DOE/SC-0025

ENERGY MATERIALS COORDINATING COMMITTEE (EMaCC)

Fiscal Year 1999

October 31, 2000

Annual Technical Report

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

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INTRODUCTION

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

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

Electrochemical Technologies - Richard Kelly, SC-13, (301) 903-6051
Metals - Sara Dillich, EE-22, (202) 586-7925
Radioactive Waste Containers - Matesh (Mat) Varma, SC-13, (301) 903-3209
Semiconductors - Jerry Smith, SC-13, (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.

Three meetings were scheduled for 1999-2000. The dates and minutes from the meetings are as follows:

Thursday, October 28, 1999, 10:15 a.m.-11:30 a.m., Room G-426/GTN

The guest speaker for the first meeting of EMaCC in FY 2000 was Dr. Joseph Carpenter, Manager of the Lightweight Vehicle Materials Program in the Office of Advanced Automotive Transportation Technologies. Dr. Carpenter first provided a brief summary of the organizational structure of the Office of Energy Efficiency and Renewable Energy and then focused on the materials research program that is funded by the following four offices: Office of Power Technologies, Office of Industrial Technologies, Office of Advanced Automotive Technologies, and Office of Heavy Vehicle Technologies. He provided a detailed description of the materials development program in the Office of Transportation Technologies.

The following upcoming events and meetings were discussed: Basic Energy Sciences Advisory Committee (BESAC) meeting: November 3-4, 1999; Metals and Ceramic Team review of M & C subprogram at the Argonne National Laboratory on November 16-17, 1999: Council on Materials Sciences meeting in Room E-401/GTN, December 13-14, 1999.

Dr. Iran Thomas discussed the possibility of involving EMaCC in supporting or sponsoring a workshop to foster collaboration in computational materials science between different program offices within the department. He suggested using the resources of a newly created organization called "Computational Materials Science Network (CMSN)." This suggestion was well received by the members.

Thursday, January 13, 2000, 10:00 a.m.-11:30 a.m., Room E-114/GTN

The guest speaker was Dr. Bruce Harmon, from the Ames National Laboratory. Dr. Harmon focused on the structure and operation of the CMSN, which is supported by the Office of Basic Energy Sciences. He provided motivation for its establishment by reviewing a number of recent developments, including the announcement by IBM of a five-year, $100M project that aims to build a 1,000,000 processor computer that will attain one petaflop (10^{15} floating point operations per second).

Dr. Matesh Varma gave a brief description of DOE's Experimental Program to Stimulate Competitive Research (EPSCoR). This program is intended to enhance the capabilities of designated states to conduct nationally competitive energy-related research and to develop science and engineering manpower to meet current and future needs in energy-related areas.

Thursday, April 11, 2000, 10:05 a.m.-11:30a.m, Room 2E-069/FORS

The guest speaker was Dr. James Daley, Manager and Team Leader of the High Temperature Superconductivity (HTS) Program in the Office of Power Technologies (OPT). The budget for this program, which performs activities in partnership with industry, is $31.4 million for FY00. Its goals are: (1) to achieve HTS wire with 100 times the current carrying capacity of copper; and (2) to complete prototype demonstration of HTS electric power equipment such as motors, power cables, and transformers.

Dr. Charles Sorrell described changes in the Materials Program supported by the Office of Industrial Technologies. The subprogram " Continuous Fiber Ceramic Composites (CFCC)" is scheduled for completion by FY02. The Advanced Industrial Materials (AIM) Program, which is currently predominately laboratory-oriented, will be transformed into a new program called "Industrial Materials of the Future (IMF)," consisting of AIM and remnants of the CFCC program. The intention is to open IMF to both laboratory and university communities by FY05.

The EMaCC reports to the Director of the Office of Science 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 1999 and describes the materials research programs of various offices and divisions within the Department.

The EMaCC Chair for FY 1999 was Dr. Tim Fitzsimmons. The compilation of this report was performed by Dr. Matesh Varma, EMaCC Executive Secretary for FY 2000, with the assistance of FM Technologies, Inc. and the RAND Corporation.

Dr. Charles Sorrell
Office of Industrial Technologies
EMaCC Chair, FY 2000

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
	Pat Hoffman, EE-23	202/586-6074
Transportation Technologies		
Automotive Propulsion System Materials	Patrick Davis, EE-32	202/586-8061
Automotive Lightweight Vehicle Materials	Joseph Carpenter, EE-32	202/586-1022
Advanced Battery Systems	Ray Sutula, EE-32	202/586-8064
Fuel Cell Systems	JoAnn Milliken, EE-32	202/586-2480
Heavy Vehicle Propulsion System Materials	Sidney Diamond, EE-34	202/586-8032
High Strength Weight Reduction Materials	Sidney Diamond, EE-34	202/586-8032
High Temperature Materials Laboratory	Sidney Diamond, EE-34	202/586-8032
Utility Technologies		
Wind/Hydro/Ocean Technologies	William Richards, EE-121	202/586-5410
Geothermal Technology	Raymond LaSala, EE-122	202/586-4198
Photovoltaic Technology	Richard King, EE-131	202/586-1693
Advanced Utility Concepts	James Daley, EE-142	202/586-1165

Table 1. Membership List

ORGANIZATION	REPRESENTATIVE	PHONE NO.
SCIENCE		
Basic Energy Sciences		
Materials Sciences	Pat Dehmer, SC-10	301/903-3081
	Iran L. Thomas, SC-13	301/903-3427
Metal and Ceramic Sciences	Robert J. Gottschall, SC-13	301/903-3428
	Alan Dragoo, SC-13	301/903-3428
	Yok Chen, SC-13	301/903-3428
	Helen Kerch, SC-13	301/903-3428
Solid State Physics and Materials Chemistry	W. Oosterhuis, SC-13	301/903-3426
	Jerry Smith, SC-13	301/903-3426
	Richard Kelly, SC-13	301/903-3426
	Manfred Leiser, SC-13	301/903-3426
	Matesh (Mat) Varma, SC-13	301/903-3209
Chemical Sciences	Robert S. Marianelli, SC-14	301/903-5808
Engineering and Geosciences	Nick Woodward, SC-15	301/903-5822
Advanced Scientific Computing Research		
Technology Research	Walter M. Polansky, SC-32	301/903-5995
	David Koegel, SC-32	301/903-3159
Laboratory Operations and Environment, Safety and Health		
Environment, Safety and Health	Ted Tomczak, SC-83	301/903-6916
Fusion Energy		
Fusion Technologies	Sam Berk, SC-52	301/903-4171
Office of Biological and Environmental Research		
Medical Sciences Division	Larry James, SC-73	301/903-7481
ENVIRONMENTAL RESTORATION AND WASTE MANAGEMENT		
Waste Operations		
Waste Management Projects	Doug Tonkay, EM-34	301/903-7212
Science and Technology		
Research and Development	Chet Miller, EM-34	202/586-3952

ORGANIZATION	REPRESENTATIVE	PHONE NO.
NUCLEAR ENERGY, SCIENCE AND TECHNOLOGY		
Disposition Technologies	William Van Dyke, NE-40 Beverly Cook, NE-40	301/903-4201 301/903-4021
Space and Defense Power Systems	William Barnett, NE-50 John Dowicki, NE-50	301/903-3097 301/903-7729
Naval Reactors	David I. Curtis, NE-60 Tom Kennedy, NE-60	703/603-5561 703/603-1754
Reactor Programs	John Warren, NE-80 Bob Lange, NE-80	301/903-6491 301/903-2915
CIVILIAN RADIOACTIVE WASTE MANAGEMENT		
Analysis and Verification	Alan Berusch, RW-37	202/586-9362
DEFENSE PROGRAMS		
Research and Advanced Technology Research and Technology Development	Bharat Agrawal, DP-16	301/903-2057
Inertial Confinement Fusion	Carl B. Hilland, DP-18	301/903-3687
FOSSIL ENERGY		
Advanced Research	Fred M. Glaser, FE-25	301/903-2786

ORGANIZATION OF THE REPORT

The FY 1999 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 1999 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 1999 funding, and detailed project summaries are presented for each Assistant Secretary office and the Office of Science. The project summaries also provide DOE, laboratory, academic and industrial contacts for each project, as appropriate.

