welding

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

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

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

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

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

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

Keywords: Plasma, CVD, Diamond

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

The High-Velocity Oxy-Fuel (HVOF) thermal spray process combines the fields of materials, combustion, and gas dynamics. It relies on combustion to melt and propel solid particles at high speeds onto a surface to be coated. The goal of this research is to understand

and improve the HVOF deposition of corrosion-resistant coatings, which are important in many energy-related industries. This involves both experimentation and modeling.

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

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

Keywords: Combustion, Oxy-Fuel

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

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

Keywords: Mixture, Convection

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

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

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

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

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

Keywords: Continuum Mechanics, Fractals, Brittle Materials

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

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

In the past, the evolution of damage has been addressed through a macroscopic theoretical model (developed as part of this effort) which attempt to predict the crack growth and failure response of material components exposed to high temperature conditions. However, 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

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

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

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

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

Keywords: Fuzzy Logic, Neural Networks

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

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

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

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

Keywords: Fracture Mechanics, Welding

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

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

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

Keywords: Nondestructive Evaluation, Superconductors

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

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

Keywords: Alloys, Phase Transformations

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

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

Under macroscopic mode I loading, strength-mismatched interface crack-tip stress and deformation fields show considerable differences from the corresponding fields in mechanically homogeneous media. In particular, both triaxial stress and plastic strain levels in the softer domain (e.g., an 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

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

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

Keywords: Thermophysical Properties, Fluids

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

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

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

Keywords: High T_c Superconductors, Contacts

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

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

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

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

Keywords: Thin Films, Superlattices, Surface Roughness

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

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

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

Keywords: Porous Media, Transport Properties

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

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

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

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

Keywords: Deformation, Viscoplasticity

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

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

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

introduced[1,2] to explain some existing experimental observations of the behavior of cracks in piezoelectric ceramics. Extensions of this work are underway.

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

Keywords: Surfaces, Interfaces, Stress Analysis, Piezoelectrics

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

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

Keywords: High T_c Superconductors, Thin Films

183. 3-D EXPERIMENTAL FRACTURE ANALYSIS AT HIGH TEMPERATURES
$76,721
DOE Contact: Robert E. Price, (301) 903-5822
University of Washington Contact: Albert Kobayashi, (206) 543-5488

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

The established procedure was used to determine T^*_ϵ's of A606 HSLA steel, single-edge notched (SEN) specimens with small stable crack growth, ≈ 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

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

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

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

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

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

Keywords: Dynamic Failure, Ductile Materials

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

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

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

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

Keywords: Fracture, Pressure Vessels, Piping

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

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

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

Keywords: Optical Waveguides, Monte Carlo

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

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

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

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

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

Keywords: Superconductors, Flux Flow, Josephson Junctions

GEOSCIENCES RESEARCH

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

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

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

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

Keywords: Surface reactions, Aluminosilicate Minerals, Adsorption Mechanisms

189. SOLUTION-REPRECIPITATION OF CALCITE AND PARTITIONING OF DIVALENT METALS
$129,999
DOE Contact: P. M. Davidson, (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 calcites, 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

190. TRANSITION METAL CATALYSIS IN THE GENERATION OF PETROLEUM AND NATURAL GAS
$109,313
DOE Contact: P. M. Davidson, (301) 903-5822
Rice University Contact: Frank D. Mango, (713) 527-4880

Light hydrocarbons in petroleum, including natural gas (C_1-C_4), are conventionally viewed as products of progressive thermal breakdown of kerogen and oil. Alternatively, transition metals, activated under the reducing conditions of diagenesis, can be proposed as catalysts in the generation of light hydrocarbons. Transition metal-rich 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

191. MINERAL DISSOLUTION AND PRECIPITATION KINETICS: A COMBINED ATOMIC-SCALE AND MACRO-SCALE INVESTIGATION
$181,477
DOE Contact: P. M. Davidson, (301) 903-5822
University of Wyoming Contact: Carrick M. Eggleston, (307) 766-6769
Lawrence Livermore National Laboratory Contact: Kevin G. Knauss, (510) 422-1372

The project combines atomic-scale and 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 and 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

192. **REACTION MECHANISMS OF CLAY MINERALS AND ORGANIC DIAGENESIS: AN HRTEM/AEM STUDY**
$139,065
DOE Contact: P. M. Davidson, (301) 903-5822
Arizona State University Contact: P. R. Buseck, (602) 965-3945

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

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

193. **INFRARED SPECTROSCOPY AND HYDROGEN ISOTOPE GEOCHEMISTRY OF HYDROUS SILICATE GLASSES**
$141,634
DOE Contact: P. M. Davidson, (301) 903-5822
Caltech Contacts: S. Epstein, (818) 356-6100 and E. Stolper, (818) 356-6504

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

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

194. **BIOMINERALIZATION: SYSTEMATICS OF ORGANIC-DIRECTED CONTROLS ON CARBONATE GROWTH MORPHOLOGIES AND KINETICS DETERMINED BY *In situ* ATOMIC FORCE MICROSCOPY**
$38,559
DOE Contact: P. M. Davidson, (301) 903-5822
Georgia Inst. Of Technology Contact: P. Dove, (404) 894-6043

The research is to investigate biomineralization mechanisms of dissolution and precipitation reactions of the two common calcium carbonate polymorphs, calcite and (metastable) aragonite. Experiments 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

195. **REACTIONS AND TRANSPORT OF TOXIC METALS IN ROCK-FORMING SILICATES AT 25°C**
$200,000
DOE Contact: P. M. Davidson, (301) 903-5822
Johns Hopkins 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 investigate 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

196. **THE CRYSTAL CHEMISTRY AND STRUCTURAL ANALYSIS OF URANIUM OXIDE HYDRATES**
$0
DOE Contact: P. M. Davidson, (301) 903-5822
University of New Mexico Contacts: D. Miller and R.C. Ewing, (505) 277-4163

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

Keywords: Uranium Oxide Hydrates, Crystal Chemistry Structural Topology

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

197. **OXYGEN AND CATION DIFFUSION IN OXIDE MATERIALS**
$180,000
DOE Contact: P. M. Davidson,(301) 903-5822
LLNL Contact: F. J. Ryerson, (510) 422-6170
University of California at Los Angeles Contact: K. D. McKeegan

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

Keywords: Diffusion, Minerals, Plastic Deformation

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

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

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

199. **CATION DIFFUSION RATES IN SELECTED MINERALS**
$150,000
DOE Contact: P. M. Davidson, (301) 903-5822
Sandia National Laboratory 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

200. **GRAIN BOUNDARY TRANSPORT AND RELATED PROCESSES IN NATURAL FINE-GRAINED AGGREGATES**
$0
DOE Contact: P. M. Davidson, (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

201. **THERMODYNAMICS OF MINERALS STABLE NEAR THE EARTH'S SURFACE**
$150,000
DOE Contact: P. M. Davidson, (301) 903-5822
UC 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

202. **NEW METHOD FOR DETERMINING THERMODYNAMIC PROPERTIES OF CARBONATE SOLID-SOLUTION MINERALS**
$133,661
DOE Contact: P.M. Davidson, (301) 803-5822
UC 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

203. **THEORETICAL STUDIES OF METAL SPECIES IN SOLUTION AND ON MINERAL SURFACES**
$55,817
DOE Contact: P. M. Davidson,(301) 903-5822
University of Maryland Contact: John Tossell, (301) 314-1868

The project involves quantum mechanical (Hartree Fock) calculations of relative stabilities of species participating in dissolution and precipitation of gold on sulfide minerals. Although the solubility and surface adsorption of aqueous Au species on sulfide minerals are important agents of ore deposition, current understanding is limited by lack of information on surface complexation sites and speciation. 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

204. **MICROMECHANICS OF FAILURE IN BRITTLE GEOMATERIALS**
$223,820
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

205. **THREE-DIMENSIONAL IMAGING OF DRILL CORE SAMPLES USING SYNCHROTRON-COMPUTED MICROTOMOGRAPHY**
$225,000
DOE Contact: P. M. Davidson, (301) 903-5822
BNL Contact: Keith Jones, (516) 282-4588
SUNY, Stony Brook Contact: W.B. Lindquist, (516) 632-8361

Synchrotron radiation makes feasible the use of high resolution computed microtomography (CMT) for non-destructive measurements of the structure of different types of drill core samples. The goal of this work is to produce three-dimensional images of rock drill core samples with spatial resolution of 1 micron.

CMT images are postprocessed (filtered) to provide specific grain/pore identification to each voxel in the image. The pore topology is analyzed statistically to yield information on disconnected pore volumes, throat areas, pore connectivity and tortuosity. Current effort is on development of software to analyze the 3-dimensional connectivity and shape of the pore space using the medial axis theorem from computational geometry.

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

206. **SHEAR STRAIN LOCALIZATION AND FRACTURE EVOLUTION IN ROCKS**
$144,987
DOE Contact: N. B. Woodward, (301) 903-5822
Northwestern University Contact: J.W. Rudnicki, (708) 491-3411

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

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

207. **DISSOLUTION RATES AND SURFACE CHEMISTRY OF FELDSPAR GLASS AND CRYSTAL**
$107,026
DOE Contact: P. M. Davidson, (301) 903-5822
Penn State Contact: S. Brantley, (814) 863-1739

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

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

208. **TRANSPORT PHENOMENA IN FLUID-BEARING ROCKS**
$0
DOE Contact: P. M. Davidson, (301) 903-5822
Renssalaer Polytechnic Institute Contact: E.B. Watson, (518) 276-6475

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

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

209. **CATION CHEMISORPTION AT OXIDE SURFACES AND OXIDE-WATER INTERFACES: X-RAY SPECTROSCOPIC STUDIES AND MODELING**
$246,861
DOE Contact: P. M. Davidson, (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, Interace Reactions, Synchrotron X-ray Absorption Spectroscopy

OFFICE OF COMPUTATIONAL AND TECHNOLOGY RESEARCH

DIVISION OF ADVANCED ENERGY PROJECTS AND TECHNOLOGY RESEARCH

LABORATORY TECHNOLOGY RESEARCH (LTR) PROGRAM

The LTR program supports research primarily at the five ER multi-program national laboratories: Argonne, Brookhaven, Lawrence Berkeley, Oak Ridge and Pacific Northwest.

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

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

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

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

210. **LUMELOID, A NEW SOLAR ENERGY CONVERSION MATERIAL (ANL94-42)**
$200,000
DOE Contact: Walter M. Polansky, (301) 903-5995
ANL Contact: Michael Wasielewski, Chemistry, (630) 252-3538

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

Keywords: Polymers, Composites, Solar Energy Conversion

211. **COLD CATHODE ELECTRON EMISSION FROM DIAMOND AND DIAMOND-LIKE CARBON THIN FILMS FOR FLAT PANEL COMPUTER DISPLAYS (ANL95-02)**
$140,000
DOE Contact: Walter M. Polansky, (301) 903-5995
ANL Contact: Alan Krauss, MSD/CHM, (630) 252-3520

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

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

212. **GIANT MAGNETORESISTANCE WIRE SENSOR (ANL95-07)**
$75,000
DOE Contact: Walter M. Polansky, (301) 903-5995
ANL Contact: Samuel Bader, Materials Science, (630) 252-4960

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

Keywords: Composites, Electrical, Magnetics, Sensors

213. **HIGH PERFORMANCE TAILORED MATERIALS FOR LEVITATION AND PERMANENT MAGNETIC TECHNOLOGIES (ANL97-02)**
$125,000
DOE Contact: Walter M. Polansky, (301) 903-5995
ANL Contact: George W. Crabtree, Materials Science, (630) 252-5509

The high temperature superconductor $Nd_{1+x}Ba_{2-x}Cu_3O_{7-y}$ has recently been recognized as a powerful new material in which strong magnetic flux pinning has been observed. This material can be used for the development of levitators and trapped-field permanent magnets, creating an opportunity to drive substantial advances in the performance and technical competitiveness of these technologies. The development of this material will shift the leading edge of materials research in this area from the two foreign laboratories (ISTEC, Japan and FZK, Germany) now dominating the field to the U.S. Although the strong pinning characteristics of this material have been recognized, the responsible pinning centers and efficient procedures for large scale fabrication of the material remain relatively obscure. ANL has identified a crucial new processing variable, the high temperature cooling rate during the growth process, which can be used to tailor the flux pinning properties of these materials. In addition, ANL has developed a low temperature oxygen anneal processing technique to control the magnetic field where maximum pinning occurs. An important objective of this project is to understand the origin of the superior flux trapping capabilities and to develop fabrication procedures using top-seeding techniques for making large samples for applications. Processing methodology will be developed based on property measurements using X-ray and neutron diffraction, magneto-optical imaging, magnetization measurements, and scanning tunneling microscopy on melt-textured material and single crystal samples. The best material will be tested in prototype levitating flywheels to assess its value and define problem areas in collaboration with our industrial partner, Superconductive Components, Inc. The development of high performance flux pinning materials will enable a new generation of levitation devices for frictionless bearings and flywheel energy storage, and of permanent trapped-field magnets. The materials performance advances achieved under this project can be applied to other developing technologies, such as coated conductors for high current carrying wires (IBAD and RABITS), and high power microwave filters for cellular communications. (1) The emission sites will be identified, and a determination of the site density will be made, using photo-electron emission microscopy (PEEM) for several varieties of electron emitting diamond and diamond-like carbon films. The project team has found that post-deposition treatment is critical in controlling emission properties, and the PEEM data will be studied in conjunction with oxygen and hydrogen plasma post-deposition processing. (2) Studies of the grain morphology of films produced both at SI Diamond and at ANL are being conducted using transmission electron microscopy. The ANL portion of these tasks will continue with funding from the Advanced Projects Research Agency as part of a program for improvement of diamond cathode materials for high resolution displays. Research in diamond structures and applications to electronics support DOE's long standing mission in materials sciences.

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

214. SYNTHESIS AND CRYSTAL CHEMISTRY OF TECHNOLOGICALLY IMPORTANT CERAMIC MEMBRANES (ANL97-06)

$125,000
DOE Contact: Walter M. Polansky, (301) 903-5995
ANL Contact: James D. Jorgensen, Materials Science Division, (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

215. COMPOSITE METAL-HYDROGEN ELECTRODES FOR METAL-HYDROGEN BATTERIES (BNL94-06)

$115,000
DOE Contact: Walter M. Polansky, (301) 903-5995
BNL Contact: Myron Strongin, Physics Department, (516) 344-3763

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

Keywords: Composite Electrodes, Metal-Hydrogen Electrodes, Batteries

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

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

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

217. **CORROSION RESISTANCE OF NEW ALLOYS FOR BIOMEDICAL APPLICATIONS (BNL94-20)**
$140,000
DOE Contact: Walter M. Polansky, (301) 903-5995
BNL Contact: Hugh Isaacs, Applied Science, (516) 344-4516

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

Keywords: Corrosion Resistance, Biomedical, Applications, Alloys

218. **CATALYTIC PRODUCTION OF ORGANIC CHEMICALS BASED ON NEW HOMOGENEOUSLY CATALYZED IONIC HYDROGENATION TECHNOLOGY (BNL97-05)**
$118,000
DOE Contact: Walter M. Polansky, (301) 903-5995
BNL Contact: Morris Bullock, Chemistry Division, (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

219. **NOVEL BIOCOMPATIBLE "SMART" CONTACT LENS MATERIAL (LBL94-28)**
$211,000
DOE Contact: Walter M. Polansky, (301) 903-5995
LBNL Contact: Carolyn Bertozzi, Materials Sciences Division, (510) 643-1682

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

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

220. **ALLOY DESIGN OF NEODYMIUM ($Nd_2Fe_{14}B$) PERMANENT MAGNETS (ORL94-15)**
$155,000
DOE Contact: Walter M. Polansky, (301) 903-5995
ORNL Contact: Joseph Horton, Metals and Ceramics, (423) 574-5575

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

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

221. **DEVELOPMENT OF ALUMINUM BRIDGE DECK SYSTEM (ORL94-56)**
$105,000
DOE Contact: Walter M. Polansky, (301) 903-5995
ORNL Contact: H. Wayne Hayden, Metals & Ceramics, (423) 574-6936

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

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

222. **MANUFACTURING OF Ni-BASE SUPERALLOYS WITH IMPROVED HIGH-TEMPERATURE PERFORMANCE (ORL95-05)**
$137,000
DOE Contact: Walter M. Polansky, (301) 903-5995
ORNL Contact: C. Liu, Metals and Ceramics Division, (423) 574-4459

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

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

223. **NEW THERMOELECTRIC MATERIALS FOR SOLID STATE REFRIGERATION (ORL95-10)**
$150,000
DOE Contact: Walter M. Polansky, (301) 903-5995
ORNL Contact: Brian Sales, Solid State Division, (423) 576-7646

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

Keywords: Thermoelectric Devices, Refrigeration, Air Conditioning, Alloys

224. **POLYMER MULTILAYER (PML) FILM APPLICATIONS IN OPTICS, ELECTROLYTES, AND GLAZINGS (PNL94-06)**
$200,000
DOE Contact: Walter M. Polansky, (301) 903-5995
PNNL Contact: John Affinito, Materials and Chemical Sciences, (509) 375-6942

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

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

225. **DEVELOPMENT OF MIXED METAL OXIDES (PNL94-28)**
$25,000
DOE Contact: Walter M. Polansky, (301) 903-5995
PNNL Contact: Larry Pederson, Materials and Chemical Sciences, (509) 375-2731

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

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

226. **DEVELOPMENT OF TAPE CALENDARING TECHNOLOGY FOR SEPARATION MEMBRANES (PNL95-04)**
$257,000
DOE Contact: Walter M. Polansky, (301) 903-5995
PNNL Contact: Timothy Armstrong, Materials & Chemical Sciences, (509) 375-3938

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

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

227. **INNOVATIVE MULTILAYER THERMAL BARRIER COATINGS FOR GAS TURBINE ENGINES (PNL95-07)**
$245,000
DOE Contact: Walter M. Polansky, (301) 903-5995
PNNL Contact: Edward Courtright, Materials & Chemical Sciences, (509) 375-6926

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

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

228. **INTERFACIAL INTERACTIONS OF BIOLOGICAL POLYMERS WITH MODEL SURFACES (PNL97-21)**
$124,000
DOE Contact: Walter M. Polansky (301) 903-5995
PNNL Contact: Allison Campbell, Materials and Chemical Sciences Division, (509) 375-2180

The adsorption of biological polymers onto surfaces affects many different industrial processes. However, the controlling mechanisms and the interfacial structure are not well understood for most systems. This project will develop and 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 monolayers will be used to construct surfaces with controlled properties such as chemistry, topography, and heterogeneity. For the first time, chemical vapor deposition methods for producing controlled surfaces of the biologically relevant calcium oxalate, carbonate, and phosphate systems will be developed. Biological polymers of human serum albumin, Protein G, and fibrinogen will be used in the adsorption experiments. These provide excellent models since 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 nuclear magnetic resonance experiments will be conducted 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. The project will contribute 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

229. **HIGHLY DISPERSED SOLID ACID CATALYSTS ON MESOPOROUS SILICA (PNL97-28)**
$125,000
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 of 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 tungstophorsphoric 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. Research under this project was initiated in August 1997. To date, efforts have been conducted to define the specific catalyst properties of interest. Initial synthesis and functionalization of the mesoporous silica supports has also been initiated.

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

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

230. **APPLICATION OF HIGH PERFORMANCE COMPUTING OF AUTOMOTIVE DESIGN AND MANUFACTURING (ANL94-54)**
$175,000
DOE Contact: Walter M. Polansky, (301) 903-5995
ANL Contact: David Weber, Reactor Engineering Division, (630) 252-8175

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

Keywords: Composites, Modeling, Analyses

231. **DEVELOPMENT OF RAPID PROTOTYPING TECHNOLOGY FOR BIOCERAMIC APPLICATIONS, (ANL 95-08)**
$276,000
DOE Contact: Walter M. Polansky, (301) 903-5995
ANL Contact: William A. Ellingson, Energy Technology Division, (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, Applications, Reverse Engineering, CAT Scans, Bones, CAD

232. **SMOOTH DIAMOND FILMS FOR FRICTION AND WEAR APPLICATIONS AND CHEMICALLY PROTECTIVE COATINGS (ANL97-05)**
$150,000
DOE Contact: Walter M. Polansky, (301) 903-5995
ANL Contact: Alan R. Krauss, D. M. Gruen, Materials Science and Chemistry Division, (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. End face mechanical seals, used to prevent the leakage of gases and liquids in equipment with rotating shafts, have been chosen as the area of application. 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, but the technology which will be developed will also be directly applicable to a large number of application areas in manufacturing and transportation, in most cases with similar benefits. This project supports DOE mission in the application of basic research developments in material sciences to improved processing technologies.

Keywords: Diamonds, Films, Coatings, Applications

233. **MICROFABRICATION OF A MULTI-AXIS MICRO-ACCELEROMETER USING HIGH ASPECT RATIO MICROFABRICATION (HARM) AND SILICON MICROMACHINING (BNL94-02)**
$100,000
DOE Contact: Walter M. Polansky, (301) 903-5995
BNL Contact: John Warren, Instrumentation, (516) 344-4203

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

Keywords: Microfabrication, Accelerometer, X-ray Detector

234. **NONDESTRUCTIVE X-RAY SCATTERING CHARACTERIZATION OF HIGH TEMPERATURE SUPERCONDUCTING WIRES (BNL95-10)**
$160,000
DOE Contact: Walter M. Polansky, (301) 903-5995
BNL Contact: Thomas Thurston, Physics, (516) 344-5534

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

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

235. **THIN FILM LITHIUM BATTERIES, (BNL95-11)**
$80,000
DOE Contact: Walter M. Polansky, (301) 903-5995
BNL Contact: James McBreen, Applied Science, (516) 344-4513

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

Keywords: Thin Films, Lithium, Batteries

236. **NEW CATALYSTS FOR DIRECT METHANOL OXIDATION FUEL CELLS (BNL95-14)**
$80,000
DOE Contact: Walter M. Polansky, (301) 903-5995
BNL Contact: Radoslav Adzic, Applied Science, (516) 344-4522

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

Keywords: Electrocatalysts, Methanol Oxidation, Fuels Cells

237. **DEVELOPMENT OF MULTI-CHANNEL ASICs FOR CdZnTe GAMMA DETECTOR ARRAYS (BNL97-06)**
$82,000
DOE Contact: Walter M. Polansky, (301) 903-5995
BNL Contact: Paul O'Connor, Instrumentation Division, (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, Application, Solid State Detectors

238. **MICROCIRCUITS AND SENSORS FOR PORTABLE, LOW-POWER DATA COLLECTION AND TRANSMISSION (BNL97-07)**
$125,000
DOE Contact: Walter M. Polansky, (301) 903-5995
BNL Contact: Paul O'Connor, Instrumentation Division, (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

239. **RECHARGEABLE ZINC/AIR BATTERIES FOR CONSUMER APPLICATIONS (LBL94-43)**
$62,000
DOE Contact: Walter M. Polansky, (301) 903-5995
LBNL Contact: Elton Cairns, Energy & Environment Division, (510) 486-5028

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

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

240. **MICROMAGNETIC STRUCTURES (LBL95-12)**
$378,000
DOE Contact: Walter M. Polansky,
(301) 903-5995
LBNL Contact: Neville Smith, Accelerator and
Fusion, (510) 486-5423

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

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

241. **DEVELOPMENT OF ZINC/NICKEL OXIDE BATTERIES FOR ELECTRIC VEHICLE APPLICATIONS (LBL95-27)**
$42,000
DOE Contact: Walter M. Polansky,
(301) 903-5995
LBNL Contact: Frank McLarnon, Energy
Conversion and Storage, (510) 486-4636

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

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

242. **CATALYTIC CONVERSION OF CHLORO-FLUOROCARBONS OVER PALLADIUM-CARBON CATALYSTS (LBL95-45)**
$275,000
DOE Contact: Walter M. Polansky,
(301) 903-5995
LBNL Contact: Gabor Somorjai, Materials
Sciences, (510) 486-4831

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

Keywords: Chlorofluorocarbons, Pd Catalysts, Hydrodechlorination, Reaction Mechanisms

243. **IONICALLY CONDUCTIVE MEMBRANES FOR OXYGEN SEPARATION (LBL97-03)**
$125,000
DOE Contact: Walter M. Polansky,
(301) 903-5995
LBNL Contact: Steven J. Visco, Materials
Sciences Division, (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. The LBNL investigator recently met with the principal investigator for the industrial partner to discuss the timeline for the development plan. A tentative date of October 1997 has be agreed upon for the LBNL team to travel to industrial partner's laboratory in order to discuss the development plan in detail, and to ensure maximum productivity of the collaborative effort. This research supports the DOE mission in materials research and applications.