FY 1999 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 1999
OFFICE OF BUILDING TECHNOLOGY, STATE AND COMMUNITY PROGRAMS	$955,000
Office of Building Systems	955,000
OFFICE OF INDUSTRIAL TECHNOLOGIES	$20,204,682
Office of Industrial Strategies	8,581,000
Aluminum Vision Team	4,475,000
Forest Products Vision Team	700,000
Steel Vision Team	450,000
Glass Vision Team	550,000
Metal Casting Vision Team	1,530,000
Mining Vision Team	876,000
Office of Crosscut Technologies	11,623,682
Advanced Industrial Materials (AIM) Program	5,350,000
Financial Assistance Program	6,273,682
Inventions and Innovations	2,472,585
National Industrial Competitiveness Through Energy, Environment and Economic (NICE^3)	3,801,097
OFFICE OF TRANSPORTATION TECHNOLOGIES	$39,832,101
Office of Advanced Automotive Technologies	31,147,500
Transportation Materials Technology	27,165,000
Propulsion Materials	1,805,000
Lightweight Vehicle Materials	25,360,000
Electric Drive Vehicle Technologies	3,982,500
Advanced Battery Materials	3,582,500
Fuel Cell Materials	400,000
Office of Heavy Vehicle Technologies	8,684,601
Transportation Materials Technology	8,684,601
Heavy Vehicle Propulsion System Materials	4,499,601
High Strength Weight Reduction Materials	4,185,000
OFFICE OF POWER TECHNOLOGIES	$56,996,000
Office of Solar Energy Technologies	24,033,000
Office of Geothermal Technologies	863,000
Office of Energy Management	32,100,000
Advanced Utility Concepts Division	32,100,000
High Temperature Superconductivity for Electric Systems	32,100,000

FY 1999 BUDGET SUMMARY FOR DOE MATERIALS ACTIVITIES (continued)

	FY 1999
OFFICE OF SCIENCE	$461,957,625
Office of Basic Energy Sciences	419,258,600
Division of Materials Sciences	407,636,000
Division of Chemical Sciences	5,000,000
Division of Engineering and Geosciences	6,622,600
Engineering Sciences Research	3,137,800
Geosciences Research	3,484,800
Office of Advanced Scientific Computing Research	32,819,025
Division of Technology Research	32,819,025
Laboratory Technology Research Program	5,240,000
Small Business Innovation Research Program	25,583,729
Small Business Technology Transfer Research Program	1,995,296
Office of Fusion Energy Sciences	9,880,000
OFFICE OF ENVIRONMENTAL MANAGEMENT	$8,708,996
OFFICE OF NUCLEAR ENERGY, SCIENCE AND TECHNOLOGY	$73,917,000
Office of Space and Defense Power Systems	3,617,000
Space and National Security Programs	3,617,000
Office of Naval Reactors	70,300,000[1]
OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT	$29,121,295
OFFICE OF DEFENSE PROGRAMS	$45,869,600
The Weapons Research, Development and Test Program	45,869,600
Sandia National Laboratories	22,264,600
Los Alamos National Laboratory	17,000,000
Lawrence Livermore National Laboratory	6,605,000
OFFICE OF FOSSIL ENERGY	$10,004,000
Office of Advanced Research	10,004,000
Fossil Energy AR&TD Materials Program	6,004,000
Advanced Metallurgical Processes Program	4,000,000
TOTAL	$747,566,299

[1]This excludes $49.2 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	$955,000	$0	$0	$0	$955,000
Office of Industrial Technologies	$5,859,358	$11,718,716	$2,424,562	$202,046	$20,204,682
Office of Transportation Technologies	$20,310,896	$13,213,497	$5,196,940	$1,110,768	$39,832,101
Office of Power Technologies	$38,596,000	$16,000,000	$1,900,000	$500,000	$56,996,000
Office of Science	$327,835,335	$93,155,290	$40,492,000	$475,000	$461,957,625
Office of Environmental Management	$6,027,022	$300,000	$2,157,974	$224,000	$8,708,996
Office of Nuclear Energy, Science and Technology	$72,820,000	$0	$1,097,000	$0	$73,917,000
Office of Civilian Radioactive Waste Management	$29,121,295	$0	$0	$0	$29,121,295
Office of Defense Programs	$45,869,600	$0	$0	$0	$45,869,600
Office of Fossil Energy	$8,912,000	$600,000	$492,000	$0	$10,004,000
Totals	$556,306,506	$134,987,503	$53,760,476	$2,511,814	$747,566,299

Table 2. Distribution of Funds by Office

OFFICE OF ENERGY EFFICIENCY AND RENEWABLE ENERGY

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

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

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

	FY 1999
OFFICE OF BUILDING TECHNOLOGY, STATE AND COMMUNITY PROGRAMS	$955,000
Office of Building Systems	955,000
OFFICE OF INDUSTRIAL TECHNOLOGIES	$20,204,682
Office of Industrial Strategies	8,581,000
Aluminum Vision Team	4,475,000
Forest Products Vision Team	700,000
Steel Vision Team	450,000
Glass Vision Team	550,000
Metal Casting Vision Team	1,530,000
Mining Vision Team	876,000
Office of Crosscut Technologies	11,623,682
Advanced Industrial Materials (AIM) Program	5,350,000
Financial Assistance Program	6,273,682
Inventions and Innovations	2,472,585
National Industrial Competitiveness Through Energy, Environment and Economic (NICE^3)	3,801,097
OFFICE OF TRANSPORTATION TECHNOLOGIES	$39,832,101
Office of Advanced Automotive Technologies	31,147,500
Transportation Materials Technology	27,165,000
Propulsion Materials	1,805,000
Lightweight Vehicle Materials	25,360,000
Electric Drive Vehicle Technologies Program	3,982,500
Advanced Battery Materials	3,582,500
Fuel Cell Materials	400,000
Office of Heavy Vehicle Technologies	8,684,601
Transportation Materials Technology	8,684,601
Heavy Vehicle Propulsion System Materials	4,499,601
High Strength Weight Reduction Materials	4,185,000
OFFICE OF POWER TECHNOLOGIES	$56,996,000
Office of Solar Energy Technologies	24,033,000
Office of Geothermal Technologies	863,000
Office of Energy Management	32,100,000
Advanced Utility Concepts Division	32,100,000
High Temperature Superconductivity for Electric Systems	32,100,000

OFFICE OF BUILDING TECHNOLOGY, STATE AND COMMUNITY PROGRAMS

	FY 1999
Office of Building Technology, State and Community Programs - Grand Total	$955,000
Office of Building Systems	$955,000
Materials Properties, Behavior, Characterization or Testing	$955,000
Evacuated Panel Superinsulation	55,000
Non-HCFC Closed-Cell Foam Insulation	250,000
Existing Materials Performance	125,000
Radiative Heat Transfer in Attic Insulation	80,000
Hygrothermal Property Measurements	225,000
Sub-Ambient Pipe Insulation Materials and Systems	70,000
Sustainable Insulation	100,000
Program Management	50,000

OFFICE OF BUILDING TECHNOLOGY, STATE AND COMMUNITY PROGRAMS

OFFICE OF BUILDING SYSTEMS

The goal of this Office is to reduce energy use of new buildings by 50 percent by 2010, achieve further reductions in energy use through retrofit of existing buildings and reduce annual energy use by 2 quads by 2010 and 5 quads by 2020. The Division's primary objectives are to support research that advances the scientific and technical options for increased energy efficiency in buildings, to promote the substitution of abundant fuels for scarce fuels in buildings, and to promulgate standards for increased efficiency of energy use. To accomplish a portion of this, the Buildings Materials program seeks to: (1) develop new and improve existing insulating materials; (2) develop and verify analytical models that are useful to building designers and researchers for predicting the thermal performance characteristics of materials; (3) develop and standardize methods for measuring the thermal performance characteristics; and (4) provide technical assistance and advice to industry and the public. The DOE contact is Arun Vohra, (202) 586-2193.