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

244. **LIGHT EMISSION PROCESSES AND DOPANTS IN SOLID STATE LIGHT SOURCES (LBL97-13)**
$125,000
DOE Contact: Walter M. Polansky, (301) 903-5995
LBNL Contact: Eugene E. Haller, Materials Sciences Division, (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 two years, Japanese companies have been manufacturing and selling blue GaN LEDs in bulk quantities. This project is a collaboration with Hewlett-Packard Company (HP), the leading producer of LEDs, to investigate the fundamental light-emitting mechanism. Epitaxial thin film growth, including specialized structures and doping series and basic parametric characterization, will be performed in the industrial research laboratories of HP. Highly homogenous, reliably reproducible, and stable metal organic vapor phase epitaxial growth processes have been established at HP laboratories. Highly specific spectroscopic characterization and analysis aimed at revealing the basic principles underlying doping and recombination will be performed by LBNL's Materials Sciences Division, supporting key DOE missions in materials research.

Keywords: LEDs, Semiconducting Materials, Gallium Nitride, Light Emitting Mechanisms, Heteroepitaxial Growth, Blue Emitting Diodes, Red Emitting Diodes, Green Emitting Diodes

245. **COMBINATORIAL DISCOVERY AND OPTIMIZATION OF NOVEL MATERIALS FOR ADVANCED ELECTRO-OPTICAL DEVICES (LBL97-18)**
$125,000
DOE Contact: Walter M. Polansky, (301) 903-5995
LBNL Contact: Xiao-Dong Xiang, Materials Sciences Division, (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, Mutli-Component Oxides, Electro-Optical Devices, Synthesis, Thin Films

246. **DEVELOPMENT OF A THIN-FILM BATTERY POWERED HAZARD CARD AND OTHER MICROELECTRONIC DEVICES (ORL94-39)**
$74,000
DOE Contact: Walter M. Polansky, (301) 903-5995
ORNL Contact: John Bates, Solid State, (423) 574-6280

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

Keywords: Thin-Film Batteries, Microelectronics, Electronic Devices

247. **ION IMPLANTATION PROCESSING TECHNOLOGIES (ORL94-72)**
$136,000
DOE Contact: Walter M. Polansky, (301) 903-5995
ORNL Contact: Tony Haynes, Solid State, (423) 574-2858

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

Keywords: Ion Implantation, Integrated Circuits, Semiconductor Manufacturing

248. **RAPID PROTOTYPING OF CERAMICS (ORL94-95)**
$153,000
DOE Contact: Walter M. Polansky, (301) 903-5995
ORNL Contact: Robert Lauf, Engineering Technology Division, (423) 241-2102

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

Keywords: Freeform Fabrication, Rapid Manufacturing, Ceramics

249. **DEVELOPMENT OF A THIN FILM BATTERY POWERED TRANSDERMAL MEDICAL DEVICE (ORL95-11)**
$187,000
DOE Contact: Walter M. Polansky, (301) 903-5995
ORNL Contact: John B. Bates, Solid State Division, (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

250. **RAPID PROTOTYPING OF BIOCERAMICS FOR IMPLANTS (ORL95-12)**
$64,000
DOE Contact: Walter M. Polansky, (301) 903-5995
ORNL Contact: Ogbemi Omatete, Metals and Ceramics Division, (423) 576-7199

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

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

251. **DEVELOPMENT OF HIGH-TEMPERATURE SUPERCONDUCTING WIRE USING RABITS COATED CONDUCTOR TECHNOLOGIES (ORL97-02)**
$100,000
DOE Contact: Walter M. Polansky, (301) 903-5995
ORNL Contact: David K. Christen, Solid State Division Donald M. Kroeger, Metals and Ceramics Division, (423) 574-6269

This project is developing a recent breakthrough at Oak Ridge National Laboratory that offers a potential new route to the fabrication of high-temperature superconducting (HTS) wires for power applications. The new process produces high-Tc coatings that have high critical-current densities at liquid nitrogen temperatures, and enable operation in substantial magnetic fields. The present approach exploits the growth of crystalline biaxially-aligned coatings on oriented metal tapes produced by simple thermo-mechanical processing. The tapes start with inexpensive polycrystalline metals or alloys that are biaxially aligned by deformation rolling and thermal annealing treatment, followed by the epitaxial deposition of thin, passivating buffer layers. The project team is investigating the scientific and technical feasibility of making long-length coated conductors that can provide operating characteristics that are currently unattainable by any electrical conductor, including present prototype HTS tapes that utilize the "powder-in-silver-tube" fabrication approach. The research focuses on both the simplification and optimization of oxide buffer layers on reactive metals, and specifically will evaluate (co)evaporation techniques for both the buffer layer(s) and the superconductor coatings. 3M has an established experience base in high-rate deposition of other materials using this manufacturing technology. Southwire is the leading U.S. manufacturer of utility wire and cable, and is a retailer of underground transmission cables (a prime first candidate for HTS insertion). A cost-effective route to high-temperature superconducting wires would provide substantial national energy benefits in the technology of electric power production, storage, and distribution. Superconducting transmission lines alone would enable 2-3 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 will help DOE's Office of Utility Technologies, Energy Efficiency and Renewable Energy program to develop high-temperature superconductors.

Keywords: Superconducting Wires, Coatings, Metalworking, Coated Conductors, Electrical Equipment, Distribution and Transmission, High Temperature

INSTRUMENTATION AND FACILITIES

252. **MICRO-SPECTROSCOPY FACILITY FOR NEW INFRARED IMAGING MATERIALS (BNL94-60)**
$91,000
DOE Contact: Walter M. Polansky, (301) 903-5995
BNL Contact: Gwyn Williams, NSLS (516) 344-7529

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

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

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

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

Keywords: Cutting Fluids, Ceramics, Machining, Environmental

254. **NOVEL METHODS FOR FABRICATION COST REDUCTION OF PRESSURE INFILTRATION CAST METAL MATRIX COMPOSITE COMPONENTS (ORL95-01)**
$192,000
DOE Contact: Walter M. Polansky, (301) 903-5995
ORNL Contact: James Hansen, Engineering Technology Division, (423) 241-2102

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

Keywords: Pressure Infiltration Casting, Manufacture, Metal Matrix Composites

255. **ULTRA-PRECISION AUTOMATED MEASUREMENT FOR MANUFACTURING (ORL95-08)**
$75,000
DOE Contact: Walter M. Polansky, (301) 903-5995
ORNL Contact: C. Thomas, Fusion Energy Division, (423) 574-1155

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

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

256. **NEURAL NETWORK MODEL (ORL95-90)**
$248,000
DOE Contact: Walter M. Polansky, (301) 903-5995
ORNL Contact: Gerald Ludtka, (423) 574-5098

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

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

257. **MICROFABRICATED INSTRUMENTATION FOR CHEMICAL SENSING IN INDUSTRIAL PROCESS CONTROL (ORL97-08)**
$99,000
DOE Contact: Walter M. Polansky, (301) 903-5995
ORNL Contact: J. Michael Ramsey, Chemical and Analytical Sciences Division, (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 micro-fabricated 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, Manufacturing Processes

258. **MODELING AND SIMULATION OF ADVANCED SHEET METAL FORMING (PNL94-38)**
$170,000
DOE Contact: Walter M. Polansky, (301) 903-5995
PNNL Contact: Mark Smith, Materials & Chemical Sciences, (509) 376-2847

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

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

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

259. NEXT GENERATION CORROSION INHIBITORS FOR STEEL IN CONCRETE (BNL95-12)

$50,000
DOE Contact: Walter M. Polansky, (301) 903-5995
BNL Contact: Hugh Isaacs, Applied Science (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

260. PREVENTION/ELIMINATION OF METAL-WATER EXPLOSIONS IN ALUMINUM CASTING PITS (ORL92-05)

$174,000
DOE Contact: Walter M. Polansky, (301) 903-5995
ORNL Contact: Rusi P. Taleyarkhan, Engineering Technology Division, (423) 576-4735

Metal-water or steam explosions in aluminum industry casting pits have caused numerous injuries and fatalities, and significant damage and destruction of infrastructure over the past fifty years. Traditionally, industry has attempted to prevent explosions by using an empirical-based approach involving the coating of sensitive surfaces with materials like Tarset Standard (TS). However, due to environmental concerns and other reasons, TS is being discontinued from production, leaving industry with the task of evaluating and finding alternate materials. As part of this project with the Aluminum Association (AA), ORNL is investigating how steam explosions initiate over specific surfaces, and what other coatings and novel methods may be appropriate as alternatives to TS. Work completed has resulted in the development and validation of a unique apparatus that, at significant cost reduction, accurately and rapidly simulates in a laboratory environment the interaction of molten aluminum contacting various submerged surfaces without attendant safety problems associated with field experiments involving molten aluminum pours in water-filled containers. While further testing and theoretical model development still need to be done, unprecedented insights have been obtained on key phenomenological issues. This has enabled the development of a novel approach for conclusive explosion prevention. A patent has been filed and granted for this novel, environmentally-friendly, cost-effective approach based on knowledge of fundamentals of the physics of explosion initiation. Field demonstrations are planned. This project supports DOE's energy-related mission to develop a more energy-efficient metal-casting operation. Additionally, this work is expected to provide a better physical understanding of entrapment-boiling heat transfer that could be applied to safety improvements in DOE and commercial nuclear reactors.

Keywords: Aluminum Production, Aluminum Casting Explosion, Molten Aluminum, Heat Transfer, Injuries and Fatalities

261. **IN-LINE ALUMINUM SENSORS (ORL95-04)**
$113,000
DOE Contact: Walter M. Polansky,
(301) 903-5995
ORNL Contact: Jack Young, Chemical & Analytical Sciences, (423) 574-5241

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

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

262. **THE ROLE OF YTTRIUM IN IMPROVING THE OXIDATION RESISTANCE IN ADVANCED SINGLE CRYSTAL NICKEL-BASED SUPERALLOYS FOR TURBINE APPLICATIONS (ORL95-07)**
$149,000
DOE Contact: Walter M. Polansky,
(301) 903-5995
ORNL Contact: Kathleen Alexander, Metals and Ceramics Division, (423) 574-0631

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

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

263. **ATOMIC SCALE STRUCTURE OF ULTRATHIN MAGNETIC MULTILAYERS AND CORRELATION WITH RESISTANCE, GIANT MAGNETORESISTANCE, AND SPIN-DEPENDENT TUNNELING (ORL97-03)**
$100,000
DOE Contact: Walter M. Polansky,
(301) 903-5995
ORNL Contact: William H. Butler, Metals and Ceramics Division, (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, Applications

264. **PROCESSING/PROPERTY RELATIONSHIPS IN CENTRIFUGALLY CAST AL-METAL MATRIX COMPOSITES (MMC) (PNL94-02)**
$245,000
DOE Contact: Walter M. Polansky, (301) 903-5995
PNNL Contact: Ed Courtright, Material Sciences, (509) 375-6926

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

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

265. **BIOACTIVE AND POROUS METAL COATINGS FOR IMPROVED TISSUE REGENERATION (PNL95-23)**
$191,000
DOE Contact: Walter M. Polansky, (301) 903-5995
PNNL Contact: Allison Campbell, Materials & Chemical Sciences, (509) 375-2180

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

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

ADVANCED ENERGY PROJECTS PROGRAM

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

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

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

266. **COMPOSITE MAGNETOSTRICTIVE MATERIALS FOR ADVANCED AUTOMOTIVE MAGNETOMECHANICAL SENSORS**
$449,000
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%. These sensors will need to meet stringent specifications such as the ability to operate over a range of temperatures between minus 40°C and plus 85°C, be able to survive unexpected mechanical shocks of up to 500 N and operate under continual vibrational forces of 150 N. In addition, the sensors must be able to sustain overload torques of 135 N.m without malfunctioning or significantly changing sensitivity over the normal operating range of +/- 10 N.m. Analysis of the relationship between the magnetomechanical effect (the change in magnetization with stress) and the magnetostriction (particularly the rate of change of strain with magnetic field) has shown that highly magnetostrictive materials with low anisotropy, and hence high permeability, form the most 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

267. **ENERGY RELATED APPLICATIONS OF SELECTIVE LINE EMITTERS**
$266,000
DOE Contact: Walter M. Polansky, 301/903-5995
Auburn University Contact: M. Frank Rose, 334/844-5894

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

Keywords: Solar Cells, Photovoltaic, MOMBE, Metalorganic Molecular Beam Epitaxy

268. **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% 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%. 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, we have measured carrier dynamics and band gap structures for GaAs, InP and their alloys, and calculated the resonant tunneling time and the barrier potential design criteria for achieving maximum energy conversion efficiency in MQW structures. Based on these measurements and calculations, we have designed several GaAs- and InP-based MQW solar cell structures which have been 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. We will investigate resonant tunneling times for GaAs/AlGaAs and InGaAs/InP MQW structures to make sure that the resonant tunneling process dominates photocarrier collection. We will measure the I-V characteristics and investigate the energy efficiencies for GaAs/AlGaAs and InGaAs/InP MQW solar cells with different well and barrier configurations to select the best one. We will study multi-unit GaAs-and InP-based MQW solar cells to further increase the range of the band gaps and the energy efficiency. The target for the energy efficiency improvement is at least 150% 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

269. **A NOVEL TANDEM HOMOJUNCTION SOLAR CELL: AN ADVANCED TECHNOLOGY FOR HIGH EFFICIENCY PHOTOVOLTAICS**
$255,000
DOE Contact: Walter M. Polansky, 301/903-5995
Colorado State University Contact:
Bruce Parkinson, 970/491-0504

A material for the construction of a solar cell must meet a number of criteria to be suitable for large scale photovoltaic applications. It must be made up of abundant elements, which are environmentally benign, and when combined into a crystal have suitable electronic properties. The required electronic properties include a bandgap in the 1.1-1.8 eV range, high absorption coefficients to minimize the amount of material required, and high mobilities of photo generated carriers to facilitate the collection of these carriers. The semiconductor, $ZnSnP_2$, meets all of the above requirements. It is isoelectronic with the III-V alloy $InGaP_2$, but has the advantage, for photovoltaic applications, of not containing expensive and rare group III elements. In addition, this material does not contain toxic heavy metals such as are found in CdTe and $CuInSe_2$/CdS thin film solar cells. The absorption coefficient for this material is also very high. The bandgap of $ZnSnP_2$ has the additional interesting and useful property of ranging from 1.24 to 1.66 eV, depending on the preparation conditions. Bulk crystal growth techniques have not yielded high mobility $ZnSnP_2$ but there is no *a priori* reason that the electronic properties of these materials cannot be as good as III-V materials, since very high mobilities were only achieved in III-V's after the development of modern epitaxial growth techniques. State-of-the-art metal-organic molecular beam epitaxy (MOMBE) will be used to grow epitaxial layers of $ZnSnP_2$ on lattice matched GaAs substrates. Studies of the order-disorder transition in the metal sublattice, using both optical and electrical techniques and especially solid state NMR to examine atomic scale local environments, will be conducted in order to find the conditions for preparing materials with various bandgap energies and to understand the basic chemistry and physics associated with this interesting order/disorder phase transition. When the conditions are established for preparing a material of a given bandgap, a "tandem homojunction" solar cell will be fabricated by variation of growth conditions in the MOMBE chamber in the appropriate way. This device should show significant efficiency advantages over a single material device or tandem heterojunction devices where lattice mismatch produces recombination-promoting interface states.

Keywords: Solar Cells, Photovoltaics, MOMBE, Metalorganic Molecular Beam Epitaxy

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

Cryogenic solid-state refrigerators based on the Ettinghausen effect can provide vastly superior performance to Peltier devices, opening up new markets in electronics and in superconductor-, and medical applications. Surprisingly, this most effective of solid-state cryogenic refrigeration processes is not being studied at present. Yet it is much less restrictive in the possible materials that can be used, is simpler to construct (even noting that a small permanent magnet must produce a field at the device), and has already achieved lower temperatures than Peltier coolers, the only devices presently under investigation. Recent discoveries of new hybridization-gap semi-conductors and semi-metals, and the commercial availability of high-strength $Nd_2Fe_{14}B$ permanent magnets, open the way for development of new ultra-high-performance, all solid-state Ettinghausen refrigerators. We will initiate studies of such coolers using modern materials to engineer the world's best solid-state cryocooler.

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

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

Very high power conversion efficiencies (8-12%) for photochemical solar cells were reported in 1991. These solar cells consist of highly porous nanocrystalline films of TiO_2 (band gap=3.0 eV) that are sensitized to the visible region of the solar spectrum through adsorption of Ru-containing metal-organic dye complexes on the TiO_2 particle surface. This represents more than two orders of magnitude improvement in the power conversion efficiency of dye-sensitized semiconductor electrodes in a photochemical cell. A dye-sensitized photochemical solar cell system based on TiO_2 powders is very attractive from the point of view of potential low cost and high semiconductor photo stability. This project is an integrated program of basic and applied development research that is funded jointly by three U.S. Department of Energy program offices: the

Division of Chemical Sciences in the Office of Basic Energy Sciences, the Photovoltaic program in the Office of Utility Technology and Advanced Energy Projects. In addition to the molecular dye-sensitized TiO_2 system, research is also occurring to study other organic heterojunctions with wide bandgap semiconductors for photovoltaic applications. The AEP portion of the project is to develop a configuration where the system is able to efficiently split water into hydrogen and oxygen, rather than to produce electricity. An inexpensive source of solar-produced hydrogen would be greatly beneficial to the energy economy of the world, and would result in the use of hydrogen as a non-polluting substitute for many of the fuels currently in use.

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

272. **EFFICIENT ENERGY UP-CONVERSION OF INFRARED TO VISIBLE LIGHT AT SEMICONDUCTOR HETEROJUNCTIONS**
$268,000
DOE Contact: Walter M. Polansky, 301/903-5995
National Renewable Energy Laboratory 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

273. **ELECTRICALLY ACTIVE LIQUID MATRIX COMPOSITES**
$300,000
DOE Contact: Walter M. Polansky, 301/903-5995
Oak Ridge National Laboratory 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. We have recently discovered 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. In this project, we 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

274. **SEMICONDUCTOR BROADBAND LIGHT EMITTERS**
$390,000
DOE Contact: Walter M. Polansky, 301/903-5995
Sandia National Laboratory Contact:
Paul Gourley, 505/844-5806

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

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

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

275. NEXT GENERATION HIGH-TEMPERATURE STRUCTURAL MATERIALS FOR HEAT EXCHANGERS AND HEATING ELEMENTS

$294,000
DOE Contact: Walter M. Polansky, 301/903-5995
Ames Laboratory 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

276. PHOTOREFRACTIVE LIQUID CRYSTALS: NEW MATERIALS FOR ENERGY-EFFICIENT IMAGING TECHNOLOGY

$289,000
DOE Contact: Walter M. Polansky, 301/903-5995
Argonne National Laboratory Contact: Gary P. Wiederrecht, 630/252-6963

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

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

277. **TRITIATED POROUS SILICON: A STAND-ALONE POWER SOURCE**
$250,000
DOE Contact: Walter M. Polansky, 301/903-5995
Argonne National Laboratory 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

278. **SUPPORTED MOLTEN METAL CATALYSTS: DEVELOPMENT OF A NEW CLASS OF CATALYSTS**
$322,000
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, we will initially 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

279. **COMBINATORIAL SYNTHESIS OF HIGH T_c SUPERCONDUCTORS**
$250,000
DOE Contact: Walter M. Polansky, 301/903-5995
Lawrence Berkeley National Laboratory:
X. D. Xiang, 510/486-6640

Currently, there is a tremendous interest in materials such as high temperature superconductors, organic conductors, permanent magnets, nonlinear optical materials and zeolites. However, even 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. We will develop a new approach to materials discovery that will significantly increase the rate at which novel materials are discovered as well as increase our ability to correlate physical properties with structure. Specifically, we will develop the ability to rapidly synthesize and analyze large libraries, or collections, of solid state materials for specific electronic, magnetic, optical and structural properties. The aim of this project is twofold: (1) to develop the technology to the point where it can be used effectively for materials discovery; and (2) to apply the technology to the discovery of new superconducting materials.

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

280. **FABRICATION AND CHARACTERIZATION OF MICRON SCALE FERROMAGNETIC FEATURES**
$106,000
DOE Contact: Walter M. Polansky, 301/903-5995
University of Nebraska Contact:
Peter A. Dowben, 402/472-9838

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

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

281. **MICRO-HOLLOW CATHODE DISCHARGE ARRAYS: HIGH PRESSURE, NONTHERMAL PLASMA SOURCES**
$259,000
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 ten's 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 (VOC's).