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

1. **EVACUATED PANEL SUPERINSULATION**
   $55,000
   DOE Contact: Arun Vohra, (202) 586-2193
   ORNL Contact: Therese Stovall, (865) 574-0329

This project is to continue long term ageing measurements of vacuum insulation panels. Current technology produces R-30 per inch panels. Cost effective applications, including the walls and doors of refrigerators/freezers and building envelopes, are being explored.

Keywords: Insulation, Vacuum, Heat Transfer, Refrigerators

2. **NON-HCFC CLOSED-CELL FOAM INSULATION**
   $250,000
   DOE Contact: Arun Vohra, (202) 586-2193
   ORNL Contact: Ken Wilkes, (865) 574-5931

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

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

3. **EXISTING MATERIALS PERFORMANCE**
   $125,000
   DOE Contact: Arun Vohra, (202) 586-2193
   ORNL Contact: Therese Stovall, (865) 574-0329

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

Keywords: Insulation, Buildings

4. **RADIATIVE HEAT TRANSFER IN ATTIC INSULATION**
   $80,000
   DOE Contact: Arun Vohra, (202) 586-2193
   ORNL Contact: Ken Wilkes, (865) 574-5931

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

Keywords: Fibrous Insulation, Attics, Radiation, Models

5. **HYGROTHERMAL PROPERTY MEASUREMENTS**
$225,000
DOE Contact: Arun Vohra, (202) 586-2193
ORNL Contact: Ken Wilkes, (865) 574-5931

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

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

6. **SUB-AMBIENT PIPE INSULATION MATERIALS AND SYSTEMS**
$70,000
DOE Contact: Arun Vohra, (202) 586-2193
ORNL Contact: Ken Wilkes, (865) 574-5931

Pipe thermal insulations are rated by the thermal resistance as measured in pipe testing apparatus in conformance with ASTM C 335. The scope of ASTM C 335 limits its use to piping systems operating at temperatures above ambient. Numerous ASTM material specifications specify the use of these materials on pipes operating below ambient conditions. There are no test methods or test facilities available for undertaking these measurements.

Pipe insulations applied to piping operating at sub-ambient conditions is also a major concern within ASHRAE. These insulation systems can have severe moisture-related problems due to the unidirectional nature of their vapor drive. Attempts to address the rash of failures to these systems due to moisture ingress leading to loss in energy efficiency as well as mechanical failure are planned.

Keywords: Piping, Moisture, Insulation, Properties

7. **SUSTAINABLE INSULATION**
$100,000
DOE Contact: Arun Vohra, (202) 586-2193
ORNL Contact: Ken Wilkes, (865) 574-5931

The objective of this task is to develop very low-cost sustainable insulation materials that require a minimum of physical or chemical processing for use in building envelope systems. This information will be provided to ASHRAE for inclusion in a revision of Chapter 24 of the Handbook of Fundamentals.

Keywords: Building Materials, Environment, Sustainable, Properties

8. **PROGRAM MANAGEMENT**
$50,000
DOE Contact: Arun Vohra, (202) 586-2193
ORNL Contact: Andre Desjarlais, (865) 574-0022

This task provides for the field management of the Building Materials Program. This includes preparation of the field work proposal, program statement of work, monthly progress reports, management of subcontracts, and responses to other requests from the DOE Program Manager.

Keywords: Building Materials, Moisture, Insulation, Energy, Properties

OFFICE OF INDUSTRIAL TECHNOLOGIES

	FY 1999
Office of Industrial Technologies - Grand Total	$20,204,682
Office of Industrial Strategies	$8,581,000
Aluminum Vision Team	$4,475,000
Device or Component Fabrication, Behavior or Testing	$287,000
Innovative Vertical Floatation Melter (VFM)	600,000
Technology for Converting Spent Potliner (SPL) to Useful Glass Fiber Products	132,000
Inert Metal Anode Life in Low Temperature Aluminum Reduction Process	402,000
Advanced Anodes and Cathodes Utilized in Energy Efficient Aluminum Production Cells	1,334,000
Detection and Removal of Molten Salts from Molten Aluminum Alloys	65,000
Intelligent Potroom Operation	75,000
Development of a Novel Non-Consumable Anode for Electrowinning Primary Aluminum	147,000
High-Efficiency, High-Capacity, Low-NO_x Aluminum Melting Using Oxygen-Enhanced Combustion	0
Potlining Additives	115,000
Materials Properties, Behavior, Characterization or Testing	$730,000
Molten Aluminum Explosion Prevention	250,000
Semi Solid Aluminum Alloys	405,000
Integrated Numerical Methods and Design Provisions for Aluminum Structures	75,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$3,458,000
Recycling Aluminum Salt Cake	1,650,000
Processing and Recycling of Aluminum Wastes	436,000
Wettable Ceramic-based Drained Cathode Technology for Aluminum Electrolysis Cells	1,116,000
Improved Grain Refinement Process for Aluminum	246,000
Spray Rolling Aluminum Strip	10,000
Forest Products Vision Team	$700,000
Materials Properties, Behavior, Characterization or Testing	$700,000
Corrosion in Kraft Digesters: Characterization of Degradation and Evaluation of Corrosion Control Methods	300,000
Selection and Development of Refractory Structural Materials for Black Liquor Gasification	400,000
Steel Vision Team	$450,000
Device or Component Fabrication, Behavior or Testing	$450,000
Intermetallic Alloy Development Related to the Steel Industry	450,000

OFFICE OF INDUSTRIAL TECHNOLOGIES (continued)

	FY 1999
Office of Industrial Strategies (continued)	
Glass Vision Team	$550,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$220,000
Chemical Vapor Deposition Ceramic Synthesis	220,000
Materials Properties, Behavior, Characterization or Testing	$330,000
Development of Improved Refractories	30,000
Synthesis and Design of $MoSi_2$ Intermetallic Materials	300,000
Metal Casting Vision Team	$1,530,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$132,000
Creep Resistant Zinc Alloy Development	132,000
Materials Properties, Behavior, Characterization or Testing	$1,398,000
Clean Cast Steel: 1) Machinability of Cast Steel; 2) Accelerated Transfer of Clean Steel Technology	261,000
Thin Section Steel Castings	111,000
Clean Metal Processing (Aluminum)	255,000
Advanced Lost Foam Casting Technology	196,000
Mechanical Properties Structure Correlation for Commercial Specification of Cast Particulate Metal Matrix Components	91,000
Ferrite Measurements in Duplex Stainless Steel Castings	25,000
Technology for the Production of Clean, Thin Wall, Machinable Gray and Ductile Iron Castings	206,000
Enhancements in Magnesium Die Casting Die Life and Impact Properties	101,000
Mold Materials for Permanent Molding of Aluminum Alloys	92,000
Systematic Microstructural and Corrosion Performance Evaluation of High Molybdenum Stainless Steel Casting	60,000
Mining Vision Team	$876,000
Drilling and Blasting Optimization Using Seismic Analysis and X-ray Fluorescence Spectroscopy	200,000
Application of High Temperature Superconductors to Underground Communications	357,000
Hydrides for Fuel Cell Mining Vehicles	155,000
Mining Byproduct Recovery	64,000
Development of a Mine Compatible LIBS Instrument for Ore Grading	100,000

OFFICE OF INDUSTRIAL TECHNOLOGIES (continued)