Keywords: Plasma Sources, Hollow-Cathode Discharge

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

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

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

283. **EXPERIMENTAL AND THEORETICAL INVESTIGATION OF DUAL-LASER ABLATION FOR STOICHIOMETRIC LARGE-AREA MULTICOMPONENT FILM GROWTH**
$108,000
DOE Contact: Walter M. Polansky, 301/903-5995
University of South Florida Contact:
Sarath Witanachchi, 813/974-2789

We have recently discovered a novel dual-laser ablation process that dramatically alters the dynamics of the conventional single-laser ablation process. Initial experiments, using this process, allowed the production of high quality, defect-free films of Y_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 $CuIn_{1-x}Ga_xSe_2$ plumes to explore the behavior of individual elements in multi-component plumes. Investigation of spatial stoichiometric control of Ga in the $CuIn_{1-x}Ga_xSe_2$ 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

284. **SHAPE MEMORY ALLOY REINFORCEMENT OF METALS**
$405,000
DOE Contact: Walter M. Polansky, 301/903-5995
Oak Ridge National Laboratory 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. Its characteristic are that 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 the corrosion resistance of this class of composites.

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

285. **EXPLOITATION OF ROOM TEMPERATURE MOLECULE/ POLYMER MAGNETS FOR MAGNETIC AND ELECTROMAGNETIC INTERFERENCE SHIELDING AND ELECTROMAGNETIC INDUCTION APPLICATIONS**
$212,000
DOE Contact: Walter M. Polansky, 301/903-5995
Ohio State University: Arthur J. Epstein,
614/292-1133

There are increasing needs in today's society for lightweight, electromagnetic radiation shielding materials for operation at low frequencies (<MHz range). This is partially driven by the growth of electric power distribution, telecommunications, and electromechanical power devices; concerns about electromagnetic interference; and an increasing need for lightweight inductive materials for efficient and portable motors and transformers. We reported the first polymer(tetracyanoethylene)-based magnet that remained strongly magnetic up to 350 K (170°F). We also demonstrated that more-than doubling of the room temperature magnetization can be achieved using a new route. Molecule/polymer-based magnetic materials are technologically attractive due to anticipated room temperature synthesis, processing, and device manufacture. Though these materials are relatively new, we already demonstrated that unoptimized versions of the materials shield magnetic fields independent of frequency between 10 and 10^4 Hz - a range difficult to shield using electrical conductors alone - with initial room-temperature real permeabilities of 13, which is close to iron. In late 1994, a preliminary report from a French group disclosed that a second class of molecule-based magnets (based on mixed-metal Prussian Blue type materials) has magnetic transitions near room temperature. The report suggests that additional molecule-based magnetic materials may be suitable for magnetic shielding. We have now synthesized similar (but not identical) Prussian Blue type materials with vanadium replacing iron. Our preliminary results on these modified Prussian Blue-type materials revealed an even higher saturation magnetization, though a lower transition temperature than reported by the French group, indicating opportunity for chemical tuning of the magnetic properties including initial permeabilities and transition temperatures. This project involves an integrated synthesis/processing/characterization/modeling component to ascertain the feasibility of using molecule-based magnetic materials, with emphasis on

the study of the high Tc Prussian Blue-type magnetic materials, 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

286. **MOLECULAR SURFACE MODIFICATION AS A MEANS OF CORROSION CONTROL**
$292,000
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

MATERIALS, PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

PHASE I

Controlled Permeability Chemically Activated Fly Ash (CAFA) for Reactive Contaminant Barrier - DOE Contact Tom Hicks, (803) 725-2027; By-products Development Co. Contact Mr. Thomas Silverstrim, (610) 461-2961

Advanced Multilayer Braze foil for Si_3N_4 Joining - DOE Contact Yok Chen, (301) 903-3428; Eltron Research, Inc. Contact Ms. Eileen E. Sammells, (303) 440-8008

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

Fabrication of Active Braze Alloys for High Temperature Service - DOE Contact Yok Chen, (301) 903-3428; Surmet Corporation Contact Dr. Suri A. Sastri, (617) 272-3250

Diamond-Like Nanocomposites: Hard, Wear Resistant, Low Friction Coatings for Tribological Applications - DOE Contact Yok Chen, (301) 903-3428; Advanced Refractory Technologies, Inc. Contact Mr. Keith A. Blakely, (716) 875-4091

High Growth Rate Cubic Boron Nitride Deposition - DOE Contact Yok Chen, (301) 903-3428; Applied Science And Technology, Inc. Contact Mr. John M. Tarrh, (617) 937-5135

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

Nano-Layered Diboride Materials with Enhanced Hardness, Strength, and Toughness for Wear Applications - DOE Contact Yok Chen, (301) 903-3428; Hyper-therm High-temperature Composites, Inc. Contact Mr. Wayne S. Steffier, (714) 375-4085

Advanced Plasma Surface Modification System - DOE Contact Yok Chen, (301) 903-3428; Ism Technologies, Inc. Contact Mr. 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

An Ion Source Design Useful for the Production of Tribiological Thin Films - DOE Contact Yok Chen, (301) 903-3428; Stirling Technologies Inc. Contact Mrs. Bobbie C. Stirling, (423) 483-0142

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

Controlled Atmosphere Plasma Spraying of NdFeB Magnet Materials - DOE Contact Yok Chen, (301) 903-3428; Aps Material, Inc. Contact Mr. Joseph T. Cheng, (937) 278-6547

Stabilization of Nitride Magnet Material Via Sol-Gel Route - DOE Contact Yok Chen, (301) 903-3428; Chemat Technology, Inc. Contact Ms. Jenny Sajoto, (818) 727-9786

A Novel Process to Produce Nanostructured Permanent Magnetic Materials - DOE Contact Yok Chen, (301) 903-3428; Nanomaterials Research Corporation Contact Dr. Tapesh Yadav, (520) 294-7115

Coke Resistant Catalyst for the Partial Oxidation Reforming of Hydrocarbon Fuels - DOE Contact JoAnn Milliken, (202) 586-2480; Aspen Systems, Inc. Contact Mr. Hamed Borhanian, (508) 481-5058

CO Tolerant Doped-Metal Oxide Catalysts - DOE Contact JoAnn Milliken, (202) 586-2480; Giner, Inc. Contact Dr. Anthony B. LaConti, (617) 899-7270

Advanced Electrocatalysts for Direct Methanol Oxidation - DOE Contact JoAnn Milliken, (202) 586-2480; Giner, Inc. Contact Dr. Anthony B. LaConti, (617) 899-7270

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 Mr. Isy Goldwasser, (408) 328-3100

Novel Multifunctional Direct Methanol Fuel Cell Catalysts - DOE Contact JoAnn Milliken, (202) 586-2480; T/j Technologies, Inc. Contact Mr. Leslie Alexander, (313) 213-1637

Low Cost Deposition of Buffer Layers for Manufacturable YBCO HTS Conductors - DOE Contact James Daley, (202) 586-1165; American Superconductor Corporation Contact Mr. Ramesh Ratan, (508) 836-4200

Stoichiometric YBCO Epitaxial Coatings on RABITS Using Low Cost CCVD Processing - DOE Contact James Daley, (202) 586-1165; Ccvd, Inc., Dba Microcoating Technologies Contact Dr. Andrew T. Hunt, (770) 457-7767

Buffer Layers on Textured Nickel Using Commercially Viable CCVD Processing - DOE Contact James Daley, (202) 586-1165; Ccvd, Inc., Dba Microcoating Technologies Contact Mr. Jeffrey C. Moore, (770) 457-7767

Micromachined SiC Sensors For Harsh Environment Applications - DOE Contact Rolf Butters, (202) 586-0984; Advanced Technology Materials, Inc. Contact Dr. Duncan W. Brown, (203) 794-1100

Silicon Carbide Sensors for Harsh Environments - DOE Contact Rolf Butters, (202) 586-0984; Busek Company, Inc. Contact Mrs. J. Budny, (508) 655-5565

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 Ms. Faragnis Jamzadeh, (517) 349-5653

Heterogeneous Hydroformylation of Alkanes with Syngas - DOE Contact Donald Krastman, (412) 892-4720; Tda Research, Inc. Contact Mr. Michael E. Karpuk, (303) 940-2301

Advanced NZP-Ceramic Based Thermal Barrier Coatings with Enhanced Oxidation and Thermal Shock Resistance - DOE Contact Udaya Rao, (412) 892-4743; Lotec, Inc. Contact Mr. Santosh Y. Limaye, (801) 483-3100

Tubular SOFC with Deposited Nano-Scale YSZ Electrolyte - DOE Contact Udaya Rao, (412) 892-4743; Nextech Materials, Ltd. Contact Mr. William J. Dawson, (614) 766-4895

Integrated Bandpass Filter Contacts for TPV Cells - DOE Contact Bill Barnett, (301) 903-3097; Edtek, Inc. Contact Mr. William E. Horne, (206) 395-8084

In-Situ Ultrahigh-Pressure Waterjet Peening of Nuclear Reactor Internals for the Prevention of Stress Corrosion Cracking - DOE Contact John Warren, (301) 903-6491; Waterjet Technology, Inc. Contact Ms. Diana Suzuki, (206) 872-1925

Thallium-Containing III-V Quaternary Compound Semiconductor for Use in Infrared Detection - DOE Contact Karl Veith, (202) 586-6002; Astropower, Inc. Contact Mr. Thomas J. Stiner, (302) 366-0400

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 Mr. James L. Greco, 201-767-1910

AlInGaN Light Emitting Diodes for Spectroscopic Applications - DOE Contact Carl Friesen, (208) 526-1765; Svt Associates, Inc. Contact Dr. Peter Chow, (612) 934-2100

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

High Quantum Efficiency Spin-polarized Photocathodes - DOE Contact Jerry Peters, (301) 903-5228; Spire Corporation Contact Mr. Richard S. Gregorio, (617) 275-6,000

Rapid Quench Nb_3Al for High Field Accelerator Applications - DOE Contact Jerry Peters, (301) 903-5228; Plastronic, Inc. Contact Mr. 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 Mr. William O. Miller, (505) 662-0080

Epitaxial Growth of SiC on Silicon for Radiation Hard Particle Detectors - DOE Contact Richard Plano, (301) 903-4801; Lawrence Semiconductor Research Laboratory, Inc. Contact Lamonte H. Lawrence, (602) 438-2300

Development of Scintillators and Waveshifters for Detection of Ionizing Radiation - DOE Contact Richard Plano, (301) 903-4801; Ludlum Measurements, Inc. Contact Mr. Donald G. Ludlum, (915) 235-5494

Low Viscosity Organic Insulation Systems For Improved Processing and Reduced Radiation Induced Gas Evolution - DOE Contact H. Stanley Staten, (301) 903-4950; Eltron Research, Inc. Contact Ms. Eileen E. Sammells, (303) 440-8008

Radiation Resistant Joining Methods for Structural Applications in Fusion Energy Systems - DOE Contact F. W. Wiffen, (301) 903-4963; Starfire Systems, Inc. Contact Dr. Walter Sherwood, (518) 276-2112

PHASE II (FIRST YEAR)

An Attrition-Resistant Zinc Titante Sorbent for a Transport Reactor - DOE Contact Daniel C. Cicero, (304) 285-4826; Intercat Development, Inc. Contact Ms. 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 Mr. 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 Ms. 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 Mr. David A. Jackson, (609) 587-3,000

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 Ms. Susan K. Switzer, (505) 822-9186

PHASE II (SECOND YEAR)

Low Cost, Contamination-Tolerant Electrocatalysts for Low-Temperature Fuel Cells - DOE Contact David Koegel, (301) 903-5997; Aspen Systems, Inc. Contact Dr. Kang P. Lee, (508) 481-5058

A Low Cost, High Temperature Superconductor Wire Manufacturing Technology - DOE Contact James Daley, (202) 586-1165; American Superconductor Corporation Contact Mr. Ramesh Ratan, (508) 836-4200

A Low Cost Receiver Plate Manufacturing Process for High Concentration Photovoltaic Systems - DOE Contact Alec Bulawka, (202) 586-5633; Amonix, Inc. Contact Mr. Vahan Garboushian, (310) 325-8091

An Intumescent Mat Material for Joining of Ceramics to Metals at High Temperatures - DOE Contact William J. Gwilliam, (304) 285-4401; CeraMem Corporation Contact Dr. Robert L. Goldsmith, (617) 899-0467

Development of Modulator Quality Rubidium Titanyl Arsenate Crystals for Remote Sensing Laser Systems - DOE Contact Michael O'Connell, (202) 586-9311; Crystal Associates, Inc. Contact Mr. G. M. Loiacono, (201) 612-0060

A Novel Method to Recycle Thin Film Semiconductor Materials - DOE Contact Alec Bulawka, (202) 586-5633; Drinkard Metalox, Inc. Contact Mr. Fred Gallagher, (704) 332-8173

An Improved Material and Low-Cost Fabrication Options for Candle Filters- DOE Contact William J. Gwilliam, (304) 285-4401; FluiDyne Engineering Corporation Contact Dr. Gary J. Hanus, (612) 544-2721

An Integrated Catalyst/Collector Structure for Regenerative Proton-Exchange Membrane Fuel Cells - DOE Contact David Koegel, (301) 903-5997; Giner, Inc. Contact Dr. Anthony B. LaConti, (617) 899-7270

Nanostructured Interstitial Alloys as Catalysts for Direct Energy Applications - DOE Contact David Koegel, (301) 903-5997; Nanomaterials Research Corporation Contact Dr. Angelo Yializis, (602) 575-1354

Environmentally Responsible Recycling of Thin-Film Cadmium Telluride Modules - DOE Contact Alec Bulawka, (202) 586-5633; Solar Cells, Inc. Contact Mr. Frederick L. Yocum, (419) 534-3377

Low-Cost, Large-Area, High-Resistivity Substrates for Gas Microstrip Detectors - DOE Contact Richard Meyer, (301) 903-3613; Spire Corporation Contact Mr. Richard S. Gregorio, (617) 275-6000

An Economic Sorbent for the Removal of Mercury, Chlorine, and Hydrogen Chloride from Coal Combustion Flue Gases - DOE Contact Sean Plasynski, (412) 892-4867; TDA Research, Inc. Contact Michael E. Karpuk, (303) 940-2301

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

PHASE I

Nondestructive Measurements of Key Mechanical Properties of Alloy 718 Welded Structures Using Novel Stress-Strain Microprobe Technology - DOE Contact Yok Chen, (301) 903-3428; Advanced Technology Corporation Contact Mr. Fahmy M. Haggag, (423) 483-5756

Processing For Surface Hardness: Novel Characterization Techniques for Dynamic Tribological Properties of Thin Films - DOE Contact Yok Chen, (301) 903-3428; Nano Instruments, Inc. Contact Dr. Warren C. Oliver, (423) 481-8454

A Novel Mass Spectrometer for Characterization of Electrochemical Processes - DOE Contact Al Landgrebe, (202) 586-1483; Southwest Sciences, Inc. Contact Mr. Alan C. Stanton, (505) 984-1322

New Insulation Techniques for High Voltage, High Frequency Motors - DOE Contact Jim Merritt, (202) 586-0903; Satcon Technology Corporation Contact Mr. David B. Eisenhaure, (617) 661-0540

Development of Carbon Products from the Waste Stream of the Super Critical Deashing Process in Coal Liquefaction - DOE Contact Thomas Brown, (412) 892-4691; Fiber Materials, Inc. Contact Mr. David R. Audie, (207) 282-5911

Sol-Gel Coatings as Corrosion Barriers for Carbonate Fuel Cell Components - DOE Contact Udaya Rao, (412) 892-4743; Energy Research Corporation Contact Mr. Hans C. Maru, (203) 825-6006

Enhanced Flaw Detection by Time-Reversal Auto-Focusing of an Ultrasonic Array - DOE Contact John Warren, (301) 903-6491; Foster-Miller, Inc. Contact Mr. Adi R. Guzdar, (617) 684-4239

High Resolution Cryogenic Calorimeter for Beta and Gamma Ray Detection - DOE Contact Dick Meyer, (301) 903-3613; Concept Technology Contact Dr. Alan Singsaas, (619) 695-0402

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

High Current Capacity High Temperature Superconducting Film Based Tape for High Field Magnets - DOE Contact Jerry Peters, (301) 903-5228; Midwest Superconductivity, Inc. Contact Dr. Jonathan W. Wilson, (913) 749-3613

A Polycrystalline Pixel Diamond Film Particle Detector - DOE Contact Richard Plano, (301) 903-4801; Applied Science And Technology, Inc. Contact Mr. John M. Tarrh, (617) 937-5135

Resistance Welding Vanadium Alloys - DOE Contact F. W. Wiffen, (301) 903-4963; Hitech Metallurgical Co. Contact Mr. Kenneth H. Holko, (619) 586-7272

Low Cost Technique for Testing Ceramic Insulator Coatings - DOE Contact F. W. Wiffen, (301) 903-4963; Reb Research And Consulting Contact Dr. Robert E. Buxbaum, (810) 547-7942

PHASE II (FIRST 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 Mr. Ramesh Ratan, (508) 836-4200

Low Cost Multifilament Composite Process - DOE Contact James Daley, (202) 586-1165; American Superconductor Corporation Contact Mr. 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 Mrs. Anne Churchill, (540) 731-0655

Novel Fiber-Based Adsorbent Technology - DOE Contact Kristine Bilenki, (301) 903-1687; Chemica Technologies, Inc. Contact Mr. Daniel J. Brose, (541) 385-0355

Metal-Binding Silica Materials for Wastewater Cleanup - DOE Contact Kristine Bilenki, (301) 903-1687; Tpl, Inc. Contact Ms. 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 Mr. 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 Ms. Andrea Gray, (619) 453-4451

PHASE II (SECOND YEAR)

Rotating, In-Plane Magnetization and Magneto-Optic Imaging of Cracks Under Coatings on Ferromagnetic Metals - DOE Contact Dennis Harrison, (301) 903-2884; Physical Research, Inc. Contact Dr. William C. L. Shih, (310) 378-0056

Development of Laser Materials and Rugged Coatings as Components for Tunable Ultraviolet Laser Systems - DOE Contact Michael O'Connell, (202) 586-9311; Lightning Optical Corporation Contact Mr. Wayne Ignatuk, (813) 938-0092

Application of Raman Spectroscopy to Identification and Sorting of Post-Consumer Plastics for Recycling - DOE Contact Simon Friedrich, (202) 586-6759; National Recovery Technologies, Inc. Contact Dr. Charles E. Roos, (615) 734-6400

A Sensor for Automated Plastics Sorting - DOE Contact Simon Friedrich,(202) 586-6759; Radiation Monitoring Devices, Inc. Contact Dr. Gerald Entine, (617) 926-1167

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

PHASE I

Hydrocarbon Gas Sensors Based on Wide Band-Gap Semiconductors - DOE Contact Wanda Ferrell, (301) 903-0043; Svt Associates, Inc. Contact Dr. Peter Chow, (612) 934-2100

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

A Novel Technology for Si_3N_4-To Superalloy Joints With High Use Temperature Capability - DOE Contact Yok Chen, (301) 903-3428; Materials And Electrochemical Research (MER) Contact Dr. Raouf Loutfy, (520) 574-1980

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 Mr. Charles Carlberg, (303) 778-6566

A New Semi-Solid Forming Process For Fabrication of High Volume Fraction (>15 vol%) Metal/Metal Carbide Nanocomposites - DOE Contact Yok Chen, (301) 903-3428; Nanopowder Enterprises, Inc. Contact Dr. Gary S. Tompa, (908) 885-5909

Alternative Metal Forming Using Laser Engineered Net Shaping - DOE Contact Yok Chen, (301) 903-3428; Optomec Design Company Contact Mr. Thomas A. Swann, (505) 343-9139

Production of High Performance BSCCO-2223 Tapes Using Hydrostatic Pressure - DOE Contact James Daley, (202) 586-1165; American Superconductor Corporation Contact Mr. Ramesh Ratan, (508) 836-4200

Development of Long-length Fabrication Technology for High T_c Superconductors Operation in High Magnetic Fields at 77K - DOE Contact James Daley, (202) 586-1165; Ues, Inc. Contact Mr. Francis F. Williams, Jr., (937) 426-6900

Non-Linear Inductor for Power Electronics Protection - DOE Contact Jim Merritt, (202) 586-0903; Energen, Inc. Contact Dr. Chad H. Joshi, (617) 271-9876

Novel Fabrication of Low Cost Performance Bipolar Plates - DOE Contact Jim Merritt, (202) 586-0903; Materials And Electrochemical Research (MER) Contact Dr. J. C. Withers, (520) 574-1980

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

Reduced Part Count Motor Fabrication - DOE Contact Jim Merritt, (202) 586-0903; Unique Mobility, Inc. Contact Mr. Donald A. French, (303) 278-2002

Removal of Particulate and SO_x/NO_x Precursors in Integrated Gasification Combined Cycle Systems - DOE Contact Mildred Perry, (412) 892-6015; Industrial Filter And Pump Manufacturing Company Contact Mr. Jeffrey D. Burgeson, (708) 656-7800

Use of Novel, Low-Cost Additives to Improve Sorbent Efficiency for Control of Mercury Emissions in Coal-Fired Power Plant Flue Gases - DOE Contact Thomas Brown, (412) 892-4691; Physical Sciences Inc. Contact Mr. George E. Caledonia, (508) 689-0003

Mixed Phase Positive Electrodes for Long Life AMTEC Modules - DOE Contact Bill Barnett, (301) 903-3097; Tda Research, Inc. Contact Mr. Michael E. Karpuk, (303) 940-2301

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

Cost Reduction for Production of Superconducting Niobium Cavities - DOE Contact Jerry Peters, (301) 903-5228; Meyer Tool & Mfg., Inc. Contact Mr. Edward C. Bonnema, (708) 425-9080

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

Direct Adhesive Technology for Arbitrary Conductors - DOE Contact Jerry Peters, (301) 903-5228; Advanced Magnet Laboratory, Inc. Contact Mr. Mark W. Senti, (407) 728-7543

Controlled Processing for High-Performance Fine Filament Bi-2223 Conductors - DOE Contact Jerry Peters, (301) 903-5228; American Superconductor Corporation Contact Mr. Ramesh Ratan, (508) 836-4200

Development of a High Field NbTi Superconductor Using an Approach Combining Artificial Flux Pinning With Conventional Thermomechanical Processing - DOE Contact Jerry Peters, (301) 903-5228; Supercon, Inc. Contact Ms. Elaine Drew, (508) 842-0174

Conventionally Processed NbTi Superconductors with Artificial Ferromagnetic Pinning Centers for High Magnetic Field (>8 T) Application - DOE Contact Jerry Peters, (301) 903-5228; Supercon, Inc. Contact Ms. Elaine Drew, (508) 842-0174

Liquid Core Optical Scintillating Fibers - DOE Contact Richard Plano, (301) 903-4801; Nano Systems, Inc. Contact Mr. Robert W. Boerstler, (203) 881-2827

High Performance Heat Pipe Cooling of Electron Cyclotron Heating Mirrors P12-2426 - DOE Contact T. V. George, (301) 903-4957; Thermacore, Inc. Contact Mr. Donald M. Ernst, (717) 569-6551

Reaction Bonding of Silicon Carbide Composites for Fusion Applications - DOE Contact F. W. Wiffen, (301) 903-4963; Busek Company, Inc. Contact Mrs. J. Budny, (508) 655-5565

Net Shape Gradient W-Cu Plasma Facing Components by Pressure Infiltration - DOE Contact Sam E. Berk, (301) 903-4171; Foster-miller, Inc. Contact Mr. Adi R. Guzdar, (617) 684-4239

Joining of Silicon Carbide for Fusion Applications - DOE Contact F. W. Wiffen, (301) 903-4963; Lanxide Corporation Contact Mr. Marc S. Newkirk, (302) 456-6217

A Novel Divertor Design Based on a Tungsten Wire Brush Tile - DOE Contact Sam E. Berk, (301) 903-4171; Materials And Electrochemical Research (MER) Contact Dr. Raouf O. Loutfy, (520) 574-1980

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

Fabrication for Reliable Tungsten Brush Structures for Fusion Reactor Applications - DOE Contact Sam E. Berk, (301) 903-4171; Surmet Corporation Contact Dr. Suri A. Sastri, (617) 272-3250

PHASE II (FIRST 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 Mrs. 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 Mr. 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 Mr. Brian L. Sperry, (303) 427-1312

Infrared Hollow Waveguide Organic Solvent Analyzer - DOE Contact Wanda Ferrell, (301) 903-0043; Polestar Technologies, Inc. Contact Ms. 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 Mr. 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 Mr. Ed LeBaker, (408) 733-7780

High Performance X-Ray and Neutron Microfocusing Optics - DOE Contact Tim Fitzsimmons, (301) 903-9830; Hirsch Scientific Contact Mr. 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 Mr. 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 Mr. 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 Mr. 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 Ms. 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 Mr. 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 Ms. 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 Mr. Richard S. Gregorio, (617) 275-6000

Large Room Temperature $Cd_{1-x}Zn_xT_e$ 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 Mr. 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 Mr. Norman L. Duncan, (703) 516-6372

PHASE II (SECOND YEAR)

Advanced High Power Silicon Carbide Internally Cooled X-Ray - DOE Contact Bill Oosterhuis, (301) 903-3426; SSG, Inc. Contact Mr. Dexter Wang, (617) 890-0204.