	FY 1999
Office of Crosscut Technologies	$11,623,682
Advanced Industrial Materials (AIM) Program	$5,350,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$2,910,000
Intermetallic Alloy Development and Technology Transfer of Intermetallic Alloys	980,000
Development of Advanced Intermetallic Alloys	250,000
Composites and Coatings Through Reactive Metal Infiltration	440,000
Conducting Polymers: Synthesis and Industrial Applications	200,000
Membrane Systems for Efficient Separation of Light Gases	300,000
Plasma Processing - Advanced Materials for Corrosion and Erosion Resistance	300,000
Uniform Droplet Processing	440,000
Materials Properties, Behavior, Characterization or Testing	$980,000
Materials for Recovery Boilers	980,000
Materials Structure and Composition	$615,000
Metallic and Intermetallic Bonded Ceramic Composites	100,000
Advanced Materials/Processes	515,000
Device or Component Fabrication, Behavior or Testing	$845,000
Microwave Joining of SiC	45,000
Selective Inorganic Thin Films	350,000
Materials for High Temperature Filtration/Thermochemical Modeling	100,000
Metals Processing Laboratory User (MPLUS) Facility	350,000
Financial Assistance Program	$6,273,682
Inventions and Innovations	$2,472,585
Laser Sensor for Optimization of Compressor Stations and Refinery Operations	199,632
Titanium Matrix Composite Tooling Material for Enhanced Manufacture of Aluminum Die Castings	199,984
An Insoluble Titanium-Lead Anode for Sulfate Electrolytes	200,000
Development of an Innovative Energy Efficient High Temperature Natural Gas Fired Furnace	199,361
A New High Temperature Coating for Gas Turbines	200,000
Tough-Coated Hard Powders (TCHPs): A New Paradigm in Mining and Machining Tool Materials	200,000
A New Energy Saving Method of Manufacturing Ceramic Products from Waste Glass	199,977
Distillation Column Flooding Predictor	52,900
Energy Saving Lightweight Refractory	158,041
High Intensity Silicon Vertical Multi-Junction Solar Cells	142,900
Fabrication and Testing of a Prototype Ceramic Furnace Coil	199,853
Germanium Compounds as Highly Selective Fluorination Catalysts	40,000
Development of Phosphors for Use in High-Efficiency Lighting and Displays	40,000
Novel Ceramic Composition for Hall-Heroult Cell Anode Application	39,989
Functionally Graded Materials for Improved High Temperature Performance of Nd-Fe-B-Based Permanent Magnets	39,948

OFFICE OF INDUSTRIAL TECHNOLOGIES (continued)

	FY 1999
Office of Crosscut Technologies (continued)	
Financial Assistance Program (continued)	
Inventions and Innovations (continued)	
Improved Alkylation Contractor	40,000
Low Cost Synthesis and Consolidation of TiC	40,000
Development of Aluminum Iron Alloys for Magnetic Applications	40,000
Novel Frequency-Selective Solar Glazing System	40,000
A Ceramic Composite for Metal Casting	40,000
Electrochemical Method for Extraction of Oxygen From Air	40,000
Energy Saving Method for Producing Ethylene Glycol and Propylene Glycol	40,000
Improved Refractories Using Engineered Particles	40,000
Enabling Tool for Innovative Glass Applications	40,000
National Industrial Competitiveness Through Energy, Environment and Economics (NICE[3])	$3,801,097
Demonstration of a Three-Phase Rotary Separator Turbine	519,326
Ceramic Turbine Wheel Technology To Provide Economic, Efficiency and Environmental Enhancements to Microturbines	524,673
Precision Irrigation Technologies for the Agricultural Industry	455,000
Energy Conserving Tool for Combustion Dependent Industries	304,867
Energy-Saving Regeneration of Hydrochloric Acid Pickling Liquor	472,231
Supercritical Fluid Purification of Combi-Chem Libraries	500,000
Full-Scale 100 Ton/Hr Demonstration of Magnetic Elutriation Technology for Clean and Efficient Processing of Iron Ore	500,000
Reducing Foundry Emissions and Green Sand Waste Via Integrated Advanced Oxidation-Underwater Plasma Processing	525,000

OFFICE OF INDUSTRIAL TECHNOLOGIES

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

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

OFFICE OF INDUSTRIAL STRATEGIES

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

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

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

9. INNOVATIVE VERTICAL FLOATATION MELTER (VFM)
$600,000
DOE Contact: Ramesh Jain, (202) 586-2381

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

Keywords: Flotation Melter, Aluminum Scrap

10. TECHNOLOGY FOR CONVERTING SPENT POTLINER (SPL) TO USEFUL GLASS FIBER PRODUCTS
$132,000
DOE Contact: Tom Robinson, (202) 586-0139

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

- Design, fabrication, and installation of pilot-scale glass fiberizing and flue gas filtration and analysis equipment into Vortec's existing pilot-scale CMS™ testing facility
- Pilot-scale SPL vitrification test to produce glass fibers

- Testing and analysis of the fibers from the pilot-scale test with respect to commercial quality specifications
- Testing and analysis of fibers with respect to human health considerations
- Sampling and analysis of flue gas from the pilot-scale CMSJ during testing
- Preliminary design of a commercial-scale air pollution system for aluminum fluoride production.

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

11. INERT METAL ANODE LIFE IN LOW TEMPERATURE ALUMINUM REDUCTION PROCESS
$402,000
DOE Contact: Tom Robinson, (202) 586-0139

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

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

12. ADVANCED ANODES AND CATHODES UTILIZED IN ENERGY EFFICIENT ALUMINUM PRODUCTION CELLS
$1,334,000
DOE Contact: Tom Robinson, (202) 586-0139

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

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

13. DETECTION AND REMOVAL OF MOLTEN SALTS FROM MOLTEN ALUMINUM ALLOYS
$65,000
DOE Contact: Tom Robinson, (202) 586-0139

Selee Corporation and the Alcoa Technical Center are conducting this project to detect and reduce chloride salts in molten aluminum. These salts have been shown to initiate defects when they agglomerate and migrate to the surface of an ingot or casting. Because they are liquid at aluminum casting temperatures, they can pass through conventional filter systems, which are designed to capture solid inclusions. Moreover, they tend to reduce the efficiency of filters by causing the release of solid inclusions. 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 that 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. The detection and removal of molten salts will result in improved metal quality, recovery, and reliability; elimination of melt rejection and recast; and a reduction in chlorine use and release.

Keywords: Molten Salts, Molten Aluminum Alloys, Aluminum Casting

14. **INTELLIGENT POTROOM OPERATION**
$75,000
DOE Contact: Simon Friedrich, (202) 586-6759

Applied Industrial Solutions, Century Aluminum, Gensym Corporation and West Virginia University are project partners for the development of intelligent potroom operation. Aluminum smelting requires operators to oversee many refining cells. Close scrutiny of each one on a regular basis is not possible. Also, modern aluminum refining cell controllers attempt to optimize cell efficiency by controlling the concentration of alumina in the bath. Unfortunately, no direct measure of alumina concentration is yet possible. The ramifications miscalculating alumina concentration is significant from an environmental and energy efficiency stand point. One major product of this research will be the development of a Corrective Action Neural Network (CANN). Its function is to monitor and analyze data from the pots on a continuous basis, looking for cells whose performance is deteriorating. It will anticipate which cells are about to slip into degraded or out-of-control operation and dispatch the operator to intervene before trouble begins. Eventually, a closed-loop Cell Control Enhancement Module (CCEM) will be added to the individual cell controllers. The CCEM will use an enhanced instrumentation package and powerful data analysis techniques to provide a more complete picture of instantaneous cell status to the CANN. The CANN and CCEM will work in concert to continuously improve the database on each cell, and the knowledge base on control and remediation techniques.

Keywords: Smelting, Aluminum Potroom Operation, Aluminum Refining

15. **DEVELOPMENT OF A NOVEL NON-CONSUMABLE ANODE FOR ELECTROWINNING PRIMARY ALUMINUM**
$147,000
DOE Contact: Simon Friedrich, (202) 586-6759

Gas Research Institute, Kaiser Aluminum, Ohio State University, Siemens-Westinghouse and TDA Research are project partners for the development of a novel non-consumable anode. Since the patenting of the Hall-Héroult Cell (HHC) in 1886 for electrowinning aluminum, the basic features have remained essentially the same. Although significant optimization has occurred, industry acknowledges that there are many problems associated with the use of the consumable carbon anode. This project is developing a novel non-consumable (gas) anode that will displace today's carbon anode (eliminating the carbon plant), and serve as a retrofit into the current HHC. The anode is comprised of a thin, dense oxide-ion-conducting membrane with an electrocatalytic porous internal anode where reformed natural gas is electrochemically oxidized. Application of such a non-consumable anode retrofitted into the HHC would significantly increase the energy efficiency, reduce the emissions, and reduce the cost of producing primary aluminum compared to the best current and emerging anode replacement technologies.

Keywords: Carbon Anode, Aluminum Production, Smelting

16. **HIGH-EFFICIENCY, HIGH-CAPACITY, LOW-NO_x ALUMINUM MELTING USING OXYGEN-ENHANCED COMBUSTION**
$0
DOE Contact: Ramesh Jain, (202) 586-2381

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

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

Keywords: Aluminum Melting, Combustion, Burner

17. **POTLINING ADDITIVES**
$115,000
DOE Contact: Tom Robinson, (202) 586-0139

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

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

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

18. **MOLTEN ALUMINUM EXPLOSION PREVENTION**
$250,000
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. Oak Ridge National Laboratory has designed and developed the Steam Explosion Triggering Studies (SETS) facility, an experimental test site where the fundamental issues of explosions will be investigated with emphasis on triggering events. Solid tungsten, an element that has thermophysical properties similar to those of liquid aluminum, is used during the experiments to allow the apparatus to be instrumented and the phenomena associated with the breakdown of steam film and triggering investigated without the hazards associated with experiments performed with large amounts of liquid aluminum. ORNL has produced significant data to assess suppression capability for various coatings with full curing times. However, the impact of shorter curing times as well as the study of impact of bare spots is issues that need resolution. Further collection of data for selected coatings with different degrees of curing, together with the effects of the introduction of non-condensable gasses, remain the subjects of Phase II.

Keywords: Explosions, Molten Aluminum, Water

19. **SEMI SOLID ALUMINUM ALLOYS**
$405,000
DOE Contact: Tom Robinson, (202) 586-0139

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

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

20. **INTEGRATED NUMERICAL METHODS AND DESIGN PROVISIONS FOR ALUMINUM STRUCTURES**
$75,000
DOE Contact: Simon Friedrich, (202) 586-6759

Project partners for this research effort are the Aluminum Association and Cornell University. Aluminum's competitive edge arises from the ease with which shapes can be extruded. Yet, this advantage cannot be fully exploited by designers because they do not have the tools to predict the strength of many extrudable shapes. Suggested specifications for the structural design of parts made of various aluminum alloys were developed in 1962 and published in 1967 in Specifications for Aluminum Structures (Aluminum Association). The document has been revised five times, most recently in 1994, but methods for determining the buckling strength of extrusions are essentially unchanged. Many types of stiffeners, such as web stiffeners and multiple intermediate stiffeners, thickness changes and other cross-sectional peculiarities cannot be addressed by the current specification even though they add significantly to the load carrying capacity. Researchers from Cornell University will develop and demonstrate a design methodology using finite strip analysis. It will result in design rules applicable to many extrudable or cold-rolled shapes. Columns, beams, and beam columns will be studied. A wide variety of failure modes such as local, distortional, torsional, torsional-flexural, and lateral buckling will be researched. Failures involving the interaction of these modes, such as the local and overall buckling will be included in the study as well.

Keywords: Aluminum Extrusions, Aluminum Structures, Design Provisions

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

21. **RECYCLING ALUMINUM SALT CAKE**
$1,650,000
DOE Contact: Tom Robinson, (202) 586-0139
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 electro-dialysis (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 recom-pression). Increasing the market value of non-metallic product (NMP) is critical for cost-effective salt cake recycling. Impurities constitute about 10 percent of NMP and lower its market value. Research investigated hydrometallurgical processes to purify NMP, since higher NMP purity results in higher market value for refractory aggregate and other potential alumina markets. Technical and economic analysis indicated the electrodialysis process to be most promising. Pilot-scale work indicated fiber insulation materials can be made cost-effectively using NMP as a starting material. A new potential use for NMP (i.e. as alternative alumina units for the blast furnace in ironmaking) has been identified. Process flow sheet and engineering design for pilot scale testing of the electrodialysis process have been completed.

Keywords: Aluminum, Salt Cake, Recycling, Electrodialysis

22. **PROCESSING AND RECYCLING OF ALUMINUM WASTES**
$436,000
DOE Contact: Tom Robinson, (202) 586-0139

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

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

- Document the environmental acceptability of the smelting by-products used as concrete additives and assess the environmental acceptability of the low-density concrete products made using these additives.

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

23. **WETTABLE CERAMIC-BASED DRAINED CATHODE TECHNOLOGY FOR ALUMINUM ELECTROLYSIS CELLS**
$1,116,000
DOE Contact: Tom Robinson, (202) 586-0139

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

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

Keywords: Cathode, Aluminum Production, Titanium Diboride

24. **IMPROVED GRAIN REFINEMENT PROCESS FOR ALUMINUM**
$246,000
DOE Contact: Tom Robinson, (202) 586-0139

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

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

25. **SPRAY ROLLING ALUMINUM STRIP**
$10,000
DOE Contact: Ramesh Jain, (202) 586-2381
INEEL Contact: Kevin McHugh, (208) 525-5877

Alcoa Incorporated, Century Aluminum, Colorado School of Mines, Idaho National Engineering and Environmental Laboratory, Inductotherm, Metals Technology, and University of California are project partners for the development of a new process that combines benefits of twin-roll casting and spray forming. Aluminum's competitive edge arises from the ease with which shapes can be extruded. Nearly all aluminum strip is manufactured commercially by conventional ingot metallurgical (I/M) processing, also known as continuous casting. This method accounts for about 70% of domestic production. However, it is energy and capital equipment intensive. Spray forming is a competitive low-cost alternative to ingot metallurgy for manufacturing ferrous and non-ferrous alloy shapes. It produces materials with a reduced number of processing steps, while maintaining materials properties, with the possibility of near-net-shape manufacturing. However, there are several hurdles to large-scale commercial adoption of spray forming: 1) ensuring strip is consistently flat, 2) eliminating porosity, particularly at the deposit/substrate interface, and 3) improving material yield. Researchers are investigating a spray rolling approach to overcome these hurdles. It should represent a processing improvement over conventional spray forming for strip production. Spray rolling is an innovative manufacturing technique to produce aluminum net-shape products. It requires less energy and generates less scrap than conventional processes and, consequently, enables the development of materials with lower environmental impacts in both processing and final products. It combines benefits of twin-roll casting and conventional spray forming.

Keywords: Aluminum, Spray Forming, Aluminum Strip and Sheet

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

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION, OR TESTING

26. **CORROSION IN KRAFT DIGESTERS: CHARACTERIZATION OF DEGRADATION AND EVALUATION OF CORROSION CONTROL METHODS**
 $300,000
 DOE Contact: Valri Robinson, (202) 586-0937
 ORNL Contact: James Kaiser, (423) 475-4453

This project will correlate chemical pulping digester conditions with material performance. Digester conditions will be evaluated using a computational fluid dynamics model of flow within a digester. This flow model will be supplemented with a model for the chemical reactions occurring in the digester. In-situ and laboratory corrosion studies will be used to provide information about the corrosion behavior of conventional materials. An assessment of corrosion control methods and alternative materials will be performed. This is a 5-year project with an expected completion date of 9/30/03.

Keywords: Digester, Corrosion, Pulp and Paper

27. **SELECTION AND DEVELOPMENT OF REFRACTORY STRUCTURAL MATERIALS FOR BLACK LIQUOR GASIFICATION**
 $400,000
 DOE Contact: Valri Robinson, (202) 586-0937
 ORNL Contact: James Kaiser, (423) 475-4453

This project will identify refractory materials that have acceptable life to allow gasifiers to efficiently and economically operate using black liquor or biomass as feedstocks. Working with industrial partners, the investigators will identify and address the most serious material problems associated with the top three emerging biomass and black liquor gasification technologies. Studies will be performed to identify or develop more suitable materials for these applications. This is a 4-year project with an expected completion date of 9/30/03.

Keywords: Gasification, Black Liquor, Refractory, Pulp and Paper

STEEL VISION TEAM - DOE Steel Team leader, Peter Salmon-Cox, (202) 586-2380

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

28. **INTERMETALLIC ALLOY DEVELOPMENT RELATED TO THE STEEL INDUSTRY**
 $450,000
 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 1999: (1) the melting and centrifugal casting of FeAl was successfully performed at AEC, (2) the evaluation and operation of two Ni_3Al radiant burner tubes prepared for testing in commercial furnaces in Timken and Ford continued; (3) additional castings from various suppliers were evaluated and various types of rolls were introduced at Bethlehem Steel.