Chemical Microsensor Arrays as Integrated Chip Compatible Devices for Chemical Weapons Nonproliferation Inspection - DOE Contact Robert Marianelli, (301) 903-5808; Microsensor Systems, Inc. Contact Dr. Hank Wohltjen, (502) 745-0099

A High Resolution Multi-hit Time to Digital Converter Integrated Circuit - DOE Contact Robert Woods, (301) 903-3367; Lecroy Corporation Contact Mr. Joseph Migliozzi, (914) 578-6006

A Helium-Cooled Faraday Shield Using Porous Metal Cooling - DOE Contact T. V. George, (301) 903-4957; Thermacore, Inc. Contact Mr. Donald M. Ernst, (717) 569-6551

Low Cost Fabrication of Large Silicon Carbide/Silicon Carbide Composite Structures - DOE Contact F. W. Wiffen, (301) 903-4963; Lanxide Corporation Contact Dr. Christopher Kennedy, (302) 456-6320

Bandgap-Engineered Thermophotovoltaic Devices for High Efficiency Radioisotope Power - DOE Contact Bill Barnett, (301) 903-3097; Edtek, Inc. Contact Mr. W. E. Horne, (206) 395-8084

Rugged, Tunable Infrared Laser Sources - DOE Contact Michael O'Connell, (202) 586-9311; Deacon Research Contact Dr. Olive Lee, (415) 493-6100

An Innovative Membrane and Process for Removal and Recovery of Natural Gas Liquids - DOE Contact William J. Gwilliam, (304) 285-4401; Membrane Technology And Research, Inc. Contact Ms. E. G. Weiss, (415) 328-2228

A Lower Cost Molten Carbonate Matrix - DOE Contact William J. Gwilliam, (304) 285-4401; M-C Power Corporation Contact Mr. Patrick F. McSweeney, (708) 986-8040

SMALL BUSINESS TECHNOLOGY TRANSFER PROGRAM

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

PHASE I

Improved Beta-Alumina Fabrication Using Rapid Plasma Sintering - DOE Contact David Koegel, (301) 903-3159; Advanced Modular Power Systems, Inc. Contact Dr. Thomas Hunt, (313) 677-4260

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

PHASE II (FIRST YEAR)

Cabled Monofilament Subelements for Improved Multifilament Niobium Tin Performance and Reduced Cost - DOE Contact Jerry Peters, (301) 903-5228; Supercon, Inc. Contact Ms. Elaine Drew, (508) 842-0174

PHASE II (SECOND YEAR)

Laser Processing of Thermal Sprayed Beryllium Plasma Facing Components - DOE Contact T. V. George, (301) 903-4957; Plasma Processes, Inc. Contact Mr. Tim McKechnie, (205) 851-7653

Amorphous Silicon/Crystalline Silicon Heterojunctions for Nuclear Radiation Detector Applications - DOE Contact Richard Rinkenberger, (301) 903-3613; Quantrad Sensor, Inc. Contact Dr. Nicholas J. Szluk, (408) 727-7827

Low Loss Sapphire Windows for High Power Microwave Transmission - DOE Contact T. V. George, (301) 903-4957; Thoughtventions Unlimited Contact Dr. Stephen C. Bates, (203) 657-9014

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

PHASE 1

Novel Thin Film Scintillator for Intermediate Energy Photons Detection and Imaging - DOE Contact Dick Meyer, (301) 903-4398; NZ Applied Technologies, Inc. Contact Mr. Peter Norris, (617) 935-0300

Silicon Carbide Heat Exchanger for Advanced Coal-Based Power Systems - DOE Contact Udaya Rao, (412) 892-4743; Busek Company, Inc. Contact Dr. Vlad Hruby, (508) 655-5565

Advanced Ceramic Hot Gas Filters - DOE Contact Theodore McMahon, (304) 285-4865; LoTec, Inc. Contact Mr Santosh Y. Limaye, (801) 483-3100

PHASE II (FIRST YEAR)

High Speed Motor Alternators for Hybrid Electric Vehicle Energy Storage - DOE Contact Jim Merritt, (202) 586-0903, SatCon Technology Corporation Contract Mr. Michael Turmelle, (617) 349-0861

A Flywheel Motor Alternator for Hybrid Electric Vehicles - DOE Contact Jim Merritt, (202) 586-0903; Visual Computing Systems Corporation Contact Mr. Robert J. Westerkamp, (812) 923-7474

PHASE II (SECOND YEAR)

Environmentally Benign Manufacturing of Compact Disk Stampers - DOE Contact Helen Kerch, (301) 903-2346; Prism Company Contact Mr. Peter Ciriello, (508) 785-2511

OFFICE OF FUSION ENERGY SCIENCES

The mission of the Office of Fusion Energy Sciences (OFES) is to advance plasma science, fusion science and fusion technology—the knowledge base needed for an economically and environmentally attractive fusion energy source. The policy goals that support this mission are: (1) advance plasma science in pursuit of national science and technology goals; (2) develop fusion science, technology and plasma confinement innovations as the central theme of the domestic program; and (3) pursue fusion energy science and technology as a partner in the international effort.

A significant component of the fusion energy program is the development and validation of the materials required for the fusion systems. Materials must be developed that will meet the unique requirements of fusion, as well as the standard requirements of a high efficiency, high reliability power generating system. The unique requirements of fusion are the result of the intense neutron environment, dominated by the 14 MeV neutrons characteristic of the deuterium-tritium fusion reaction. For performance, the materials must have slow and predictable degradation of properties in this neutron environment. For safety and environmental considerations, materials must be selected with activation products that neither decay too rapidly (affecting such safety factors as system decay heat) nor too slowly (affecting the waste management concerns for end-of-life system components). Materials that meet these requirements are referred to as "Low Activation Materials." Programs to develop the materials for plasma-facing components, for diagnostic and control systems, for structures in the high neutron flux regions, for the production of tritium in the blanket, and for the superconducting magnets required for confinement are sponsored by OFES.

The fusion 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 usefull 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. More than one-half of the materials work sponsored by OFES is in support of the ITER collaboration.

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

287. **STRUCTURAL MATERIALS DEVELOPMENT**
$670,000
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

288. **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

289. **FUSION SYSTEMS MATERIALS**
$3,270,000
DOE Contact: F. W. Wiffen, (301) 903-4963
ORNL Contacts: E. E. Bloom, (423) 574-5053 and A. F. Rowcliffe, (423) 574-5057

This program is directed at the development and qualification of structural materials and insulating ceramics for use in components of fusion power systems exposed to the intense neutron flux. Candidate low activation structural material systems include ferritic/martensitic steels, vanadium alloys and SiC/SiC composites. Investigations focus on the most critical questions or limiting properties in each of these systems: ferritic/ martensitic steels—DBTT transition shifts and fracture toughness; vanadium alloys—welding processes, effects of irradiation on fracture toughness, and compatibility in proposed coolant systems; SiC/SiC composites—definition of the effects of irradiation on properties and structure and evaluation of advanced composite fibers and coatings. The insulating ceramic activity is initially developing an understanding of irradiation effects in alumina, spinel and other materials. The greatest concern is to establish the permanent and transient changes in electrical properties, requiring measurement while the specimen is under irradiation. Work on these material classes involves irradiation in fission reactors, including HFIR, HFBR, and other test reactors, as partial simulation of the fusion environment.

Keywords: Ceramics, Steels, Vanadium, Silicon Carbide, Composites, Irradiation Effects, Electrical Properties

290. **STRUCTURAL MATERIALS FOR FUSION SYSTEMS**
$960,000
DOE Contact: F. W. Wiffen, (301) 903-4963
PNNL Contacts: R. H. Jones, (509) 376-4276 and R. 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

291. **DEVELOPMENT OF RADIATION-HARDENED CERAMIC COMPOSITES FOR FUSION APPLICATIONS**
$28,000
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

292. **DAMAGE ANALYSIS AND FUNDAMENTAL STUDIES FOR FUSION REACTOR MATERIALS DEVELOPMENT**
$150,000
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 ITER and other fusion systems.

Keywords: Vanadium, Steels, Irradiation Effects Fracture

293. **DEVELOPMENT OF LITHIUM-BEARING CERAMIC MATERIALS FOR TRITIUM BREEDING IN FUSION REACTORS**
$100,000
DOE Contact: S. Berk, (301) 903-4171
ANL Contact: C. Johnson, (630) 252-7533

Research activities are focused on critical issues of ceramic breeder blankets for fusion reactors, including ceramic breeder material tritium retention and release, ceramic breeder and beryllium irradiation response, chemical compatibility of ceramic breeder materials and beryllium with blanket coolant and structural materials, and heat transfer and temperature control in ceramic breeder materials. Computer models are tested against data on irradiation of lithium-oxide and lithium-zirconate materials in a fast-spectrum fission reactor. There is good agreement between model predictions and experimental data in the area of transient tritium release.

Keywords: Ceramics, Compatibility, Tritium Release, Modeling, Lithium Ceramics

294. **POST-IRRADIATION EXAMINATION OF LITHIUM-BEARING CERAMIC MATERIALS FOR TRITIUM BREEDING IN FUSION REACTORS**
$20,000
DOE Contact: S. Berk, (301) 903-4171
PNNL Contact: G. Hollenberg, (509) 376-5515

Research activities are for post-irradiation examinations (PIE) of the ceramic breeder materials irradiated in the Fast Flux Test Facility. The PIE was conducted as part of the BEATRIX-II program under an International Energy Agency agreement between the US, Japan and Canada. PIE involved capsule disassembly, neutron radiography, plenum gas analysis, photography, mensuration characterization, tritium inventory measurements, microstructural characterization and thermal conductivity measurements. PIE for specimens from the BEATRIX-II Phase 1 irradiation (lithium-oxide irradiated to 5 percent lithium atom burnup) and the

Phase 2 irradition (lithium-oxide and lithium-zirconate irradiated to 5 percent lithium atom burnup) was completed in FY 1995.

Keywords: Ceramics, Lithium Ceramics, Tritium Release

295. **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

296. **ITER MATERIALS EVALUATION**
$330,000
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

297. **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

298. **DEVELOPMENT OF Nb_3Sn SUPERCONDUCTING WIRE FOR THE ITER MAGNET PROGRAM**
$200,000
DOE Contact: T. V. George, (301) 903-4957
MIT Contact: J. Minervini, (617) 253-5503

A major development and industrial procurement activity of a high critical current density Nb_3Sn superconducting wire for use in the ITER Model Coil program was completed recently. Intermagnetics General Corporation/Advanced Superconductors Inc. (IGC/ASI) delivered over 5 metric tons of superconducting wire to the ITER HP1 strand specification. The strand was subsequently cabled by BIW, Inc. into 4 cables of greater than 1000 strands, each over 200m long, for use in the US Inner Coil Module of the ITER CS Model Coil. The strand procurement program was supported by characterization and acceptance measurements of strand critical superconducting properties and ac losses by several university and national laboratories. Further work is continuing to enhance the wire performance while reducing production costs.

Keywords: Superconductors, Magnet Materials, Nb_3Sn

299. **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. IAI has recently delivered over 60 metric tons of this material in the shape of square extrusions with a circular hole, in unit lengths up to 10m, for the ITER CS Model Coil Program. 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 1997
Office of Environmental Management - Grand Total	$6,870,939
Materials Properties, Behavior, Characterization or Testing	$6,870,939
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 Repository	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
Photooxidation of Organic Wastes Using Semiconductor Nanoclusters	417,000
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 Solution	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
Ion-Exchange Processes and Mechanisms in Glasses	300,333
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

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), a joint program of EM and the Office of Energy Research (ER). Basic research under the EMSP contributes to environmental management activities that decrease risk to the public and workers, provide opportunities for major cost reductions, reduce time required to achieve EM's mission goals, and, in general, address problems that are considered intractable without new knowledge. This program is designed to inspire "breakthroughs" in areas critical to the EM mission through basic research and is managed in partnership with ER. ER's well-established procedures are used for merit review of applications to the EMSP. Subsequent to the formal scientific merit review, applications that are judged scientifically meritorious are evaluated by DOE for relevance to the objectives of the EMSP. The current EMSP portfolio consists of 202 awards amounting to a total of $160 million in three-year funding. Twenty-one of those awards were in scientific disciplines related to materials issues that have potential to solve Environmental Management challenges. The 1997 component of materials research amounts to $6,870,939. This figure is smaller than that reported for FY96 because of a redefinition of the materials research component. 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

300. **THE INFLUENCE OF RADIATION AND MULTIVALENT CATION ADDITIONS ON PHASE SEPARATION AND CRYSTALLIZATION OF GLASS**
$241,000
DOE Contact: Chet Miller, (202) 586-3952
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

301. **CHEMICAL AND CERAMIC METHODS TOWARD SAFE STORAGE OF ACTINIDES USING MONAZITE**
$429,000
DOE Contact: Chet Miller, (202) 586-3952
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

302. **ATMOSPHERIC-PRESSURE PLASMA CLEANING OF CONTAMINATED SURFACES**
$404,000
DOE Contact: Chet Miller, (202) 586-3952
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 μm/hour, and tantalum at between 1 and 2 μm/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 NF_3, CF_4, C_2F_6, O_2,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

303. **CHEMICAL DECOMPOSITION OF HIGH-LEVEL NUCLEAR WASTE STORAGE/DISPOSAL GLASSES UNDER IRRADIATION**
$163,000
DOE Contact: Chet Miller, (202) 586-3952
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

304. **ANALYSIS OF SURFACE LEACHING PROCESSES IN VITRIFIED HIGH-LEVEL NUCLEAR WASTES USING IN-SITU RAMAN IMAGING AND ATOMISTIC MODELING**
$186,333
DOE Contact: Chet Miller, (202) 586-3952
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

305. **INVESTIGATION OF MICROSCOPIC RADIATION DAMAGE IN WASTE FORMS USING ODNMR AND AEM TECHNIQUES**
$232,667
DOE Contact: Chet Miller, (202) 586-3952
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 $^{238,239}Pu$, $^{241,243}Am$, and $^{243,244}Cm$ and the beta- and alpha-decay of ^{249}Bk(^{249}Cf) 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

306. **IN-SITU SPECTRO-ELECTROCHEMICAL STUDIES OF RADIONUCLIDE CONTAMINATED SURFACE FILMS ON METALS AND THE MECHANISM OF THEIR FORMATION AND DISSOLUTION**
$335,000
DOE Contact: Chet Miller, (202) 586-3952
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

307. **DETERMINATION OF TRANSMUTATION EFFECTS IN CRYSTALLINE WASTE FORMS**
$304,328
DOE Contact: Chet Miller, (202) 586-3952
Argonne National Laboratory Contact:
Denis M. Strachan, (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 ^{137}Cs 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 α-decay will give support to the selection of alternate waste forms for separated ^{137}Cs and give information on the long-term behavior of candidate waste forms.

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

308. **RADIATION EFFECTS ON MATERIALS IN THE NEAR-FIELD OF NUCLEAR WASTE REPOSITORY**
$136,000
DOE Contact: Chet Miller, (202) 586-3952
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

309. **AN ALTERNATIVE HOST MATRIX BASED ON IRON PHOSPHATE GLASSES FOR THE VITRIFICATION OF SPECIALIZED NUCLEAR WASTE FORMS**
$208,278
DOE Contact: Chet Miller, (202) 586-3952
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

310. **MICROSTRUCTURAL PROPERTIES OF HIGH LEVEL WASTE CONCENTRATES AND GELS WITH RAMAN AND INFRARED SPECTROSCOPIES**
$155,000
DOE Contact: Chet Miller, (202) 586-3952
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

311. **FUNDAMENTAL THERMODYNAMICS OF ACTINIDE-BEARING MINERAL WASTE FORMS**
$383,333
DOE Contact: Chet Miller, (202) 586-3952
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

312. **PHOTOOXIDATION OF ORGANIC WASTES USING SEMICONDUCTOR NANOCLUSTERS**
$417,000
DOE Contact: Chet Miller, (202) 586-3952
SNL Contact: J. P. Wilcoxon, (505) 844-3939
Colorado State University Contact: D. F. Kelley, (970) 491-6381

Solar detoxification is a process wherein sunlight is captured by a semiconductor particle in suspension to create electrons and holes that then diffuse to the particulate surface to effect the oxidation and reduction of toxic pollutants. Using solar energy to oxidize organic chemicals to carbon dioxide and dilute mineral acids is very energy efficient compared to other methods such as incineration. Finding an efficient particulate has thus been a focus of research, which has had only limited success, the fundamental problem being that materials that efficiently absorb in the visible portion of the solar spectrum also photocorrode.

Past solar detoxification efforts have relied almost exclusively on titanium dioxide, and although it is photostable, it is a *white* material with a UV bandgap that absorbs less than 7% of the solar spectrum. It also suffers from electron-hole recombination in commercially available forms. Recent research has made possible the synthesis of photostable semiconductor nanoclusters with *visible* band gaps that can be tuned by adjusting the cluster size. Thus bulk materials with near IR absorbence edges can be made into visible band-edge materials with stronger redox potentials.

The rate of electron-hole recombination is small in nanoclusters, so they have the potential to act as highly efficient solar detoxification agents. In effect, they act more like molecular organic photoredox catalysts, but with significant advantages in chemical stability because they are inorganic. This project is investigating the use of these materials in practical detoxification applications.

Keywords: Photooxidation, Nanoclusters

313. OPTIMIZATION OF THERMOCHEMICAL, KINETIC, AND ELECTROCHEMICAL FACTORS GOVERNING PARTITIONING OF RADIONUCLIDES DURING MELT DECONTAMINATION OF RADIOACTIVELY CONTAMINATED STAINLESS STEEL
$400,000
DOE Contact: Chet Miller, (202) 586-3952
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

314. MECHANISM OF PITTING CORROSION PREVENTION BY NITRITE IN CARBON STEEL EXPOSED TO DILUTE SALT SOLUTIONS
$216,667
DOE Contact: Chet Miller, (202) 586-3952
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

315. STABILITY OF HIGH-LEVEL WASTE FORMS
$254,000
DOE Contact: Chet Miller, (202) 586-3952
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

316. **RADIATION EFFECTS IN NUCLEAR WASTE MATERIALS**
$960,000
DOE Contact: Chet Miller, (202) 586-3952
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

317. **NEW SILICOTITANATE WASTE FORMS: DEVELOPMENT AND CHARACTERIZATION**
$400,000
DOE Contact: Chet Miller, (202) 586-3952
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 ^{137}Cs and ^{90}Sr) 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

318. **ION-EXCHANGE PROCESSES AND MECHANISMS IN GLASSES**
$300,333
DOE Contact: Chet Miller, (202) 586-3952
PNL Contact: B. Peter McGrail, (509) 376-9193
LBNL Contact: David K. Shuh, (510) 486-6937

Recent performance assessment calculations of a disposal system at Hanford, Washington for low activity waste glass show that a Na ion-exchange reaction can effectively increase the radionuclide release rate by over a factor of 1000 and so is a major factor that currently limits waste loading. However, low temperature ion exchange has not been thought to be important in recent analyses of waste glass durability. The objective of this work is to develop an understanding of the processes and mechanisms controlling alkali ion exchange and to correlate the kinetics of the ion-exchange reaction with glass structural properties.

Ion-exchange reaction mechanisms are being studied by using nuclear reaction analysis techniques to probe the distribution of isotopically-labeled elements in the hydrated layers on glass surfaces. Differences in the uptake and distribution of these isotopes provide a signature characteristic of specific ion-exchange reactions. X-ray absorption spectroscopy is used to identify and correlate key structural properties, such as the number of nonbridging oxygens, bonding of alkali to other elements in the glass, and alkali coordination, with differences in measured rates of alkali exchange. The fundamental understanding of the ion-exchange process developed under this study will provide a sound scientific basis for formulating low exchange rate glasses with higher waste loading, resulting in substantial production and disposal cost savings.

Keywords: Ion-exchange, Glasses

319. **DISTRIBUTION & SOLUBILITY OF RADIO-NUCLIDES & NEUTRON ABSORBERS IN WASTE FORMS FOR DISPOSITION OF PLUTONIUM ASH & SCRAPS, EXCESS PLUTONIUM, AND MISCELLANEOUS SPENT NUCLEAR FUELS**
$600,000
DOE Contact: Chet Miller, (202) 586-3952
PNNL Contact: Xiangdong Feng, (509) 373-7284
Australian Nuclear Science & Technology Organisation Contact: Eric R. Vance
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) 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

320. **MODELING OF DIFFUSION OF PLUTONIUM IN OTHER METALS AND OF GASEOUS SPECIES IN PLUTONIUM-BASED SYSTEMS**
$145,000
DOE Contact: Chet Miller, (202) 586-3952
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 situ*ations 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 situ*ations, 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

OFFICE OF NUCLEAR ENERGY, SCIENCE AND TECHNOLOGY

	FY 1997
Office of Nuclear Energy, Science and Technology - Grand Total	$65,080,000
Office of Engineering and Technology Development	$ 2,080,000
Space and National Security Programs	$ 2,080,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 1,815,000
Development of an Improved Process for the Manufacture of DOP-26 Iridium Alloy Blanks, Product Characterization and Exploratory Alloy Improvement Studies	1,425,000
Carbon-Bonded Carbon Fiber Insulation Production Maintenance, Manufacturing Process Development and Product Characterization	390,000
Materials Properties, Behavior, Characterization or Testing	$ 265,000
Development of Materials for Advanced Radioisotope Power Systems	265,000
Office of Naval Reactors	$63,000,000[1]

[1]This excludes $47 million for the cost of irradiation testing in the Advanced Test Reactor (ATR).