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

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

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

29. **CHEMICAL VAPOR DEPOSITION CERAMIC SYNTHESIS**
 $220,000
 DOE Contact: Charles A. Sorrell, (202) 586-1514
 Sandia National Laboratories - Livermore Contact: M. D. Allendorf, (415) 294-2895

Comprehensive models, including detailed gas-phase and surface chemistry coupled with reactor fluid mechanics, are required to optimize and scale-up chemical vapor deposition (CVD) processes. In FY1999 the CRADA with Libby- Owens-Ford Co. on developing new CVD techniques for depositing coatings on glass was continued and completed. The effort focuses on (1) characterized the thermal stability and reactivity of indium containing precursors use din float glass operations, (2) designed an operated a field portable system for monitoring stability of precursors, (3) a field portable unit mass spectrometer unit was constructed in preparation for field testing.

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

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

30. **DEVELOPMENT OF IMPROVED REFRACTORIES**
$30,000
DOE Contact: Charles A. Sorrell, (202) 586-1514
Oak Ridge National Laboratory Contacts:
A. A. Wereszczak, (423) 574-7601 and
Peter Angelini, (423) 574-4565

Refractories are critical for various industrial processes. For example glass melting furnaces are fabricated with various types of refractories which enable the furnaces to be operated at very high temperatures. The goal of this project is to develop improved refractories and to determine critical mechanical and thermophysical and mechanical properties. The results form this R&D will accelerate the use of oxy-fuel firing throughout the glass industry. In FY 1999, the compression creep and corrosion resistance performance of the conventional silica refractory category was completed. Six silica brands were analyzed. For this type of refractory, concurrent changes in materials properties including phase changes have a larger affect on changes in dimensions than creep mechanisms. Partners in this activity include the Oak Ridge National Laboratory, Alfred University Center for Glass Research (CGR) Satellite Center at the University of Missouri-Rolla, and an industrial technical team representing glass and refractories manufacturers.

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

31. **SYNTHESIS AND DESIGN OF $MOSi_2$ INTERMETALLIC MATERIALS**
$300,000
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 1999 included (1) laminate composite tubes of molybdenum disilicide were successfully fabricated including functionally graded composite tube geometries, (2) $MoSi_2$ –coated Al_2O_3 thermocouple sheaths were fabricated and their oxidation resistance and thermal shock behavior characterized.

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

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

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

32. **CREEP RESISTANT ZINC ALLOY DEVELOPMENT**
$132,000
DOE Contact: Ehr Ping HuangFu, (202) 586-1493
International Lead Zinc Research Organization
Frank Goodwin, (919) 361-4647, Ext. 3018

The objective of this project is to develop a hot chamber castable zinc die casting alloys that is capable of satisfactory service at 1400°C and preferably at moderately elevated temperatures 160°C. The target strength at this temperature is 4,500 psi during an exposure time of 1,000 hours. The project will be accomplished by enhancing a previously existing computer model relating zinc alloy composition to creep strength, followed by preparation of selected zinc die casting metal alloys and pressure die casting of these alloys. Mechanical testing will be carried out. An optimization task will then be conducted and these alloys will then be characterized in a manner similar to the first group of alloys. This task will be followed by technology transfer to die casters and their customers, concerning properties and processing of these enhanced alloys.

Keywords: Zinc Alloys, Zinc Die Casting, Creep Resistant

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

33. **CLEAN CAST STEEL: 1) MACHINABILITY OF CAST STEEL; 2) ACCELERATED TRANSFER OF CLEAN STEEL TECHNOLOGY**
$261,000
DOE Contact: Ehr Ping HuangFu, (202) 586-1493
University of Alabama - Birmingham Contact:
Charles Bates, (205) 975-8011

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

Keywords: Metalcasting, Steel Casting, Machinability

34. **THIN SECTION STEEL CASTINGS**
$111,000
DOE Contact: Ehr Ping HuangFu, (202) 586-1493
Pennsylvania State University Contact:
Robert C. Voigt, (814) 863-7290

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

Keywords: Metalcasting, Steel Casting, Thin Section

35. **CLEAN METAL PROCESSING (ALUMINUM)**
$255,000
DOE Contact: Ehr Ping HuangFu, (202) 586-1493
Worcester Polytechnic Institute Contact:
Diran Apelian, (508) 831-5992

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

Keywords: Metalcasting, Clean Metal, Aluminum

36. **ADVANCED LOST FOAM CASTING TECHNOLOGY**
$196,000
DOE Contact: Ehr Ping HuangFu, (202) 586-1493
University of Alabama - Birmingham Contact:
Charles Bates, (205) 975-8011

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

Keywords: Metalcasting, Lost Foam Casting

37. **MECHANICAL PROPERTIES STRUCTURE CORRELATION FOR COMMERCIAL SPECIFICATION OF CAST PARTICULATE METAL MATRIX COMPONENTS**
$91,000
DOE Contact: Ehr Ping HuangFu, (202) 586-1493
University of Wisconsin - Milwaukee Contact:
Pradeep Rohadgi, (414) 229-4987

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

Keywords: Metalcasting, Metal Matrix Composite, Mechanical Testing

38. **FERRITE MEASUREMENTS IN DUPLEX STAINLESS STEEL CASTINGS**
$25,000
DOE Contact: Ehr Ping HuangFu, (202) 586-1493
University of Tennessee Contact: Carl Lundin, (423) 974-5310

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

Keywords: Metalcasting, Calibration, Duplex Stainless Steel

39. **TECHNOLOGY FOR THE PRODUCTION OF CLEAN, THIN WALL, MACHINABLE GRAY AND DUCTILE IRON CASTINGS**
$206,000
DOE Contact: Ehr Ping HuangFu, (202) 586-1493
University of Alabama - Birmingham Contact:
Charles Bates, (205) 975-8011

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

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

40. **ENHANCEMENTS IN MAGNESIUM DIE CASTING DIE LIFE AND IMPACT PROPERTIES**
$101,000
DOE Contact: Ehr Ping HuangFu, (202) 586-1493
Case Western Reserve University Contact:
Jack Wallace, (216) 368-4222

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

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

41. **MOLD MATERIALS FOR PERMANENT MOLDING OF ALUMINUM ALLOYS**
$92,000
DOE Contact: Ehr Ping HuangFu, (202) 586-1493
Case Western Reserve University Contact:
Jack Wallace, (216) 368-4222

The primary goals of this project are to extend the life and improve quality of permanent molds utilized in casting aluminum. The relative mold life under the thermal conditions that prevail in permanent molds that experience exposure to molten aluminum will be determined for a range of materials such as gray iron, ductile iron, and compacted graphite iron. These materials may be used plain or alloyed to provide microstructures with different life and stabilities at elevated temperatures. Other candidate materials are cast and wrought 4140 type steels, and cast and wrought H-13 steels. An additional goal is to reduce the cost of the molds and improve the surface and soundness quality of the aluminum castings by selective application of coatings.

Keywords: Aluminum Casting, Permanent Mold, Mold Life

42. **SYSTEMATIC MICROSTRUCTURAL AND CORROSION PERFORMANCE EVALUATION OF HIGH MOLYBDENUM STAINLESS STEEL CASTING**
$60,000
DOE Contact: Ehr Ping HuangFu, (202) 586-1493
University of Tennessee Contact: Carl Lundin, (423) 974-5310

In this project, the University of Tennessee will systematically document the microstructural phase evolution (constituent type, morphology, extent and distribution) in two types of high molybdenum stainless castings as a function of solution heat treatment parameters, and then relate the microstructure to corrosion performance. The nature of the second phase particles and constituents will be thoroughly studied as to the origin of the secondary phases. In particular, the effect of re-oxidation during pouring of casting will be investigated and the source of the re-oxidation products will be defined by close cooperation with participating foundries.

Keywords: Metalcasting, Microstructure, Molybdenum Stainless Steel, Corrosion Performance

MINING VISION TEAM - The DOE Mining Team leader is Toni Marechaux, (202) 586-8501

43. **DRILLING AND BLASTING OPTIMIZATION USING SEISMIC ANALYSIS AND X-RAY FLUORESCENCE SPECTROSCOPY**
$200,000
DOE Contact: Toni Marechaux, (202) 586-8501
Lawrence Berkeley National Laboratory Contact: Deborah Hopkins, (510) 486-4922

This project will examine the physical and mechanical properties of rock before and after blasting. Implementation of more efficient blast technology will use a very energy-efficient process using explosives to save substantial energy during grinding and crushing of extracted rock.

Keywords: Mining, Rock Mechanics, Seismic Analysis, X-ray Fluorescence Spectroscopy, Modeling

44. **APPLICATION OF HIGH TEMPERATURE SUPERCONDUCTORS TO UNDERGROUND COMMUNICATIONS**
$357,000
DOE Contact: Toni Marechaux, (202) 586-8501
Los Alamos National Laboratory Contact: Dave Reagor, (505) 667-3091

This project will develop new materials and applications for high-power and small antennas for personal communication underground. This technology can also be used for equipment control and positioning. The development and application of underground communication for both safety and productivity will result in substantial energy savings. Improved communication will not only improve safety to workers, but will reduce transportation costs as well.

Keywords: Mining, High Temperature Superconductors, Squid, Yttria Stabilized Zirconia (YSZ)

45. **HYDRIDES FOR FUEL CELL MINING VEHICLES**
$155,000
DOE Contact: Toni Marechaux, (202) 586-8501
Savannah River Technology Center: Contact: Ed Danko, (803) 725-4264

This project will develop optimized hydride material for underground hydrogen storage for mining vehicle fuel cells. The use of fuel cells to replace diesel engines in mining vehicles will save substantial energy and has the potential to shift the energy source for mining transportation away from fossil fuels. The energy savings from reduced ventilation needs in underground mining alone make this emerging technology economically feasible.

Keywords: Mining, Metal Hydrides, Fuel Cell, Hydrogen Storage

46. **MINING BYPRODUCT RECOVERY**
$64,000
DOE Contact: Toni Marechaux, (202) 586-8501
Oak Ridge National Laboratory: Contact: Jan Berry, (865) 241-1939

This project will develop a continuous process to remove trace metals from mining by-products. This innovative process will increase the amount of product generated per ton of material removed for many commodities, including coal, copper, and lead. This will reduce the amount of overall mining waste, and will also reduce the toxicity of the waste.

Keywords: Mining, Trace Metal Separation, Mercury, Selenium, Recovery, By-product

47. **DEVELOPMENT OF A MINE COMPATIBLE LIBS INSTRUMENT FOR ORE GRADING**
$100,000
DOE Contact: Toni Marechaux, (202) 586-8501
Idaho National Engineering and Environmental Laboratory: Contact: Jerry May, (208) 526-6674

LIBS, or Laser Induced Breakdown Spectroscopy, will enable miners to determine the composition of ore at the rockface and during transportation to processing facilities, and will result in substantial energy savings by limiting extraction of unnecessary overburden and low-grade material and by determining the most efficient processing methods for the extracted ore.

Keywords: Mining, Laser Induced Breakdown Spectroscopy (LIBS), Characterization, In-Situ, Calibration

OFFICE OF CROSSCUT TECHNOLOGIES

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 activities and of crosscutting industries including carbon products, forging, heat treating, and welding. Efforts in FY 1999 were focused on partnerships between industry and the National Laboratories for commercialization of new materials and processes. The DOE program manager is Charles A. Sorrell, (202) 586-1514.

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

48. **INTERMETALLIC ALLOY DEVELOPMENT AND TECHNOLOGY TRANSFER OF INTERMETALLIC ALLOYS**
$980,000
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 1999 included: (1) thermal expansion and selected creep and fatigue data were developed on the cast eutectic free alloy IC-438; specific data generated assisted in determining various applications and specimens were prepared and are being evaluated in industry; (2) melting and centrifugal casting of iron aluminide were made at various casting companies and several specimens were sent for industrial testing and evaluation, (3) welding and brazing studies were made on various nickel aluminide alloys especially IC 438, and (4) dissimilar metal welds were successfully made and evaluated on Ni_3Al.

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

49. **DEVELOPMENT OF ADVANCED INTERMETALLIC ALLOYS**
$250,000
DOE Contact: Charles A. Sorrell, (202) 586-1514
ORNL Contacts: P. J. Maziasz, (423) 574-5082, M. L. Santella, (423) 574-4805 and V. K. Sikka, (423) 574-5112; C. T. Liu, (423) 574-4459
University of Cincinnati Contacts: A. Jordan and O. N. C. Uwakweh, (513) 556-3108

The objectives of this project are to develop advanced intermetallic alloys including FeAl and Ni_3Si. The FeAl effort is focused on alloys with improved weldability and mechanical and corrosion properties for use in structural applications; and the development of weldable FeAl alloys for use in weld-overlay cladding applications. The Ni_3Si effort focuses on alloy composition, welding and processing. Developments made in FY 1999 include; (1) a number of new Ni_3Si alloys were made. Beneficial elements were discovered to increase the intermediate temperature ductility and fabricability of the alloys, (2) the Ni_3Si alloys were shown to have excellent weldability, and (3) dissimilar metal welds were developed with FeAl.

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

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

Ceramic-metal composites have advantages as engineering materials because of their high stiffness-to-weight ratios, good fracture toughness, and because their electrical and thermal properties can be varied through control of their composition and microstructure. Reactive metal infiltration is a promising new route to synthesize and process a wide range of ceramic and metal-matrix composites to near-net-shape with control of both composition and microstructure. In FY1999 (1) the technique was used to prepare dense high-strength composites with compositions that were previously impossible, for example, Al_2O_3-$MoSi_2$, Al_2O_3-Ni, and others, (2) coatings of Al/Al_2O_3, Zn/SiO_2, and TiO_2/Al_2O_3 combined excellent corrosion resistance and hardness, and (3) a collaboration was initiated with National Refractories and Minerals Corp.

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

51. **CONDUCTING POLYMERS: SYNTHESIS AND INDUSTRIAL APPLICATIONS**
$200,000
DOE Contact: Charles A. Sorrell, (202) 586-1514
Los Alamos National Laboratory Contact:
S. Gottesfeld, (505) 667-0853

In FY 1999, 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 1999, a new flow-field element was introduced in the cathode structure resulting in a full order of magnitude increase in the time of stable operation of the oxygen polarized chlor-alkali cells. A patent disclosure has been submitted.

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

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

Ethylene and Propylene are two of the largest commodity chemicals in the U.S. and are major building blocks for other chemicals. More energy efficient 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 1999, the CRADA with BP Amoco was continued. Amoco will develop characterization capabilities and design criteria for ht membrane systems. A number of systems have been tested including C_1 through C_4 hydrocarbons with nitrogen and hydrogen.

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

53. **PLASMA PROCESSING-ADVANCED MATERIALS FOR CORROSION AND EROSION RESISTANCE**
$300,000
DOE Contact: Charles A. Sorrell, (202) 586-1514
Los Alamos National Laboratory: 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 are being developed as the coating technology. In FY 1999, (1) a CRADA between LANL and Pratt and Whitney was in progress, (2) coatings of TiN and Cr-O-C have been produced on a variety of substrate materials, (3) wetting experiments show that Cr-C-O coatings provide effective protection against reactions between molten aluminum and steel substrates.

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

54. **UNIFORM DROPLET PROCESSING**
$440,000
DOE: Contact: Charles A. Sorrell, (202) 586-1514
ORNL Contacts: 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 1999: (1) efforts at ORNL focused on alternate methods of obtaining uniform spheres of various high temperature materials including 308 Stainless Steel (2mm diameter). Additional effort was placed in working with a licensee of the uniform droplet process, Uniform Metals Technologies which has capabilities to produce spheres up to 1400°C, (2) the UDS system at Northeastern University was modified to permit processing of engineering alloys up to 1100°C with particular interest to aluminum, copper and their alloys, (3) at MIT, microdroplet spreading sensors were developed to measure the spreading velocity of molten metal droplets on impact on surfaces; and a multi-orifice nozzle was prepared.