OFFICE OF NUCLEAR ENERGY, SCIENCE AND TECHNOLOGY

OFFICE OF ENGINEERING AND TECHNOLOGY DEVELOPMENT

SPACE AND NATIONAL SECURITY PROGRAMS

Space and National Security Programs include the development and production of radioisotope power systems for both space and terrestrial applications and the technical direction, planning, demonstration and delivery of space nuclear reactor power and propulsion systems. During FY 1997, space nuclear reactor power and propulsion activities remained dormant. Essentially all materials programs were aimed at: (1) support of the production of General Purpose Heat Source-Radioisotope Thermoelectric Generators for the NASA Cassini Mission, (2) maintenance of iridium alloy and carbon bonded carbon fiber insulation heat source components manufacturing capability, (3) continued improvement in heat source materials and their production processes and product characterization, and (4) materials (non-thermoelectric) support for future high efficiency advanced radioisotope power systems.

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

321. DEVELOPMENT OF AN IMPROVED PROCESS FOR THE MANUFACTURE OF DOP-26 IRIDIUM ALLOY BLANKS, PRODUCT CHARACTERIZATION AND EXPLORATORY ALLOY IMPROVEMENT STUDIES
$1,425,000
DOE Contact: W. Barnett, (301) 903-3097
ORNL Contacts: E. P. George, (615) 574-5085 and E. K. Ohriner, (615), 574-8519

An iridium alloy, DOP-26 (i.e., Ir-0.3 wt.% W with Th and Al dopant additions), serves as the fuel clad or capsule material for isotope heat sources employed in recent and contemporary space power systems for NASA deep space missions. This program is aimed at the optimization of the new improved process route previously selected for the production of DOP-26 iridium alloy sheet, namely a consumable vacuum arc cast/extrusion/"warm" rolling route. The effectiveness of this production process was further demonstrated in the 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 initiated. 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.

Keywords: Consumable Arc Melt, Extrusion, Noble Metal, Rolling, Forming

322. CARBON-BONDED CARBON FIBER INSULATION PRODUCTION MAINTENANCE, MANUFACTURING PROCESS DEVELOPMENT AND PRODUCT CHARACTERIZATION
$390,000
DOE Contact: W. Barnett, (301) 903-3097
ORNL Contacts: R. Dinwiddie, (615) 574-9978 and 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 1997 program encompassed (1) continued maintenance of capability for both tube and plate billet production, (2) continued characterization of Cassini CBCF insulation high temperature thermal conductivity, and (3) study of the role of inert additives on high temperature thermal conductivity.

Keywords: Insulators/Thermal, High Temperature Service, Fibers

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

323. DEVELOPMENT OF MATERIALS FOR ADVANCED RADIOISOTOPE POWER SYSTEMS
$265,000
DOE Contact: W. Barnett, (301) 903-3097
Oak Ridge National Laboratory Contact: J. King, (423) 574-4807

Materials support was provided for two advanced radioisotope power systems, namely a heat source for a small Stirling Engine and an Alkali metal Thermal to Electric Converter (AMTEC) Cell.

Long-term intermediate temperature creep properties of T-111 tantalum alloy were continued. Evaluation of the high temperature reflectivity of rhodium plated Haynes-25 alloy was initiated.

Keywords: Tantalum Alloy, Creep, Rhodium Plate, Reflectivity

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 $110 million in FY1997 including approximately $47 million as the cost for irradiation testing in the Advanced Test Reactor. The Naval Reactors contact is David I. Curtis, (703) 603-5565.

OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT

	FY 1997
Office of Civilian Radioactive Waste Management - Grand Total	$15,400,000
Materials Properties, Behavior, Characterization or Testing	$15,400,000
Waste Packages	$15,400,000

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

324. **WASTE PACKAGES**
$15,400,00
DOE Contact: David Haught, (702) 794-5474
M&O Contacts: Hugh Benton,
(702) 295-4389 and David Stahl,
(702) 295-4383

The development of the nation's high-level waste repository has been delegated to DOE's Yucca Mountain Site Charactization Project Office. Framatome Cogema Fuels (formerly B&W Fuel Company), as part of the Civilian Radioactive Waste Management System Management & Operating (M&O) Contractor, is responsible for designing the waste package and related portions of the engineered barrier system. The advanced conceptual design was completed in 1996. Progress on the waste package and the supporting materials studies has been documented in various reports.

The waste package design effort includes the development of waste packages to accommodate uncanistered commercial spent nuclear fuel (SNF), canistered SNF, canistered defense high-level waste, Navy fuel, and other DOE owned spent nuclear fuel. The analytical process that is underway to support these designs included thermal, structural, and neutronic analyses. Also included are materials selection and engineering development. The waste package materials effort includes the testing and modeling of materials being considered for inclusion in the waste package and the engineered barrier system. The testing includes general aqueous and atmospheric testing, localized attack such as pitting and service corrosion, microbiologically-influenced corrosion, galvanic corrosion, and stress corrosion cracking. The corrosion test facility started the long-term (at least five-year) test program in FY 1996 with corrosion-allowance materials. Corrosion-resistant materials were added in FY 1997. Waste form materials are also being evaluated for alteration and leaching under repository-relevant conditions. Chemical simulations have been performed to evaluate the performance of engineered barrier materials. These latter efforts support both design and performance assessment.

Keywords: Yucca Mountain Repository, Waste Package, Engineered Barrier System

OFFICE OF DEFENSE PROGRAMS

	FY 1997
Office of Defense Programs - Grand Total	$96,633,600
The Weapons Research, Development and Test Program	$96,633,600
Sandia National Laboratories	$23,183,600
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 6,231,000
Materials Processing	2,999,000
Sol-Gel Preservation of Mankind's Cultural	137,000
Synthesis and Modeling of Field-Structured Anisotropic Composites	370,000
Molecular Imprinting in Aerogels for Remote Sensing of Chemical Weapons and Pesticides	390,000
Smart Interface Bonding Alloys (SIBA): Tailoring Thin Film Mechanical Properties	455,000
Atomically-Engineered Nanostructures: An Interdisciplinary Approach 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
System Studies in Electrochemical Processing Properties	100,000
Materials Properties, Behavior, Characterization or Testing	$11,227,000
Aging and Reliability	1,997,000
Nanoscale Structures and Phenomena	1,070,000
Applications-Driven Interdisciplinary Research	885,000
Materials Stability and Thin Coatings	2,483,000
Catalytic Membrane Sensors	361,600
Photonic Band Gap Structures as a Gateway to Nano-Photonics	375,000
Model Determination and Validation for Reactive Wetting Processes	351,000
Ultra-hard Multilayer Coatings Properties	472,000
Molecular-Scale Lubricants for Micromachine Applications	475,000
Understanding and Control of Energy Transfer Mechanisms in Optical Ceramics Properties	400,000
Integrated Thin Film Structures for IR Imaging Properties	430,000
The Initiation and Propagation of Nano-Scale Cracks at an Adhesive/Solid Interface Properties	400,000
Monolithic Structures for Nanoseparation Properties	339,000
Fundamental Aspects of Micromachine Reliability	350,000
Intelligent Polymers for Nanodevice Performance Control	439,000
Quantum Dot Arrays	400,000
Device or Components Fabrication, Behavior or Testing	$ 1,522,600
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
Modeling Electrodeposition for Metal Microdevice Fabrication Properties	265,000
Instrumentation and Facilities	$ 4,203,000
Advanced Analytical Techniques	998,000
Nanostructures, Advanced Materials and Ion Beam Sciences	2,792,000
Physico-Chemical Stability of Solid Surfaces	413,000

OFFICE OF DEFENSE PROGRAMS (continued)

	FY 1997
The Weapons Research, Development and Test Program (continued)	
Lawrence Livermore National Laboratory	$20,250,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 7,775,000
Engineered Nanostructure Laminates	2,000,000
Sol Gel Coatings	335,000
KDP and DKDP Crystal Development and Production	4,000,000
Energetic Materials Strategic Chemistry	350,000[1]
CHEETAH Thermochemical Code	190,000[1]
Explosives Development	900,000[1]
Materials Properties, Behavior, Characterization or Testing	$ 2,250,000
Interfaces, Adhesion, and Bonding	250,000
Laser Damage: Modeling and Characterization	1,000,000
KDP Characterization	1,000,000
Instrumentation and Facilities	$10,225,000
Scanning Tunneling Microscopy (STM) and Atomic Force Microscopy (AFM)	250,000
Fatigue of Metal Matrix Composites	500,000
Materials Produced with Dynamic High Pressure	50,000
Properties of Hydrogen at High Shock Pressures and Temperatures	400,000
Atomic Level Explosive Calculations	400,000
Metastable Solid-Phase High Energy Density Materials	535,000
AFM Investigations of Crystal Growth	290,000
Uranium Casting Program	1,000,000
Uranium Spin Forming	1,500,000
Plutonium Near Net Shape Casting	2,500,000
Electron Beam Cold Hearth Melting of Uranium	900,000
NIF Capsule Mandrel R&D	800,000
Polyimide Coating Technology for ICF Targets	500,000
Beryllium Ablator Coatings for NIF Targets	600,000
Los Alamos National Laboratory	$53,200,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 2,500,000
Rapid Solidification Processing	500,000
Structural Alloy Development	2,000,000
Materials Structure or Composition	$ 3,300,000
National High Magnetic Field Laboratory	1,800,000
Neutron Diffraction	1,500,000

[1]This activity is jointly funded (50:50) by DOE DP and the DoD.

OFFICE OF DEFENSE PROGRAMS (continued)

	FY 1997
The Weapons Research, Development and Test Program (continued)	
Los Alamos National Laboratory (continued)	
Materials Properties, Behavior, Characterization or Testing	$18,300,000
Dynamic Mechanical Properties of Weapons Materials	2,000,000
Deformation Characterization and Modeling	5,000,000
Materials Aging	11,000,000
Powder Characterization	300,000
Device or Component Fabrication, Behavior or Testing	$29,100,000
Manufacturing Process Development	8,000,000
Advanced Engineering Methods Development	1,100,000
Component Fabrication	10,000,000
Laser Target Fabrication	5,000,000
Pulsed Power Target Fabrication	3,000,000
Advanced Strategic Computing Initiative Materials Modeling	2,000,000

THE WEAPONS RESEARCH, DEVELOPMENT AND TEST PROGRAM

SANDIA NATIONAL LABORATORIES

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

325. **MATERIALS PROCESSING**
$2,999,000
DOE Contact: Robin Staffin, (202) 586-7590
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

326. **SOL-GEL PRESERVATION OF MANKIND'S CULTURAL**
$137,000
DOE Contact: Maurice J. Katz, (202) 586-6385
SNL Contact: William Hammetter, (505) 272-7603

Our cultural heritage, as reflected in artifacts and works of art, is being lost at an astonishing rate due to the ravages of nature and especially mankind. Since the industrial revolution, chemical by-products of man's technological advances have caused the deterioration of our most precious cultural treasures. Most vulnerable are stone objects that are subjected to outdoor environments in industrialized or urban settings. This research comprises three basic elements: (1) molecular modeling of the weathering mechanisms and resultant surface structure of model limestones, (2) mineral-specific passivation of the weathered surface to prevent further hydrolytic attack, and (3) *in situ* polymerization (within the weathered surface) to form a UV stable network that imparts strength and hydrophobicity. This research has been conducted in collaboration with The Metropolitan Museum of Art (MMA) and The Getty Conservation Institute (GCI), who have provided samples and ensured relevance to the conservation communities. In addition to solving the urgent need to preserve our cultural treasures, the methodology developed here can be applied to other mineral-corrosion problems such as the degradation of concrete infrastructure, environmental contamination by leached mine tailings, protection of ship hulls, and scale formation in petroleum wells.

Keywords: Conservation, Sol-Gel

327. **SYNTHESIS AND MODELING OF FIELD-STRUCTURED ANISOTROPIC COMPOSITES**
$370,000
DOE Contact: Maurice J. Katz, (202) 586-6385
SNL Contact: James Martin, (505) 844-9125

The modeling, synthesis and processing capability is being developed to create novel anisotropic polymer/ceramic and polymer/metal composite materials by applying external electric or magnetic fields to systems consisting of a polymerizable continuous phase into which particles having an electric permittivity or magnetic permeability mismatch are suspended. A linear field will create one-dimensional particle chains, a well known effect. This project used the recent discovery that rotating fields create two-dimensional particle sheets in the plane of the field. These unique structures can be captured by polymerizing the continuous phase during a field anneal. A key aspect of this program is modeling and controlling the evolution of structure in these materials.

Keywords: Polymer, Ceramic, Metal, Composite

328. **MOLECULAR IMPRINTING IN AEROGELS FOR REMOTE SENSING OF CHEMICAL WEAPONS AND PESTICIDES**
$390,000
DOE Contact: Maurice J. Katz, (202) 586-6385
SNL Contact: Roger Lee Clough (505) 844-3492

Recent events in Japan, Iraq, and elsewhere have underlined the need for reliable, inexpensive sensors for chemical warfare agents. Warfare agents, such as sarin, belong to a general class of phosphate and phosphonate esters that have a very broad range of activities including materials for nuclear weapons production, pesticides, genetic material, and biological cellular signals. Current methods to detect these agents are limited to laboratory analysis. An in-field, real-time sensor-based approach with remote sensing capability is highly desired.

Under this project, highly sensitive and specific optical sensors for phosphate and phosphonate esters are being designed and developed using molecular recognition sites in high surface area aerogels. Molecular recognition sites are engineered using computer aided molecular design and generated via the powerful "template imprinting" technique in aerogels. The material is designed with active fluorophores at the receptor site reporting on target molecule recognition via fluorescence signal through complexation with the phosphonate guest. From these materials are developed various toxic gas sensor motifs, such as visual detectors that monitor color changes, or extremely low level sensing applications that follow fluorescence lifetimes. Granular bulk aerogels will also be developed for our "smart pebbles" concept. Application of this inconspicuous material to an area of interest will provide a remote sensing system for covert chemical warfare agent production facilities, battlefield alert for chemical weapons release, and agricultural pesticide application and runoff.

Keywords: Aerogel, Remote Sensing

329. **SMART INTERFACE BONDING ALLOYS (SIBA): TAILORING THIN FILM MECHANICAL PROPERTIES**
$455,000
DOE Contact: Maurice J. Katz, (202) 586-6385
SNL Contact: Stephen Foiles, (925) 294-2898

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

This project includes growth, characterization and modeling of films grown using SIBA templates. Characterization includes atomic imaging of the dislocations structure, measurement of the mechanical properties of the film using interface force microscopy (IFM) and the nanoindenter, and measurement of the electronic structure of the SIBA with synchrotron photoemission. Resistance of films to sulfidation and oxidation is also being examined. The Paragon parallel processing computer is being used to calculate the structure of the SIBA and thin films in order to develop ability to predict and tailor SIBA and thin film behavior.

This work will lead to the development of a new class of thin film materials with properties tailored by varying the composition of the SIBA, serving as a buffer layer to relieve the strain between the substrate and the thin film. Such films will have improved mechanical and corrosion resistance allowing application as protective barriers for weapons applications. They will also exhibit enhanced electrical conductivity and reduced electromigration making them particularly suitable for application as interconnects and other electronic needs.

Keywords: Joining, Smart Materials

330. **ATOMICALLY-ENGINEERED NANOSTRUCTURES: AN INTERDISCIPLINARY APPROACH PROPERTIES**
$400,000
DOE Contact: Maurice J. Katz, (202) 586-6385
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 heterogeneoous 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 unambiquous, 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 A and B tasks, 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

331. **ENABLING SCIENCE & TECHNOLOGY FOR COLD SPRAY DIRECT FABRICATION PROPERTIES**
$330,000
DOE Contact: Maurice J. Katz, (202) 586-6385
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 (finer grain size, no brittle phases, minimal oxidation, less residual stress, etc.). With CSP, one might also deposit functionally graded or layered materials at low temperatures, thus eliminating joining operations, simplifying design/fabrication, reducing part counts, and decreasing stress cracking. (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, weapons, etc.

This project explores the use of cold spray processing for direct fabrication of simple proof-of-concept shapes.

Keywords: Cold Spray Processing, Direct Fabrication

332. **ATOMIC-LEVEL STUDIES OF SURFACTANT-DIRECTED MATERIALS GROWTH**
$400,000
DOE Contact: Maurice J. Katz, (202) 586-6385
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

333. **FREEFORMING OF CERAMICS AND COMPOSITES FROM COLLOIDAL SLURRIES**
$450,000
DOE Contact: Maurice J. Katz, (202) 586-6385
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

334. **LASER ASSISTED ARC WELDING FOR ALUMINUM ALLOYS**
$200,000
DOE Contact: Maurice J. Katz, (202) 586-6385
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

335. **SYSTEM STUDIES IN ELECTROCHEMICAL PROCESSING PROPERTIES**
$100,000
DOE Contact: Maurice J. Katz, (202) 586-6385
SNL Contact: Martin Carr, (505) 844-6070

The objective of this project is to develop physical models and associated analytical tools that will allow a number of electrochemical processes of interest to be more effectively characterized. In addition to the availability of new models and tools, the important contribution of this activity is the determination of the conceptual feasibility of using this type of approach to solve engineering-level electrochemical problems. Because of the limited scope of the project, two very specific processes have been selected for detailed study. Four primary tasks are included: (1) detailed analysis of relevant literature information, (2) planning and execution of required experiments, (3) formulation of analytical models, and (4) laboratory demonstration/ validation of the models using untested configuration.

Keywords: Electrochemical Processing, Modeling

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

336. **AGING AND RELIABILITY**
$1,997,000
DOE Contact: Robin Staffin, (202) 586-7590
SNL Contact: Richard J. Salzbrenner, (505) 844-9408

The Materials Aging and Reliability and Aging 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

337. **NANOSCALE STRUCTURES AND PHENOMENA**
$1,070,000
DOE Contact: Robin Staffin, (202) 586-7590
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

338. **APPLICATIONS-DRIVEN INTERDISCIPLINARY RESEARCH**
$885,000
DOE Contact: Robin Staffin, (202) 586-7590
SNL Contact: Samuel T. Picraux, (505) 844-5829

The Applications-Driven Interdisciplinary Research works with the National Security sector [including Micromechanical (IMEMS) reliability and high-reliability neutron tube fabrication and mid-IR based chemical sensors] and focuses on collaboration. Research specifically focuses on National Security and building on emerging technology core capabilities.

Keywords: Sensors, Micromechanical, Infrared

339. **MATERIALS STABILITY AND THIN COATINGS**
$2,483,000
DOE Contact: Robin Staffin, (202) 586-7590
SNL Contact: Terry A. Michalske, (505) 844-5829

The Materials Stability Thin Coatings research seeks to develop and apply atomic- and molecular-level microscopies, spectroscopies, and theoretical models to examine fundamental materials processes that control phenomena, including: interfacial adhesion, lubrication, wear thermal stability, thin-film and surface kinetics, radiation effects, corrosion, hydrogen effects, curing, fracture, and chemical and physical vapor deposition processes. Also, this research seeks to develop a scientific basis for design, manufacture, and application of small, smart products; new models to predict useful lifetimes for currently used materials and structures; and transfers of technology regarding degradation of resistant/stable materials to U.S.

Keywords: Coatings, Stability

340. **CATALYTIC MEMBRANE SENSORS**
$361,600
DOE Contact: Maurice J. Katz, (202) 586-6385
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. In FY 1997, the project met the following milestones toward the synthesis and processing of these CMSs: (1) synthesis and characterization of double alkoxides, (2) membrane modified sensor (H2 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

341. **PHOTONIC BAND GAP STRUCTURES AS A GATEWAY TO NANO-PHOTONICS**
$375,000
DOE Contact: Maurice J. Katz, (202) 586-6385
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 nano-meter length scale for the control and confinement of light. The low loss, highly reflective and quantum interference nature of a PBG material makes it one of the most promising candidates for realizing an extremely high-Q resonant cavity, >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

342. **MODEL DETERMINATION AND VALIDATION FOR REACTIVE WETTING PROCESSES**
$351,000
DOE Contact: Maurice J. Katz, (202) 586-6385
SNL Contact: Frederick Yost, (505) 844-5278

This work was undertaken to develop a computational model of reactive wetting processes. Although wetting and spreading have been studied in great detail, most of this work pertains only to inert or nonreactive wetting. Inert wetting is driven by an imbalance of surface tension forces with no other interaction between the wetting liquid and the substrate. In reactive wetting other processes such as diffusion, intermetallic reactions, and environmental reactions may drive or hinder the continuous advance of the wetting front. Additional aspects of reactive wetting are being investigated to determine the driving and dissipation forces that are thought to control the spreading behavior in reactive wetting systems. With this understanding wetting problems of technological significance can be controlled and processes can be improved.

Keywords: Wetting, Computation

343. **ULTRA-HARD MULTILAYER COATINGS PROPERTIES**
$472,000
DOE Contact: Maurice J. Katz, (202) 586-6385
SNL Contact: Ellen Stechel, (505) 844-2436

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

This project uses a combination of growth, analysis and theoretical modeling capabilities at Sandia that could possibly lead to a revolutionary jump in both materials understanding and performance—a material harder than diamond.

Keywords: Multilayer, Ultrahard

344. **MOLECULAR-SCALE LUBRICANTS FOR MICROMACHINE APPLICATIONS**
$475,000
DOE Contact: Maurice J. Katz, (202) 586-6385
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

345. **UNDERSTANDING AND CONTROL OF ENERGY TRANSFER MECHANISMS IN OPTICAL CERAMICS PROPERTIES**
$400,000
DOE Contact: Maurice J. Katz, (202) 586-6385
SNL Contact: Clifford Renschler, (505) 844-0324

A radically new material strategy for rare-earth (RE) hosts was developed. In this approach, the optical performance of the dopant is modified through atomic-level engineering of its local structural environment in a nanocomposite, optical ceramic host material. This program examines the influence of nanoscale hetero-geneities on ion-ion and ion-lattice energy transfer dynamics through atomic-level engineering of the RE ion local environment. Both direct optical evaluation of the dopant behavior and theoretical structural modeling and simulation were employed evaluate these novel host materials. The local atomic structure in the vicinity of RE dopants was successfully modeled using a powerful Sandia-developed (QUEST) computational approach based on local density functional theory. In Al_2O_3, this technique is being extended to model the difference in tetrahedral versus octahedral site symmetry on the density of electronic and vibrational states, to allow the investigation of a variety of dopant site types characteristic of multiphase hosts (e.g., interfaces and clusters). This work will result in a new, computer-based, predictive materials modeling capability in both single and multiphase candidate hosts, before fabrication, and will yield an improved class of materials at the junction between fundamental solid-state physics and nanophase science to enable RE optics in photonic integrated circuits.

Keywords: Energy Transfer, Optics, Ceramics

346. **INTEGRATED THIN FILM STRUCTURES FOR IR IMAGING PROPERTIES**
$430,000
DOE Contact: Maurice J. Katz, (202) 586-6385
SNL Contact: Alan Hurd, (505) 272-7642

Uncooled pyroelectric IR imaging systems, such as night vision goggles, offer important strategic advantages in battlefield scenarios and reconnaissance surveys. Unfortunately, the current technology for fabricating these devices is limited by low throughput and high cost which ultimately limit the availability of these sensor devices.

This project is developing an alternative design for pyroelectric IR imaging sensors that utilizes a multilayer thin film deposition scheme to create a fully integrated thin film element on an active silicon substrate for the first time. The approach combines a thin film pyroelectric imaging element with a thermally insulating SiO_2 aerogel thin film to produce a new type of uncooled IR sensor that offers significantly higher thermal, spatial, and temporal resolutions at a substantially lower cost per unit.

Keywords: Thin Films, IR Imaging

347. **THE INITIATION AND PROPAGATION OF NANO-SCALE CRACKS AT AN ADHESIVE/SOLID INTERFACE PROPERTIES**
$400,000
DOE Contact: Maurice J. Katz, (202) 586-6385
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

348. **MONOLITHIC STRUCTURES FOR NANOSEPARATION PROPERTIES**
$339,000
DOE Contact: Maurice J. Katz, (202) 586-6385
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

349. **FUNDAMENTAL ASPECTS OF MICROMACHINE RELIABILITY**
$350,000
DOE Contact: Maurice J. Katz, (202) 586-6385
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, electrostatics, etc.). Issues to be addressed include auto-adhesion (stiction), friction and wear. Microbridge structures with varying geometry and surface properties (roughness, chemical coatings etc.) 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 foundation. The tool set can be used to calculate and characterize reliability of micromachines for integrated microsystem applications.

Keywords: Micromachine, Reliability

350. **INTELLIGENT POLYMERS FOR NANODEVICE PERFORMANCE CONTROL**
$439,000
DOE Contact: Maurice J. Katz, (202) 586-6385
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

351. **QUANTUM DOT ARRAYS**
$400,000
DOE Contact: Maurice J. Katz, (202) 586-6385
SNL Contact: George Samara

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

352. **WIDE-BANDGAP COMPOUND SEMICONDUCTORS TO ENABLE NOVEL SEMICONDUCTOR DEVICES PROJECT**
$290,000
DOE Contact: Maurice J. Katz, (202) 586-6385
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 bandstructure and development of a model for optical gain and lasing which will include an exact treatment of Coulomb effects. Steady state and time-resolved luminescence 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 bandstructure 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

353. SCANNING PROBE-BASED PROCESSES FOR NANOMETER-SCALE DEVICE FABRICATION
$442,600
DOE Contact: Maurice J. Katz, (202) 586-6385
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

354. SURFACE MICROMACHINED FLEXURAL PLATE WAVE DEVICE INTEGRATED ON SILICON
$525,000
DOE Contact: Maurice J. Katz, (202) 586-6385
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

355. MODELING ELECTRODEPOSITION FOR METAL MICRODEVICE FABRICATION PROPERTIES
$265,000
DOE Contact: Maurice J. Katz, (202) 586-6385
SNL Contact: Jill Hruby, (925) 294-2596

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

To help understand and optimize the electroforming portion of the LIGA process, this project is developing a one-dimensional numerical model describing the electrodeposition of metal into high aspect-ratio molds having lateral dimensions on the micron scale. To guide model development, and later to validate this model, a series of one and two-dimensional laboratory experiments are being coordinated.

Keywords: *Micromachines, Electrodeposition*

INSTRUMENTATION AND FACILITIES

356. **ADVANCED ANALYTICAL TECHNIQUES**
$998,000
DOE Contact: Robin Staffin, (202) 586-7590
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

357. **NANOSTRUCTURES, ADVANCED MATERIALS, AND ION BEAM SCIENCES**
$2,792,000
DOE Contact: Robin Staffin, (202) 586-7590
SNL Contact: George A. Samara, (505) 844-6653

This research keeps Sandia at the forefront of experimental and theoretical materials science relevant to National Security needs and includes experiment and theory of new materials (e.g., nanoclusters, nanostructures, polymeric ferro electrics, amorphous diamond films, and shock wave-induced phenomena) of proven or potential application in current or future weapon systems. The program also develops new ion-beam based tools required to fully characterize or modify these new materials systems (e.g., radiation effects microscopy) and new computational tools for improved structural/electronic/photonic property simulations.

Keywords: Nanostructures, Ion Beam

358. **PHYSICO-CHEMICAL STABILITY OF SOLID SURFACES**
$413,000
DOE Contact: Maurice J. Katz, (202) 586-6385
SNL Contact: Terry Michalske, (505) 844-5829

The application of physico-chemical phenomena to either increase machinability of hard materials, improve the wear resistance of cutting surfaces, or enhance sintering of particle compacts can have large economic impact on technologies ranging from materials forming processes to oil well drilling. Unfortunately, the broad application of these physico-chemical principles is limited by the ability to predict the optimum conditions for a wide variety of materials surfaces. Predictive models must be built upon understanding of the elementary events involved in surface damage and mobility. The project is developing a new approach to examine the fundamental mechanisms controlling physico-chemical surface stability that combines: (1) atomic-scale control of surface contact forces and displacements under well controlled adsorbate conditions using the Interfacial Force Microscope; (2) atomic-level imaging of surface and near-surface structure and defects using Field Ion Microscopy and Transmission Electron Microscopy; and (3) first-principles modeling of the effect surface stress on adsorbate bonding interactions and the subsequent generation of surface damage.

Keywords: Stability, Surface, Wear

LAWRENCE LIVERMORE NATIONAL LABORATORY

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

359. **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 (0.2 nm) to hundreds of monolayers (>100 nm). At this time more than 75 of the 92 naturally occurring elements have been incorporated in multilayers in elemental form or as components of alloys or compounds. In this work deposits containing up to 225,000 layers of each of two materials to form up to 500μ thick samples have been synthesized for mechanical property studies of multilayer structures.

These unique man-made materials have demonstrated extremely high mechanical performance as a result of the inherent ability to control both composition and structure at the near atomic level. Also, mechanically active flaws that often limit mechanical performance are controllable so that the full potential of the structural control available with multilayer materials is accessible. Systematic studies of a few multilayer structures have resulted in free-standing foils with strengths approaching those of whiskers, approximately 70 percent of theory. Also, new mechanisms for mechanically strengthening materials are accessible with nanostructure laminates.

Applications now under development include: coatings for aircraft gas turbine engines; EUV, soft X-ray and X-ray optics spectroscopy and imaging; high performance capacitors for energy storage; capacitor structures for industrial applications; high performance tribological coatings; strength materials; integrated circuit interconnects; machine tool coatings; projection X-ray lithography optics.

Keywords: Thin Films, Multilayer Technology

360. **SOL GEL COATINGS**
$335,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LLNL Contact: I. M. Thomas, (925) 423-4430 and J. Britten, (925) 423-7653

This project investigates the preparation of multilayer sol-gel high reflection (HR) coatings using colloidal SiO_2 with either HfO_2 or ZrO_2. The incorporation of an organic polymer binder such as polyvinyl alcohol or polyvinyl pyrolidinone into the high index component has resulted in an increase in the damage threshold and a decrease in the number of layer pairs required for high reflection. A laboratory size meniscus coater was evaluated and found to produce mirrors of high optical performance and adequate damage threshold. This is now the preferred method of application, and a large machine capable of producing Beamlet and NIF size mirrors is in place.

Keywords: Sol Gel Coatings, Meniscus Coater, HR Coatings

361. **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

362. **ENERGETIC MATERIALS STRATEGIC CHEMISTRY**
$350,000[1]
DOE Contact: Bharat Agraval, (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

363. **CHEETAH THERMOCHEMICAL CODE**
$190,000[1]
DOE Contact: Bharat Agraval, (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

364. **EXPLOSIVES DEVELOPMENT**
$900,000[1]
DOE Contact: Bharat Agraval, (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

365. **INTERFACES, ADHESION, AND BONDING**
$250,000
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 described above, 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-

---

[1]*General energetic materials-related input.* This activity is jointly funded (50:50) by DOE DP and the DoD.

vacuum diffusion bonding machine has been developed in parallel with this research project.

Keywords: Interfaces, Bonding, Electronic Structure

366. **LASER DAMAGE: MODELING AND CHARACTERIZATION**
$1,000,000
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). Materials of primary concern are optical coatings and polished fused silica surfaces. The primary characterization tools used in the studies include Atomic Force Microscopy (AFM), Total internal Reflection Microscopy (TIRM), Near-field Scanning Optical Microscopy (NSOM), Secondary Ion Mass Spectroscopy (SIMS) and Photothermal Microscopy (PTM). Efforts are focused on the development of characterization tools that have improved resolution and detection limits and that can differentiate between damaging and non-damaging defects.

An understanding is also needed of the growth of damage resulting from illumination pulses after the initial onset of damage. 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 are being determined. Also of interest is the influence of optic environment (air vs. Vacuum) on the damage processes.

Keywords: Coatings, Atomic Force Microscopy, Laser Damage

367. **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

368. **SCANNING TUNNELING MICROSCOPY (STM) AND ATOMIC FORCE MICROSCOPY (AFM)**
$250,00
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 spectroscopy (STS) are being used for the following studies:

Uranium Hydriding - Understanding the early stages of uranium hydriding and the effect of surface impurities is of paramount importance in science based stockpile stewardship. The UHV STM/AFM is used to determine the effect of local impurities on uranium hydriding.

Electronic Properties of Nano-scale Particles - Nm-scale clusters various materials, deposited by laser ablation and by evaporation in a noble gas atmosphere onto the basal plane of graphite are analyzed by STM to determine their size distribution and by optical spectroscopy and electron spectroscopy to determine their size-dependent optical properties and electronic structure.

- Dissolution Rate of Uranium Oxide - The dissolution of uranium oxide by ground is being determined by AFM on single crystal uranium oxide by monitoring the rate of recession of the U02 surface with reference to a gold marker.
- Combined Scanning Probe Microscopy/Nano-Indentation - Used to identify the local mechanical properties of composite materials such as fiber reinforced plastics, bone-, tooth- and arterial-tissue from healthy and diseased arteries.

Keywords: NDE, Chemical Reaction, Uranium Hydriding, Stockpile Stewardship, Uranium Oxide Dissolution, Nuclear Waste Disposal, Etching, Cluster, Nano-indentation, Mechanical Properties, Biomaterials, Tooth, Artery, Bone

369. **FATIGUE OF METAL MATRIX COMPOSITES**
$500,000
DOE Contact: Warren Chernock, (202) 586-7590
LLNL Contact: Donald Lesuer, (925) 422-9633

This project involves Lawrence Livermore National Laboratory and General Motors. The project is studying the mechanisms of high cycle fatigue in squeeze cast metal matrix composites. The life limiting microstructural features are being determined and the processing-structure-property correlations are being established. Models that can predict lifetimes will be developed.

Keywords: Materials Properties, Behavior, Characterization or Testing

370. **MATERIALS PRODUCED WITH DYNAMIC HIGH PRESSURE**
$50,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LLNL Contact: William Nellis, (925) 422-7200

This project produces novel materials (crystal structures, microstructures, and properties) using high shock pressures. The terms dynamic and shock are used synonymously in this context. Tuneable shock pressure pulses are produced by the impact of a projectile launched from a small two-stage light-gas gun. Shock pressures range from 0.01-1 Mbar, temperatures range from 50 up to a few 1000°C, strain rates on loading range above 10^8/s and quench rates on release of pressure are 10^{12} bar/s and 10^9 K/s in specimens which are recovered intact for investigation. A gas gun is used to achieve these high shock pressures. Specimens range from 1 micron to 3 mm thick and from 3 to 23 mm in diameter. The observed material structures are correlated with computational simulations to enhance understanding of the effects produced. For example, a computational model of the dynamic compaction of nanocrystalline Al particles was shown to be in good agreement with the structure of compacts produced experimentally. A wide variety of materials characterization measurements are made both before and after application of high dynamic pressures, including X-ray diffraction, TEM, SEM, magnetization, NMR, and neutron scattering. Over the past few years nanocrystalline Al, ceramic, and magnetic powders have been dynamically compacted, unusual glass has been produced in bulk and nanocrystalline Si in grain boundaries by shock compressing quartz single crystals, and impacts in nature have been investigated by studying structural effects in shocked minerals. A new gas breach to achieve shock pressures of <50 Kbar to induce high densities of defects and compact powders was built in FY 1997.

Keywords: Shock Pressures, Gas Gun, Materials Characterization, Ceramics, Magnets, Nanocrystalline Si, Glass

371. **PROPERTIES OF HYDROGEN AT HIGH SHOCK PRESSURES AND TEMPERATURES**
$400,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LLNL Contacts: William Nellis, (925) 422-7200 and Neil Holmes, (925) 422-7213

The properties of hydrogen at high pressures and temperatures are a "Holy Grail" issue for laser fusion, condensed matter physics, and planetary physics. Hydrogen in the form of deuterium-tritium is the fuel in laser fusion targets; the metallization of hydrogen by electronic bandgap closure has been a key goal of condensed matter physics since the early part of this century: and Jupiter with its 300 Earth masses is 90 percent hydrogen at high pressures and temperatures. This project measures temperatures and electrical conductivities of cryogenic liquid hydrogen and deuterium shock-compressed to pressures up to 2 Mbar ($2x10^6$ bar) and temperatures up to 5000 K with a two-stage light-gas gun. These conditions are achieved by impact of projectiles accelerated to velocities up to 8 km/s. Shock temperatures up to 5000 K at 1 Mbar were measured by a fast optical spectrometer and show that hydrogen undergoes a continuous dissociative phase transition above 200 kbar. This continuous dissociation absorbs energy, which causes lower temperatures and higher densities in the Mbar shock pressure range than was thought previously.

Electrical conductivities were measured using metal electrodes at pressures in the range 1 to 2 Mbar at calculated temperatures of 2000 to 4000 K. A novel technique was used to produce just enough shock heating to excite just enough electronic carriers to be able to measure the electrical conductivity of hydrogen at Mbar pressures in the short time duration of the experiment. These are the only electrical conductivity measurements on condensed hydrogen at any pressure. This project, for the first time, metallized hydrogen at 1.4 Mbar and 3000 K in the fluid and determined the density dependence of the electronic bandgap in the molecular fluid phase. The observed metallization pressure in the fluid is about one-half what was predicted for the solid at 0 K.

Keywords: Shock Pressures, Shock Temperatures, Electrical Conductivities, Gas Gun, Hydrogen, Cryogenics, Equation of State, Dissociation, Metallization

372. **ATOMIC LEVEL EXPLOSIVE CALCULATIONS**
$400,000
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. The target is to provide 10 to 15 percent more detonation energy than CL-20 with no decrease in sensitivity.

Keywords: Energetic Materials, High Explosives, Molecular Design, Detonation

373. **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.

The existence of a new extended solid (polymeric) phase of CO has been verified at about 50 kbar. This new material is recoverable at ambient conditions, and is believed to be energetic. The equation-of-state of various candidate structures for CO have been calculated, but further experimental constraints are needed in the structure and bond nature. Accordingly, Raman measurements of absorption in the visible and infrared have been performed. This information has provided important insights as to the character of the bonds present in this material. During FY 1997 techniques for generating "large" samples of the extended-solid phase of CO at high pressures have been developed, in order to measure stoichiometry and energy content.

Keywords: Energetic Materials, High Energy Density Materials

374. **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. We are using atomic force microscopy (AFM) to investigate the growth of single crystal surfaces from solution in order to determine the mechanism of growth, the kinetics of step advancement, the effect of impurities, and the origin of defects.

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

375. **URANIUM CASTING PROGRAM**
$1,000,000
DOE Contact: Marshall Sluyter, (301) 903-5491
LLNL Contact: Jeff Kass, (925) 422-4831

The uranium casting program is addressing the use of permanent molds for near net shape castings, controlled cooling for segregation and microstructure control and the effect of alloy additions and subsequent heat treatment on microstructure. Process modeling has played a key role in producing high quality castings in uranium and uranium alloys.

Keywords: Uranium Casting

376. **URANIUM SPIN FORMING**
$1,500,000
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

377. **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

378. **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

379. **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 2 mm thin-walled plastic shells that will serve as the mandrel for the production of capsule targets for the National Ignition Facility (NIF). The mandrels must be extremely spherical (<1 μm out of round), have wall thickness uniformity better than 1 μm, and have a surface finish of less than 10 nm (rms over modes >9). Several routes are being explored.

Keywords: Polymers, Laser Fusion Targets, Microencapsulation, Microshells

380. **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) 422-4373

This program has as its objective the development of a vapor based, high strength polyimide coating technology that will allow us to produce a smooth, 150 to 200 μm polyimide ablator coating on a 2 mm diameter capsule target for the National Ignition Facility (NIF). Such targets should be strong enough to hold the full DT fuel load (about 300 atm) at room temperature, allowing us important flexibility in fielding these capsules for ignition experiments.

Keywords: Polymers, Laser Fusion Targets, Polyimide, Ablator

381. **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 sputter deposition techniques that will allow us to deposit 150 to 200 μm of a strong, smooth, Cu-doped Be ablator on a spherical plastic mandrel shell. These Be coated capsule targets have been shown by calculation to offer some important advantages as ignition targets for the National Ignition Facility (NIF).

Keywords: Beryllium, Laser Fusion Targets, Ablator, Sputter Deposition

LOS ALAMOS NATIONAL LABORATORY

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

382. **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

383. **STRUCTURAL ALLOY DEVELOPMENT**
$2,000,000
DOE Contact: Yok Chen, (301) 903-4174
LANL Contact: D.M. Parkin, (505) 667-8455

Alloy development for high temperature applications has focused on laves phase and silicide-based materials. Synthesis incorporates rapid solidification, plasma arc melting, vacuum arc melting, and powder synthesis techniques. Characterization is performed to detail phase stability and transformation thermodynamics, microstructure evolution, mechanical properties and high-temperature oxidation.

Keywords: Laves Phase, Silicide, Rapid Solidification, Plasma Arc Melting, Vacuum Arc Melting, Powder Synthesis

MATERIALS STRUCTURE OR COMPOSITION

384. **NATIONAL HIGH MAGNETIC FIELD LABORATORY**
$1,800,000
DOE Contact: J.J. Smith, (301) 903-4269
LANL Contact: D.M. Parkin, (505) 667-8455

The objective of the thrust is to apply high magnetic fields to the solution of unresolved fundamental problems in many body physics of condensed matter. Particular attention is given to electronic structure and many-body phenomena in 5f systems, with special emphasis on plutonium. There are two major components of the thrust: (1) an examination of static or mean-field properties of correlated-electron systems and (2) an examination of rapid femtosecond dynamics of electron-electron correlations (many-body phenomena) in high magnetic fields.

The world's longest-pulse, high-field magnet, funded by DOE, will be collocated with the other components of the Los Alamos NHMFL Pulsed-Field Facility, funded by the National Science Foundation (NSF). This interagency DOE/NSF collaboration will provide a unique user facility to users from DOE laboratories, industry, and universities. The magnet, when completed in 2000, will provide nondestructive 100-tesla magnetic fields for periods lasting up to 10 milliseconds, which is a thousand times longer than is available anywhere else. The magnet is a uniquely powerful tool for studying high-temperature superconductors and the electronic structure of materials at unprecedented resolution.

Keywords: High Magnetic Fields, Electronic Structure, Electron-electron Correlations, Plutonium

385. **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 demonstrate. 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

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

386. **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

387. **DEFORMATION CHARACTERIZATION AND MODELING**
$5,000,000
DOE Contact: Yok Chen, (301) 903-4174
LANL Contact: D.M. Parkin, (505) 667-8455

This program is focused on experimental measurements and computer modeling of elastic-plastic deformation paths incorporating dislocation dynamic and crystallographic texture to define multi-dimensional yield surfaces. Program success will result in an improved understanding of materials properties incorporating theories and modeling to extrapolate from microscopic to mesoscopic properties of materials.

Keywords: Elastic-Plastic Deformation, Dislocations, Crystallographic Texture

388. **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

389. **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

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

390. **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: Radioactive Materials, Plutonium Alloys, Beryllium, Uranium, Lithium Salts, Polymers, High Explosives, Tritium, Welding, Forming, Casting, Uranium Purification

391. **ADVANCED ENGINEERING METHODS DEVELOPMENT**
$1,100,000
DOE Contact: R. Jones (301) 903-6688
LANL Contact: C.A. Spirio, (505) 667-4772

The project is focused on developing tools and methods to support a models-based engineering-manufacturing (MBE-M) approach (solid models, assembly animation, spline algorithms, sensitivity analysis of secondaries, and manufacturing applications) to both the above ground experimental program, and as-built or remanufactured stockpile systems.

Keywords: Solid Model, Spline, Model-based Engineering, As-built, Remanufacturing, Stockpile

392. **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

393. **LASER TARGET FABRICATION**
$5,000,000
DOE Contact: C. Keane , (301) 903-4323
LANL Contact: L.R. Foreman, (505) 667-1846

The fabrication of complex and ultra-precision targets, mm-sized, for laser drive experiments related to inertial confinement fusion and nuclear weapons research. Efforts include the development and characterization of special alloys and tritium loading techniques along with the application of manufacturing processes of rapid solidification, powder consolidation, physical vapor deposition, chemical vapor deposition, polymer and polymer foam synthesis, precision machining and micro-assembly. Characterization includes examinations of microstructure, mechanical properties, physical properties, nondestructive examinations (radiography and ultrasonic), dimensional inspection, and optical interferometry.

Keywords: Physical Vapor Deposition, Chemical Vapor Deposition, Polymer Chemistry, Polymer Foam Synthesis, Precision Machining, Micro-assembly, Beryllium, Tritium, Plastics

394. **PULSED POWER TARGET FABRICATION**
$3,000,000
DOE Contact: C. Keane, (301) 903-4323
LANL Contact: W.E. Anderson, (505) 665-3981

Fabrication and characterization of precision liners for high explosive or capacitive discharge pulsed power experiments. Technologies employed include ingot metallurgy processing, physical deposition of coatings, precision machining and micro-assembly. Characterization techniques include microscopy, mechanical properties, nondestructive examinations (radiography and ultrasonic), dimensional inspection, and optical interferometry.

Keywords: Aluminum, Platinum, Gold, Physical Deposition of Coatings, Precision Machining and Micro-assembly

395. **ADVANCED STRATEGIC COMPUTING INITIATIVE MATERIALS MODELING**
$2,000,000
DOE Contact: G.G. Weigand, (202) 586-0568
LANL Contact: R.A. LeSar, (505) 665-0420

The development and bench-marking of advanced computer codes for the prediction of materials performance or processing technology influences on product quality. Models are being developed utilizing a full-three-dimensional first-principles approach to explore sensitivities to performance or processing variables. This includes the demonstration and baseline of engineering analysis codes to predict the engineering performance and reliability margin of the nuclear explosives package to satisfy its stockpile to target sequence requirements.

Keywords: Modeling, Constitutive Relationships, Fracture, Casting, Reliability Margin, Nuclear Explosives Package

OFFICE OF FOSSIL ENERGY

	FY 1997
Office of Fossil Energy - Grand Total	$4,914,000
Office of Advanced Research	$4,914,000
Fossil Energy AR&TD Materials Program	$4,914,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$1,905,000
Coating Process Development for Cr-Nb Alloys	20,000
Procurement of Advanced Austenitic and Aluminide Alloys	50,000
Development of Iron Aluminides	105,000
Development of Cr-Nb Alloys	105,000
High-Strength Iron Aluminide Alloys	PYF[1]
Low-Aluminum Content Iron-Aluminum Alloys	54,000
Mo-Si Alloy Development	47,000
Development of Improved and Corrosion Resistant Surfaces for Fossil Power System Components	35,000
Commercial-Scale Melting and Processing of Low-Aluminum Content Alloys	PYF[1]
Development of a Modified 310 Stainless Steel	84,000
Application of Advanced Austenitic Alloys to Fossil Power System Components	135,000
Development of Recuperator Materials	51,000
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	150,000
Compliant Oxide Coating Development	100,000
Development of Oxidation/Corrosion-Resistant Composite Materials and Interfaces	150,000
Optimization of the Chemical Vapor Infiltration Technique for Ceramic Composites	PYF[1]
Transport Properties of Ceramic Composites	50,000
Modeling of Fibrous Preforms for CVD Infiltration	50,000
Corrosion Protection of SiC-Based Ceramics with CVD Mullite Coatings	30,000
Feasibility of Synthesizing Oxide Films on Ceramic and Metal Substrates	44,000
Ceramic Coating and Native Oxide Scales Evaluation	70,000
Carbon Fiber Composite Molecular Sieves	150,000
Activation of Carbon Fiber Composite Molecular Sieves	PYF[1]
Carbon Fiber Composite Molecular Sieves Technology Transfer	100,000
Materials Properties, Behavior, Characterization or Testing	$1,202,000
Investigation of the Weldability of Polycrystalline Iron Aluminides	40,000
Friction Welding of Iron Aluminides	20,000
Evaluation of the Intrinsic and Extrinsic Fracture Behavior of Iron Aluminides	44,000
Investigation of Iron Aluminide Weld Overlays	6,000
Fireside Corrosion Tests of Candidate Advanced Austenitic Alloys, Coatings, and Claddings	33,000

[1]PYF denotes that funding for this project, active in FY 1997, was provided from prior year allocations.

OFFICE OF FOSSIL ENERGY (continued)

	FY 1997
Office of Advanced Research (continued)	
Fossil Energy AR&TD Materials Program (continued)	
Materials Properties, Behavior, Characterization or Testing (continued)	
Joining Techniques for Advanced Austenitic Alloys	PYF[1]
Fatigue and Fracture Behavior of Cr-Nb Alloys	35,000
Corrosion and Mechanical Properties of Alloys in FBC and Mixed-Gas Environments	180,000
High Temperature Environmental Effects on Iron Aluminides	170,000
Investigation of Moisture-Induced Embrittlement of Iron Aluminides	9,000
Reduction of Defect Content in ODS Aloys	30,000
Corrosion Protection of Ultrahigh Temperature Intermetallic Alloys	130,000
Oxide Dispersion Strengthened (ODS) Iron Aluminides	295,000
Materials Support for HITAF	PYF[1]
Support Services for Ceramic Fiber-Ceramic Matrix Composites	30,000
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	$1,361,000
Materials and Components in Fossil Energy Applications Newsletter	50,000
Development of Ceramic Membranes for Gas Separation and Fuel Cells	450,000
Extrusion Press Equipment	75,000
High-Temperature Heat Exchanger and Hot-Gas Filter Development	PYF[1]
Investigation of the Mechanical Properties and Performance of Ceramic Composite Components	PYF[1]
Solid State Electrolyte Systems	553,000
Oxide-Dispersion-Strengthened Fe_3Al-Based Alloy Tubes	33,000
ODS Fe_3Al Tubes for High-Temperature Heat Exchangers	50,000
Iron Aluminide Filters for IGCCs	PYF[1]
Iron Aluminide Filters for PFBCs	50,000
Ceramic Tubesheet Design Analysis	PYF[1]
Dense Ceramic Tube Development	100,000
Instrumentation and Facilities	$ 446,000
Management of the Fossil Energy AR&TD Materials Program	406,000
General Technology Transfer Activities	35,000
Gordon Research Conference Support	5,000

[1]PYF denotes that funding for this project, active in FY 1997, was provided from prior year allocations.

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:

1. 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.

2. 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.

3. The third is to pursue a global technology strategy to support the increased competitiveness of the U.S. in fossil fuel technologies, to maintain world leadership in our fossil fuel technology base, and provide expanded markets for U.S. fuels and technology. This crosscutting goal is supported by the activities in the above two technology goals.

OFFICE OF ADVANCED RESEARCH

FOSSIL ENERGY AR&TD MATERIALS PROGRAM

Fossil Energy (FE) materials-related research is conducted under an Advanced Research and Technology Development (AR&TD) Materials sub-activity and is an integral part of the R&D conducted by the Office of Advanced Research and Special Technologies. The AR&TD Materials program includes cross-cutting research to obtain a fundamental understanding of materials and how they perform in fossil-based process environments and the development of new classes of generic materials that will allow the development of new fossil energy systems or major improvements in existing systems. The present program is focused on ceramics (composite structural ceramics, catalyst supports, solid state electrolytes, membranes, and ceramic filters), new alloys (aluminides, filters, advanced austenitic steels, and coatings and claddings), corrosion research, and technology development and transfer.

The AR&TD research is carried through development and technology transfer to industry. Special emphasis is given to technology transfer to ensure that the materials will be available for subsequent fossil commercial applications. This also enhances U.S. technological competitiveness not only in the fossil area but in the materials industry in general and other technology application areas as well. The research is conducted in industry, universities, not-for-profit agencies, and national laboratories. This widespread participation also helps maintain the U.S. materials technology capabilities.

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

396. **COATING PROCESS DEVELOPMENT FOR Cr-Nb ALLOYS**
$20,000
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: R. R. Judkins, (423) 574-4572
Ohio State University Contact: R. A. Rapp, (614) 292-6178

Cr-Nb alloys are being developed for high temperature service, but require protection from high temperature environments, such as oxidation. Previously developed $MoSi_2$-base coatings have shown some promise for protecting Nb, and the principles learned may have applicability for protective coatings of Cr-Nb. The purpose of this work is to examine the protection of Cr-Nb alloys with either silicides or aluminides.

Keywords: Alloys, Aluminizing, Chromizing, Corrosion, Coatings

397. **PROCUREMENT OF ADVANCED AUSTENITIC AND ALUMINIDE ALLOYS**
$50,000
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: R. R. Judkins, (423) 574-4572

This task provides funds for the procurement of alloys necessary for alloy development and testing activities of the AR&TD Materials Program.

Keywords: Alloys, Aluminides, Austenitic

398. **DEVELOPMENT OF IRON ALUMINIDES**
$105,000
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: G. M. Goodwin, (423) 574-4809

The objective of this task is to develop low-cost and low-density intermetallic alloys based on Fe_3Al with an optimum combination of strength, ductility, weldability, and corrosion resistance for use as components in advanced fossil energy conversion systems. Emphasis is on the development of iron aluminides for heat recovery applications in coal gasification systems.

Keywords: Alloys, Aluminides, Intermetallic Compounds

399. **DEVELOPMENT OF Cr-Nb ALLOYS**
$105,000
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: C. T. Liu, (423) 574-4459

The objective of this task is to develop high-strength, corrosion-resistant intermetallic alloys for use as hot components in advanced fossil energy conversion and power generation systems. The successful development of these alloys is expected to improve the thermal efficiency of fossil energy conversion systems through increased operating temperatures and to increase the service life of hot components exposed to corrosive environments at elevated temperatures (1000°C). The work is focused on *in situ* composite alloys based on the $Cr-Cr_2Nb$ system.

Keywords: Alloys, Chromium-Niobium, Corrosion, Intermetallic Compounds

400. **HIGH-STRENGTH IRON ALUMINIDE ALLOYS**
$0 - PYF[1]
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: C. G. McKamey, (423) 574-6917

The objective of this task is to use microalloying techniques to further develop the Fe_3Al-based alloys. Emphasis is on producing a low-cost, low-density, precipitation-strengthened Fe_3Al-based intermetallic alloy with improved high-temperature creep resistance while maintaining an optimum combination of room-temperature and high-temperature (600-700°C) tensile properties, weldability, and corrosion resistance for use as structural components of advanced fossil energy conversion systems.

Keywords: Alloys, Aluminides, Microalloy

401. **LOW-ALUMINUM CONTENT IRON-ALUMINUM ALLOYS**
$54,000
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: V. K. Sikka, (423) 574-5112

The objective of this task is to develop a conventionally-fabricable low-cost and lower density iron-aluminum-based alloy with a good combination of strength, ductility, weldability, and corrosion resistance for use as components in advanced fossil energy systems. Initial emphasis is on the development of iron-aluminum alloys for heat-recovery applications in coal gasification systems.

Keywords: Alloys, Iron-Aluminum

402. **Mo-Si ALLOY DEVELOPMENT**
$47,000
DOE Contacts: F. M. Glaser, (301) 903-2784 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 power generation systems. The successful development of Mo-Si alloys is expected to improve the thermal efficiency and performance of fossil energy systems through increased operating temperature and to increase the service life of hot components exposed to corrosive environments at high temperatures (to 1600°C). The initial effort is devoted to Mo_5Si_3-base alloys containing boron additions.

Keywords: Alloys, Molybdenum, Silicon

403. **DEVELOPMENT OF IMPROVED AND CORROSION RESISTANT SURFACES FOR FOSSIL POWER SYSTEM COMPONENTS**
$35,000
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: V. K. Sikka, (423) 574-5112

A Cooperative Research and Development Agreement (CRADA) has been established with ABB Combustion Engineering for the development of corrosion-resistant surface protection for fossil power systems.

Keywords: Alloys, Iron-Aluminum, Corrosion, Technology Transfer

[1]PYF denotes that funding for this project, active in FY 1997, was provided from prior year allocations.

404. **COMMERCIAL-SCALE MELTING AND PROCESSING OF LOW-ALUMINUM CONTENT ALLOYS**
$0 - PYF[1]
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: V. K. Sikka, (423) 574-5112

The purpose of this activity is the preparation and evaluation of castings of low-aluminum content, iron-aluminum alloys. The castings will be prepared in several types of molds including: (1) graphite, (2) sand, and (3) investment. Castings will be prepared primarily from the air-induction-melted material. Selected graphite and investment castings will also be prepared from the vacuum-induction-melted material. The graphite and sand castings will be prepared at ORNL and will also be procured from the commercial foundries. The castings will be evaluated for porosity, grain structure, mechanical properties, and weldability. The mechanical property evaluation will consist of Charpy impact, tensile, and creep testing.

Keywords: Alloys, Iron-Aluminum, Melting, Casting

405. **DEVELOPMENT OF A MODIFIED 310 STAINLESS STEEL**
$84,000
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: R. W. Swindeman, (423) 574-5108

The purpose of this task is to evaluate structural alloys for improved performance of high-temperature components in advanced combined-cycle and coal-combustion systems.

Keywords: Materials, Mechanical Properties, Austenitics, Hot-Gas

406. **APPLICATION OF ADVANCED AUSTENITIC ALLOYS TO FOSSIL POWER SYSTEM COMPONENTS**
$135,000
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: R. W. Swindeman, (423) 574-5108

A Cooperative Research and Development Agreement (CRADA) has been established with ABB Combustion Engineering for the development of advanced austenitic alloys for fossil power systems.

Keywords: Alloys, Austenitics, Technology Transfer

407. **DEVELOPMENT OF RECUPERATOR MATERIALS**
$51,000
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: R. W. Swindeman, (423) 574-5108

A Cooperative Research and Development Agreement (CRADA) has been signed with Solar Turbines, Inc. to develop a materials technology for recuperators operating at gas inlet temperatures to 730°C.

Keywords: Alloys, Austenitics, Technology Transfer

408. **INFLUENCE OF PROCESSING ON MICROSTRUCTURE AND PROPERTIES OF ALUMINIDES**
$175,000
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: I. G. Wright, (423) 574-4451
Idaho National Engineering and Environmental Laboratory Contact: R. N. Wright, (208) 526-6127

The purpose of this program is to determine the influence of processing on the properties of alloys based on the intermetallic compound Fe_3Al. Thermo-mechanical processing of these alloys is pursued to improve their properties. The response of the microstructure to elevated temperature deformation and subsequent annealing is characterized in terms of the establishment of equilibrium phases and equilibrium degree of long-range order. The role of dislocation and antiphase boundary structures in enhancing ductility of Fe_3Al is investigated. The tensile properties are determined at room and elevated temperature and related to the microstructure. Reaction synthesis is investigated as a novel joining method and as a process to fabricate porous iron aluminides for filter applications. Oxide dispersion strengthened alloys, fabricated by reaction synthesis, are developed for improved high temperature strength. Compositions of the Fe_3Al alloys and details of the processing are determined in collaboration with the program at Oak Ridge National Laboratory (ORNL).

Keywords: Aluminides, Processing, Microstructure

[1]PYF denotes that funding for this project, active in FY 1997, was provided from prior year allocations.

409. **INVESTIGATION OF ELECTROSPARK-DEPOSITED COATINGS FOR PROTECTION OF MATERIALS IN SULFIDIZING ATMOSPHERES**
$100,000
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: R. R. Judkins, (423) 574-4572
Pacific Northwest National Laboratory Contact: R. N. Johnson, (509) 375-6906

The purpose of this task is to examine the use of the electrospark deposition coating process for the application of corrosion-, erosion-, and wear-resistant coatings to candidate heat exchanger (including superheater and reheater) alloys. Materials to be deposited may include MCrAl, MCrAlY, highly wear-resistant carbides, and other hardsurfacing materials.

Keywords: Coatings, Materials, Deposition

410. **TECHNOLOGY TRANSFER OF ELECTRO-SPARK DEPOSITED COATINGS FOR PROTECTION OF MATERIALS IN SULFIDIZING ATMOSPHERES**
$50,000
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: I. G. Wright, (423) 574-4451
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

411. **FABRICATION OF FIBER-REINFORCED COMPOSITES BY CHEMICAL VAPOR INFILTRATION AND DEPOSITION**
$150,000
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: 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.

Keywords: Composites, Fiber-Reinforced, Ceramics

412. **COMPLIANT OXIDE COATING DEVELOPMENT**
$100,000
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: D. P. Stinton, (423) 574-4556

Monolithic SiC heat exchangers and fiber-reinforced SiC-matrix composite heat exchangers and filters are susceptible to corrosion by alkali metals at elevated temperatures. Protective coatings are currently being developed to isolate the SiC materials from the corrodents. Unfortunately, these coatings typically crack and spall when applied to SiC substrates. The purpose of this task is to determine the feasibility of using a compliant material between the protective coating and the substrate. The low-modulus compliant layer could absorb stresses and eliminate cracking and spalling of the protective coatings.

Keywords: Ceramics, Oxides, Coatings

413. **DEVELOPMENT OF OXIDATION/CORROSION-RESISTANT COMPOSITE MATERIALS AND INTERFACES**
$150,000
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: R. A. Lowden, (423) 576-2769

Fiber-reinforced SiC-matrix composites have been observed to fail in fossil energy applications for two reasons. First, the mechanical properties of composites deteriorate under stressed oxidation because oxidants such as steam penetrate cracks formed in the SiC matrix and react with the carbon or boron nitride interface. The mechanical properties of composites may degrade because of corrosion due to sodium species typically present in fossil systems. Therefore, the purposes of this task are to first, develop fiber-matrix interfaces that are resistant to oxidation and yet optimize the mechanical behavior of composites, and second, to develop protective overcoats or oxide matrices that are resistant to oxidation and corrosion.

Keywords: Composites, Ceramics, Fiber-Reinforced, Interfaces

414. OPTIMIZATION OF THE CHEMICAL VAPOR INFILTRATION TECHNIQUE FOR CERAMIC COMPOSITES
$0 - PYF[1]
DOE Contacts: F. M. Glaser, (301) 903-2784 and
M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact:
D. P. Stinton, (423) 574-4556
University of Tennessee Contact: P. K. Liaw,
(423) 974-6356

This project is focused on an optimization of the forced chemical vapor infiltration technique for fabrication of ceramic matrix composites (CMCs) using process models. In particular, a process model developed at the Georgia Tech Research Institute shall be thoroughly investigated. Experimental verification of the process model shall be conducted in light of microstructural characterization using both destructive and nondestructive evaluation techniques. An optimized process for manufacturing CMCs shall be demonstrated. Moreover, mechanistic understanding regarding the effects of processing parameters on microstructural features, and fatigue and fracture behavior of CMCs shall be provided.

Keywords: Composites, Fiber-Reinforced, Ceramics

415. TRANSPORT PROPERTIES OF CERAMIC COMPOSITES
$50,000
DOE Contacts: F. M. Glaser, (301) 903-2784 and
M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact:
D. P. Stinton, (423) 574-4556
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

416. MODELING OF FIBROUS PREFORMS FOR CVD INFILTRATION
$50,000
DOE Contacts: F. M. Glaser, (301) 903-2784 and
M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact:
D. P. Stinton, (423) 574-4556
Georgia Institute of Technology Contact:
T. L. Starr, (404) 894-0579

The purpose of this project is to conduct a theoretical and experimental program to develop an analytical model for the fabrication and infiltration of fibrous preforms. The analytical model will: (1) predict preform structure (density, porosity, fiber orientation, etc.) based on fabrication technique and fundamental fiber parameters (diameter, aspect ratio, etc.), and (2) predict permeation and heat conduction through the preform structure and, thus, predict the CVD infiltration performance.

Keywords: Ceramics, Composites, Modeling

417. CORROSION PROTECTION OF SiC-BASED CERAMICS WITH CVD MULLITE COATINGS
$30,000
DOE Contacts: F. M. Glaser, (301) 903-2784 and
M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact:
D. P. Stinton, (423) 574-4556
Boston University Contact: Vinod Sarin,
(617) 353-6451

This project involves the growth of dense mullite coatings on SiC-based substrates by chemical vapor deposition. SiC and SiC-based composites have been identified as the leading candidate materials for stringent elevated temperature applications. At moderate temperatures and pressures, the formation of a thin self-healing layer of SiO_2 is effective in preventing catastrophic oxidation by minimizing the diffusion of O_2 to the substrate. The presence of impurities can increase the rate of passive oxidation by modifying the transport rate of oxygen through the protective scale, can cause active oxidation via formation of SiO which accelerates the degradation process, or can produce compositions such as Na_2SO_3 which chemically attack the ceramic via rapid corrosion. There is therefore a critical need to develop adherent oxidation/corrosion-resistant, and thermal-shock-resistant coatings that can withstand such harsh environments. Mullite has been identified as an excellent candidate material due to its desirable properties of toughness, corrosion resistance, and a good coefficient of thermal expansion match with SiC.

Keywords: Ceramics, Coatings

[1]PYF denotes that funding for this project, active in FY 1997, was provided from prior year allocations.

418. **FEASIBILITY OF SYNTHESIZING OXIDE FILMS ON CERAMIC AND METAL SUBSTRATES**
$44,000
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: D. P. Stinton, (423) 574-4556
Lawrence Berkeley 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

419. **CERAMIC COATING AND NATIVE OXIDE SCALES EVALUATION**
$70,000
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: P. F. Tortorelli, (423) 574-5119

The purpose of this work is to generate the information needed for the development of improved (slow growing, adherent, sound) protective oxide coatings and scales. The specific objectives are to systematically investigate the relationships among substrate composition and surface oxide structure, adherence, soundness, and micromechanical properties, (2) use such information to predict scale and coating failures, and (3) identify and evaluate compositions and synthesis routes for producing materials with damage-tolerant scales and coatings.

Keywords: Coatings, Corrosion

420. **CARBON FIBER COMPOSITE MOLECULAR SIEVES**
$150,000
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: T. D. Burchell, (423) 576-8595

Hydrogen recovery technologies are required to allow the upgrading of heavy hydrocarbons to transport fuels, thus reducing the amount of carbon rejected during the conversion of fossil resources into hydrocarbon products. The purpose of this work is to develop carbon molecular sieves (CMS) starting with porous carbon fiber composites (CFC) manufactured from petroleum pitch derived carbon fibers. The carbon fiber composite molecular sieves (CFCMS) will be utilized in pressure swing adsorption units for the efficient recovery of hydrogen from synthesis gas, refinery purge gases, and for other gas separation operations associated with hydrogen recovery.

Keywords: Carbon Fibers, Sieves, Composites

421. **ACTIVATION OF CARBON FIBER COMPOSITE MOLECULAR SIEVES**
$0 - PYF[1]
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact:
R. R. Judkins, (423) 574-4572
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

[1]PYF denotes that funding for this project, active in FY 1997, was provided from prior year allocations.

422. **CARBON FIBER COMPOSITE MOLECULAR SIEVES TECHNOLOGY TRANSFER**
$100,000
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: T. D. Burchell, (423) 576-8595

Hydrogen and methane gas recovery technologies are required to: (1) allow the upgrading of heavy hydrocarbons to transport fuels, thus reducing the amount of carbon rejected during crude oil refining and (2) to improve the yield and process economics of natural gas wells. The purpose of this work is to develop carbon fiber composite molecular sieves (CFCMS) from porous carbon fiber composites manufactured from solvent extracted coal tar pitch derived carbon fibers. The work will be performed in collaboration with other members of the Cooperative Research Partnership on Carbon Products and the Non Fuel Uses of Coal.

Keywords: Consortium, Carbon Products

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

423. **INVESTIGATION OF THE WELDABILITY OF POLYCRYSTALLINE IRON ALUMINIDES**
$40,000
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: R. W. Swindeman, (423) 574-5108
Colorado School of Mines Contact: G. R. Edwards, (303) 273-3773

The purpose of this project is the investigation of the weldability of polycrystalline aluminides. The major thrust of the project is to determine the role of microstructure in the intergranular cracking of aluminides, with special emphasis on weld cracking susceptibility. The weldability of polycrystalline Fe_3Al-X alloys is being evaluated, and the weldability is correlated with composition, phase equilibria, grain size and morphology, domain size, and degree of long-range order.

Keywords: Joining, Welding

424. **FRICTION WELDING OF IRON ALUMINIDES**
$20,000
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: I. G. Wright, (423) 574-4451
The Welding Institute Contact: P. L. Threadgill, 8-0-11-44-1223-891162

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

425. **EVALUATION OF THE INTRINSIC AND EXTRINSIC FRACTURE BEHAVIOR OF IRON ALUMINIDES**
$44,000
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: I. G. Wright, (423) 574-4451
West Virginia University Contact: B. R. Cooper, (304) 293-3423

The purpose of this activity is the evaluation of the intrinsic and extrinsic fracture behavior of iron aluminides and the study of atomistic simulations of defect concentrations, dislocation mobility, and solute effects in Fe_3Al. The work also involves an experimental study of environmentally-assisted crack growth of Fe_3Al at room and at elevated temperatures. The combined modeling and experimental activities are expected to elucidate the mechanisms controlling deformation and fracture in Fe_3Al in various environments.

Keywords: Alloys, Aluminides, Fracture

426. **INVESTIGATION OF IRON ALUMINIDE WELD OVERLAYS**
$6,000
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: R. W. Swindeman, (423) 574-5108
Lehigh University Contact: J. N. DuPont, (610) 758-3942

The objective of this activity is the investigation of iron aluminide weld overlays. Specific tasks include: (1) filler wire development, (2) weldability, (3) oxidation and sulfidation studies, (4) erosion studies, (5) erosion-corrosion studies, and (6) field exposures.

Keywords: Alloys, Aluminides, Overlay, Welding, Joining

427. **FIRESIDE CORROSION TESTS OF CANDIDATE ADVANCED AUSTENITIC ALLOYS, COATINGS, AND CLADDINGS**
$33,000
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: R. W. Swindeman, (423) 574-5108
Foster Wheeler Development Corporation Contact: J. L. Blough, (201) 535-2355

The purpose of this project is to provide comprehensive corrosion data for selected advanced austenitic tube alloys in simulated coal ash environments. ORNL-modified alloys and standard comparison alloys have been examined. The variables affecting coal ash corrosion and the mechanisms governing oxide breakdown and corrosion penetration are being evaluated. Corrosion rates of the test alloys are determined as functions of temperature, ash composition, gas composition, and time.

Keywords: Austenitics, Alloys, Corrosion

428. **JOINING TECHNIQUES FOR ADVANCED AUSTENITIC ALLOYS**
$0 - PYF[1]
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: R. W. Swindeman, (423) 574-5108
University of Tennessee Contact: C. D. Lundin, (423) 974-5310

Weldability is an important consideration in the selection of a suitable alloy for the fabrication of boiler components such as superheaters and reheaters. It is often a challenge to select joining materials and establish procedures that will allow advanced materials to function at their full potential. The purpose of this research is to examine important aspects of newly developed austenitic tubing alloys intended for service in the temperature range 550-700°C.

Keywords: Alloys, Austenitics, Joining, Welding

429. **FATIGUE AND FRACTURE BEHAVIOR OF Cr-Nb ALLOYS**
$35,000
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: I. G. Wright, (423) 574-4451
University of Tennessee Contact: Peter Liaw, (423) 974-6356

The objective of this research 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

430. **CORROSION AND MECHANICAL PROPERTIES OF ALLOYS IN FBC AND MIXED-GAS ENVIRONMENTS**
$180,000
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: I. G. Wright, (423) 574-4451
Argonne National Laboratory Contact: K. Natesan, (708) 252-5103

The purposes of this task are to: (1) evaluate the corrosion mechanisms for chromia- and alumina-forming alloys in mixed-gas environments, (2) develop an understanding of the role of several microalloy constituents in the oxidation/sulfidation process, (3) evaluate transport kinetics in oxide scales as functions of temperature and time, (4) characterize surface scales that are resistant to sulfidation attack, and (5) evaluate the role of deposits in corrosion processes.

Keywords: Corrosion, Gasification, Creep Rupture, Fluidized-Bed Combustion

431. **HIGH-TEMPERATURE ENVIRONMENTAL EFFECTS ON IRON ALUMINIDES**
$170,000
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: P. F. Tortorelli, (423) 574-5119

The purpose of this task is to evaluate the high-temperature corrosion behavior of iron-aluminum alloys as part of the effort to develop highly corrosion-resistant iron-aluminide alloys and coatings for fossil energy applications. A primary objective is to investigate the resistance of the alloys to mixed-oxidant (oxygen-sulfur-chlorine-carbon) environments that arise in the combustion or gasification of coal. This includes the determination of the influence of sulfur and other reactive gaseous species on corrosion kinetics and oxide microstructures and the effects of alloying additions and oxide dispersoids on sulfidation and oxidation resistance.

Keywords: Corrosion, Aluminides, Mixed-Gas, Scales

[1]PYF denotes that funding for this project, active in FY 1997, was provided from prior year allocations.

432. **INVESTIGATION OF MOISTURE-INDUCED EMBRITTLEMENT OF IRON ALUMINIDES**
$9,000
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: I. G. Wright, (423) 574-4451
Rensselaer Polytechnic Institute Contact: N. S. Stoloff, (518) 276-6371

The purpose of this work is to study hydrogen embrittlement of iron aluminide alloys. Moisture in air can significantly reduce the room-temperature tensile ductility of Fe_3Al-based alloys by combining with the aluminum in the alloys to form atomic hydrogen. The atomic hydrogen diffuses rapidly into the material causing embrittlement. Experiments are being conducted on selected Fe_3Al alloys that will lead to an understanding of the phenomenon. The work focuses on the effects of moisture on relevant mechanical properties such as fatigue and tensile strengths, and correlates important microstructural variables such as degree of order, grain size, and phases present with the alloy's susceptibility to embrittlement.

Keywords: Aluminides, Embrittlement, Moisture

433. **REDUCTION OF DEFECT CONTENT IN ODS ALLOYS**
$30,000
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: I. G. Wright, (423) 574-4451
The University of Liverpool Contact: A. R. Jones

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

434. **CORROSION PROTECTION OF ULTRAHIGH TEMPERATURE INTERMETALLIC ALLOYS**
$130,000
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: P. F. Tortorelli, (423) 574-5119

The objective of this task is to develop high-strength, corrosion-resistant intermetallic alloys for use as hot components in advanced fossil energy conversion and combustion systems. The successful development of these alloys is expected to improve the thermal efficiency of fossil energy conversion systems through increased operating temperatures and to increase the service life of hot components exposed to corrosive environments at elevated temperatures (1000°C). The initial effort will be devoted to *in situ* composite alloys based on the $Cr\text{-}Cr_2Nb$ system.

Keywords: Corrosion, Chromium-Niobium, Mixed-Gas, Scales

435. **OXIDE DISPERSION STRENGTHENED (ODS) IRON ALUMINIDES**
$295,000
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: I. G. Wright, (423) 574-4451

The purpose of this task is to develop fabrication procedures for making oxide dispersion-strengthened (ODS) iron-aluminum alloys based on Fe_3Al. The suitability of the procedures is measured in terms of the high-emperature oxidation and sulfidation resistance and creep strength of the ODS alloys compared with Fe_3Al alloys fabricated by conventional ingot and powder processes.

Keywords: Aluminides

436. **MATERIALS SUPPORT FOR HITAF**
$0 - PYF[1]
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: K. Breder, (423) 574-5089

This task involves the measurement of selected mechanical and physical properties of structural ceramics which are proposed for use in the construction of the High Temperature Advanced Furnace (HITAF) air heater design being developed under the Combustion 2000 Program. The purpose of the research is to evaluate candidate structural ceramics for this application by studying the fast fracture and fatigue (both dynamic and interrupted static) properties at temperatures from 1100 to 1400°C in air, their corrosion behavior, property uniformity of components and long term degradation of ceramic properties due to exposure in prototype HITAF systems.

Keywords: Furnace, Materials, HITAF

[1]PYF denotes that funding for this project, active in FY 1997, was provided from prior year allocations.

437. **SUPPORT SERVICES FOR CERAMIC FIBER-CERAMIC MATRIX COMPOSITES**
$30,000
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: D. P. Stinton, (423) 574-4556
University of North Dakota Energy and Environmental Research Center Contact: J. P. Hurley, (701) 777-5159

This task will review and, if appropriate, propose modifications to plans, materials, and tests planned by researchers on the AR&TD Materials Program in work to test materials for coal-fueled energy systems. The changes shall be suggested in order to make the corrosion experiments more reflective of the actual conditions that will be encountered by the materials in the energy systems. UNDEERC shall accomplish this task by reviewing the major advanced energy system projects being funded by the DOE, and by working with the company's technical monitor and staff to prepare a summary of the expected corrosion problems. Both gasification and combustion systems will be included. Ceramic materials in two subsystems will be the focus of this work: (1) hot gas cleanup systems and (2) high-temperature heat exchangers. UNDEERC shall review and suggest improvements to materials testing procedures that are used to determine material behavior when used in hot-gas cleanup or heat exchanger applications. A limited amount of computer modeling and laboratory experimentation shall be a part of this effort.

Keywords: Composites, Ceramics, Fibers

438. **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 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

439. ***MATERIALS AND COMPONENTS IN FOSSIL ENERGY APPLICATIONS* NEWSLETTER**
$50,000[1]
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: I. G. Wright, (423) 574-4451

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

440. **DEVELOPMENT OF CERAMIC MEMBRANES FOR GAS SEPARATION AND FUEL CELLS**
$450,000
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: R. R. Judkins, (423) 574-4572
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, Fuel Cells

[1]Matching funding provided by EPRI.

441. **EXTRUSION PRESS EQUIPMENT**
$75,000
DOE Contacts: F. M. Glaser, (301) 903-2784 and
M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact:
R. R. Judkins, (423) 574-4572
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

442. **HIGH-TEMPERATURE HEAT EXCHANGER AND HOT-GAS FILTER DEVELOPMENT**
$0 - PYF[1]
DOE Contacts: F. M. Glaser, (301) 903-2784 and
M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact:
D. P. Stinton, (423) 574-4556
Pennsylvania State University Contact:
R. E. Tressler, (814) 865-7961

This project addresses the development of ceramic heat exchanger materials with chromia surface treatments for corrosion resistance. High chromia-content refractories have been demonstrated to be resistant to corrosion by coal slags. This project will focus on improving the corrosion resistance of ceramics by incorporating chromia into the surface layers. This work has two principal parts: (1) screening analysis of candidate ceramic hot-gas filter materials, and (2) internal pressure testing of ceramic tubes exposed to coal combustion environments.

Keywords: Ceramics, Corrosion, Filters

443. **INVESTIGATION OF THE MECHANICAL PROPERTIES AND PERFORMANCE OF CERAMIC COMPOSITE COMPONENTS**
$ 0 - PYF[1]
DOE Contacts: F. M. Glaser, (301) 903-2784 and
M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact:
D. P. Stinton, (423) 574-4556
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

444. **SOLID STATE ELECTROLYTE SYSTEMS**
$553,000
DOE
DOE Contacts: F. M. Glaser, (301) 903-2784 and
M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact:
R. R. Judkins, (423) 574-4572
Pacific Northwest National Laboratory Contact:
L. R. Pederson, (509) 375-2579

The purpose of this project is to develop functional ceramic materials that will ultimately lead to the broader, cleaner, and more efficient utilization of fossil fuels, particularly coal and natural gas. This project is composed of three principal tasks:

1. Stability of Solid Oxide Fuel Cell Materials - The purpose of this task is to evaluate the stabilities of materials and interfaces in SOFCs in order to identify features that would limit system performance.

2. Mixed Oxygen Ion/Electron-Conducting Ceramics for Oxygen Separation - Compositions and physical forms are being developed that simultaneously conduct oxygen ions and electrons. Such mixed conducting ceramics can function as highly selective oxygen separation membranes, allowing high purity oxygen to be separated from air.

3. Proton-Conducting Solid Electrolytes - This task will develop perovskite compositions and physical forms, which will be used as the electrolyte in small-scale solid oxide fuel cells operating at intermediate temperatures.

Keywords: Fuel Cells, SOFC

445. **OXIDE-DISPERSION-STRENGTHENED Fe_3Al-BASED ALLOY TUBES**
$33,000
DOE Contacts: F. M. Glaser, (301) 903-2784 and
M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact:
I. G. Wright, (423) 574-4451
University of 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

[1]PYF denotes that funding for this project, active in FY 1997, was provided from prior year allocations.

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 its superior sulfidation resistance, in comparison to the competing Fe-Cr-Al base alloys and the Ni-base superalloys currently in service.

Keywords: Aluminide, Tubes

446. **ODS Fe_3Al TUBES FOR HIGH-TEMPERATURE HEAT EXCHANGERS**
$50,000
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: I. G. Wright, (423) 574-4451
PM Hochtemperatur-Metall. GmbH Contact: Dieter Sporer, 011-43-5672-70-2923

The goal of the work is to produce tubes of Fe_3Al-0.5 wt. percent Y_2O_3 which have properties suitable for application as heat transfer surfaces in very high-temperature heat exchangers. The alloy is produced by a powder metallurgical (mechanical alloying) process, the main purpose of which is to obtain a uniform distribution of sub-micron Y_2O_3 particles in the Fe_3Al matrix. The required high-temperature creep strength is derived largely by developing very large, elongated grains which are effectively pinned by the oxide dispersion. Development of the necessary grain structure is dependent on the characteristics of the mechanically-alloyed powder, and on thermo-mechanical processing of the consolidated powder.

Keywords: Aluminide, Tubes, Heat Exchangers

447. **IRON ALUMINIDE FILTERS FOR IGCCs**
$0 - PYF[1]
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: P. F. Tortorelli, (423) 574-5119

The purpose of this project is to provide technical support to the Pall Corporation in its development of porous sintered iron-aluminide filters for hot-particle removal from product streams in coal gasification systems. The ORNL role is to provide specialized expertise in the areas of corrosion analysis, micro-structural 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

[1]PYF denotes that funding for this project, active in FY 1997, was provided from prior year allocations.

448. **IRON ALUMINIDE FILTERS FOR PFBCs**
$50,000
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: P. F. Tortorelli, (423) 574-5119

The goal of this project is to determine the suitability of particular iron aluminides as materials of construction for hot-gas filters in advanced first- and second-generation PFBCs.

Keywords: Filters, Aluminides

449. **CERAMIC TUBESHEET DESIGN ANALYSIS**
$0 - PYF[1]
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: R. W. Swindeman, (423) 574-5108

The purpose of this task is to perform thermal and mechanical analyses of critical regions in a ceramic tubesheet support for barrier filters in a hot gas cleanup vessel designed for use in gasifier, carbonizer, and pressurized fluidized bed combustion gas streams.

Keywords: Ceramics, Tubesheet

450. **DENSE CERAMIC TUBE DEVELOPMENT**
$100,000
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: 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. Potentials applications for CFCCs include air heaters or recuperators, heat exchangers, catathermal or porous combustors, components for filtration systems, gas turbine components (primarily combustors), and radiant 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

451. **MANAGEMENT OF THE FOSSIL ENERGY AR&TD MATERIALS PROGRAM**
$406,000
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: R. R. Judkins, (423) 574-4572

The overall objective of the Fossil Energy Advanced Research and Technology Development (AR&TD) Materials program is to conduct a fundamental, long-range research and development program that addresses, in a generic way, the materials needs of fossil energy systems and ensures the development of advanced materials and processing techniques. The purpose of this task is to manage the Fossil Energy AR&TD Materials program in accordance with procedures described in the Program Management Plan approved by DOE. This task is responsible for preparing the technical program implementation plan for DOE approval; submitting budget proposals for the program; recommending work to be accomplished by subcontractors, other national laboratories, and by Oak Ridge National Laboratory (ORNL); placing and managing subcontracts for fossil energy materials development at industrial research centers, universities, and other government laboratories; and for reporting the progress of the program.

Keywords: Management, Materials Program

452. **GENERAL TECHNOLOGY TRANSFER ACTIVITIES**
$35,000
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: R. R. Judkins, (423) 574-4572

The task provides funds for the initiation of technology transfer activities to identify and develop relationships with industrial partners for the transfer of AR&TD Materials Program technologies to industry.

Keywords: Technology Transfer

453. **GORDON RESEARCH CONFERENCE SUPPORT**
$5,000
DOE Contacts: F. M. Glaser, (301) 903-2784 and M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: R. R. Judkins, (423) 574-4572

The task provides funds for partial support of the annual Gordon Research Conference.

Keywords: Technology Transfer

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

C. Arnold, Jr.
Division 1811
Sandia National Laboratories
Albuqeurque, NM 87185
(505) 844-8728

T. W. Arrigoni
U.S. Dept. of Energy
P.O. Box 10940
Pittsburgh, PA 15236
(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
Internl. Solar Electric Tech., Inc.
8635 Aviation Boulevard
Inglewood, CA 90301
(310) 216-4427

J. L. Bates
Pacific Northwest Laboratories
P.O. Box 999
Richland, WA 99352
(509) 375-2579

S. Bauer, Division G314
Sandia National Laboratory
P.O. Box 5800
Albuquerque, NM 87185
(505) 846-9645

M. B. Beardsley
Caterpillar, Inc.
100 N.E. Adams Street
Peoria, IL 61629
(309) 578-8514

R. L. Beatty
ORNL
P.O. Box 2008
Bldg. 4508, MS 088
Oak Ridge, TN 37831
(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) 231-1396

Dave Benson
NREL
1617 Cole Blvd
Golden, CO 80401
(303) 384-6462

Clifton G. Bergeron
University of Illinois
105 South Goodwin Avenue
204 Ceramics Building
Urbana, IL 61801
(217) 333-1770

Sam Berman
Bldg. 90, Rm. 3111
Lawerence Berkeley Laboratory
University of California
Berkeley, CA 94720
(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

R. J. Bourcier
Division 1832
Sandia National Laboratories
Albuquerque, NM 87185
(505) 844-6638

H. K. Bowen
Dept. of Mat. Science & Eng.
MIT
77 Massachusetts Avenue
Cambridge, MA 02139
(617) 253-6892

D. J. Bradley
Pacific Northwest National Laboratory
Richland, WA 99352
(509) 375-2587

R. A. Bradley
ORNL
P.O. Box 2008
Bldg. 4515
Oak Ridge, TN 37831-6067
(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

Russell Chou
Materials Research Center
Lehigh University
Bethlehem, PA 18015
(215) 861-4235

D. C. Christensen
LANL
Los Alamos, NM 87545
(505) 667-2556

Richard Christensen
LLNL
University of California
P.O. Box 808
Livermore, CA 94550
(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

Mr. Norbert B. Elsner
Hi-Z Technology, Inc.
6373 Nancy Ridge Drive
San Diego, CA 92121-2247
(619) 535-9343

James Ely, Thermophys. Prop.
Ctr. for Chemical Engineering
National Eng. Laboratory
NIST
Boulder, CO 80303
(303) 320-5467

Gerald Entine
Radiation Monitoring Devices, Inc.
44 Hunt Street
Watertown, MA 02172
(617) 926-1167

Mike Epstein
Battelle-Columbus Labs
505 King Avenue
Columbus, OH 43201
(614) 424-6424

R. H. Ericksen
Division 1813
Sandia National Laboratories
Albuquerque, NM 87185
(505) 844-8333

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

R. A. Graham
Division 1130
Sandia National Laboratories
Albuquerque, NM 87185
(505) 844-1931

Anton C. Greenwald
Spire Corporation
One Patriots Park
Bedford, MA 01730-2396
(617) 275-6000

N. Grossman
NE-42/FORS
U.S. Dept. of Energy
Washington, DC 20585
(301) 903-3745

Dieter M. Gruen
Materials Science Division
Argonne National Laboratory
9700 South Cass Avenue
Argonne, IL 60439
(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

Thomas P. Herbell
NASA Lewis Research Center
21000 Brookpark Road, 105-1
Cleveland, OH 44135
(216) 433-3246

Carl B. Hilland
DP-28/GTN
U.S. Dept. of Energy
Washington, DC 20545
(301) 903-3687

G. Duncan Hitchens
Lynntech, Inc.
7610 Eastmark Drive
Suite 105
College Station, TX 77840
(409) 693-0017

Kai-Ming Ho
Inst. for Physical
Research and Technology
Ames 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) 231-1115

M. R. Keenan
Division 1813
Sandia National Laboratories
Albuquerque, NM 87185
(505) 844-6631

J. R. Keiser
ORNL
P.O. Box 2008
Bldg. 4500-S, 156, Room 0734
Oak Ridge, TN 37830
(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

C. C. Koch
Materials Eng. Department
North Carolina State University
Raliegh, NC 27650
(919) 737-2377

Victor R. Koch
Covalent Associates, Inc.
10 State Street
Woburn, MA 01801
(617) 938-1140

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, Dean
New York State College of Ceramics
Alfred University
Alfred, NY 14802
(607) 871-2411

Robert W. McClung
ORNL
P.O. Box 2008
Bldg. 4500-S, 151, Rm. D63
Oak Ridge, TN 37831-6088
(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

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

Jack Mofett
Library of Congress
101 Independence Avenue, SW
Washington, DC 20540-7490
(202) 707-1435

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

R. Gerald Nix
NREL
1617 Cole Blvd
Golden, CO 80401
(303) 231-1757

T. A. Nolan
ORNL
P.O. Box 2008
Bldg. 4515, MS 064
Oak Ridge, TN 37831
(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

Randall B. Olsen
Chronos Research Labs, Inc.
3025 Via de Caballo
Olivenhaim, CA 92024
(619) 756-1447

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

Reinhold N. W. Strnot
KJS Associates
1616 Hillrose Place
Fairborn, OH 45324
(513) 879-0114

Thomas N. Strom
NASA Lewis Research Center
21000 Brookpark Road, MS 77-6
Cleveland, OH 44135
(216) 433-3408

David Sutter
ER-224/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

J. A. VanDenAvyle
Division 1832
Sandia National Laboratories
Albuquerque, NM 87185
(505) 844-1016

D. van Rooyen
Brookhaven National Lab.
Upton, NY 11973
(516) 282-4050

Carl R. Vander Linden
Vander Linden & Associates
AIC Materials Program
5 Brassie Way
Littleton, CO 80123
(303) 794-8309

William VanDyke
NE-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) 231-7141

INDEX

A

B

C

D

D

E

F

G

H

I

J

K

L

M

N

O

P

Q

R

S

W

X

Y

Z

U.S. Department of Energy
19901 Germantown Road
Germantown, MD 20874

EM-131