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

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

55. **MATERIALS FOR RECOVERY BOILERS**
$980,000
DOE Contact: Charles A. Sorrell, (202) 586-1514
ORNL Contact: James R. Keiser, (423) 574-4453

The purpose of this project is to determine the cause of failure of composite tubes used in Kraft Black Liquor recovery boilers during pulp and paper making, and to develop new materials to eliminate failures. The project consists of three efforts: (1) to obtain operating data and failure analyses, (2) determination of residual stresses in new and used composite tubes and microstructural characteristics of tubes, and (3) development of new materials and/or fabrication methods for improvements in boiler efficiency, service life, and safety. In FY 1999: (1) an array of 25 thermocouples were installed in a boiler floor in order to measure temperature variations as they occur; (2) a heating system was fabricated enabling the measurement of neutron residual stresses in composite tubes as a function of temperature in order to validate predictions and to understand the development of residual stresses during boiler operations, (3) neutron residual stress measurements confirmed that stainless steel yielded upon heating to the normal boiler operating temperature; (4) panels of tubes (base layer of SA210) clad with 304L, Alloy 825, and Alloy 625 were modeled and results compared with fatigue experiments, (5) stress corrosion cracking experiments were made on various alloy systems in order to understand the role of various operations including water washing the floor on tube cracking, and (6) composition of the aqueous liquid in contact with tubes as a result of water washing during shutdown was measured for various conditions and its relevance to stress corrosion cracking evaluated. Participants include Oak Ridge National Laboratory (ORNL), Institute of Paper Science and Technology (IPST), and the Pulp and Paper Research Institute of Canada (PAPRICAN), 18 pulp and paper companies, and 6 boiler and materials suppliers.

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

MATERIALS STRUCTURE AND COMPOSITION

56. **METALLIC AND INTERMETALLIC BONDED CERAMIC COMPOSITES**
$100,000
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. The efforts 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 FY1999, (1) the method of producing powder was evaluated by the use of TGA, DSC, SEM and TEM, (2) formation of tungsten powder was achieved using coated precursor without further addition of carbon, and (3) synthesis of submicron TiC powder was achieved at shorter reaction times (2h) than previously used.

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

57. **ADVANCED MATERIALS/PROCESSES**
$515,000
DOE Contact: Charles A. Sorrell, (202) 586-1514
ORNL Contact: P. Angelini, (423) 574-4459

The goals of this project are to develop new and improved materials. Many metallic, intermetallic alloys, refractories and ceramics possess unique properties and have the potential to be developed as new materials for energy related applications. In FY 1999: (1) a new 300,000 W infrared heating system and processing system has been shown to be capable of hardening steel at rates of up to 1m/min with sweep widths as large as 30cm, (2) fusing of coatings and post fusing of thermally sprayed coatings can be achieved with minimal influence on the substrate material, (3) coatings can be metallurgically bonded to substrates, and (4) coatings developed and fused by infra red processing have increased the life of die casting pins by an order of magnitude.

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

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

58. **MICROWAVE JOINING OF SiC**
$45,000
DOE Contact: Charles A. Sorrell, (202) 586-1514
FM Technologies, Inc. Contact: R. Bruce, (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 1999: (1) SiC was produced from several different slurries of the same polymer precursor with different carbon loadings, and (2) sections of commercial radiant burner tubes supplied by a manufacturer were joined and provided to the manufacture for leak testing.

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

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

The purpose of this research is to develop a new class of inorganic zeolite based membranes for light gas separation and use this technology to improve on separation efficiencies currently available with polymer membranes, particularly for light alkanes. The approach is to nucleate and crystallize zeolithic phases from sol-gel derived amorphous coatings, using porous filters and gas membranes as supports for these films. In FY1999: (1) defect free zeolite/sol-gel composite thin film membranes were successfully produced and remained thermally stable to 500°C, (2) the choice of molecular films for various target light-gases or hydrocarbon separations were determined by molecular modeling of pore sizes and shape, (3) a patent disclosure has been submitted for producing gas impermeable end seals.

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

60. **MATERIALS FOR HIGH TEMPERATURE FILTRATION/THERMOCHEMICAL MODELING**
$100,000
DOE Contact: Charles A. Sorrell, (202) 586-1514
Oak Ridge National Laboratory Contact:
T. M. Besmann, (423) 574-6852

The objectives of this project are to (1) develop high temperature materials for high temperature filtration needs, and (2) develop a method for computational modeling of molten slat system (smelt from kraft recovery boilers) and glass systems. High temperature filters are critical in many chemical and other industrial processes. The effort includes bench-scale testing and analyses of compatibility of materials in various environments up to over 1000°C. In FY 1999: (1) filter specimens were exposed for up to 1000 h periods in thermal oxidizer simulated environments, and (2) phase diagrams were calculated for many of the binary and ternary subsystems for smelt; and in case of glass, a pseudoquaternary.

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

61. **METALS PROCESSING LABORATORY USER (MPLUS) FACILITY**
$350,000
DOE Contact: Charles A. Sorrell, (202) 586-1514
Oak Ridge National Laboratory Contacts:
G. M. Mackiewicz-Ludtka, (423) 576-4652 and
H. W. Hayden, (423) 574-6936

The Metals Processing Laboratory User (MPLUS) Facility was officially designated as a DOE User Facility in February 1996. It's primary focus is related to the Office of Industrial Technologies (OIT) efforts including the "Industries of the Future," national, and cross cutting programs. The purpose of MPLUS is to assist U.S. industry and academia in improving energy efficiency and enhancing U.S. competitiveness. MPLUS includes the following user centers: Metals Processing, Metal Joining, Metals Characterization and Metals Process Modeling. As of the end of FY 1999, 135 proposals were received from 72 different companies and universities representing states across the U.S.A. and 40 MPLUS projects have been completed. Projects crosscut all of the seven industries in the Industries of the Future effort; and other crosscutting industries including forging, heat treating, and welding; and national programs.

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

FINANCIAL ASSISTANCE PROGRAM

The goal of the Financial Assistance Program of OIT is to support technologies within the areas of industry, power, transportation, or buildings that have a significant energy savings impact and future commercial market potential. OIT is particularly interested in supporting technology development and deployment in OIT's "Industries of the Future," nine of the most energy-intensive U.S. industries— agriculture, aluminum, chemicals, forest products, glass, metalcasting, mining, petroleum, and steel industries. Financial assistance through a competitive solicitation is offered to: (1) speed the development of new energy efficient inventions, and (2) leverage industry and other resources to demonstrate, and promote the benefits of energy savings, pollution prevention and cost savings possible through the adoption of clean, energy-efficient industrial technologies. OIT provides grants and assistance to independent inventors and small businesses with promising new ideas through its inventions and innovation (I&I) Program. OIT also provides grants to help fund technology demonstrations through its National Industrial Competitiveness through Energy, Environment and Economics ($NICE^3$) Program.

INVENTIONS AND INNOVATIONS - DOE Contact Lisa Barnett, (202) 586-2212

62. **LASER SENSOR FOR OPTIMIZATION OF COMPRESSOR STATIONS AND REFINERY OPERATIONS**
$199,632
DOE Contact: Roxanne Danz, (303) 275-4706
LaSen, Inc. Contact: Allen R. Geiger,
(505) 522-5110

LaSen, Inc. will develop a process to rapidly monitor and inspect leaks associated with valves and flanges within natural gas and liquid pipeline compressor stations. If a proposed detection system is installed in a petroleum refinery, product savings and associated embodied energy savings could reach $1–2 million /year.

Keywords: Laser, Leak Detection, Natural Gas, Pipeline

63. **TITANIUM MATRIX COMPOSITE TOOLING MATERIAL FOR ENHANCED MANUFACTURE OF ALUMINUM DIE CASTINGS**
$199,984
DOE Contact: Roxanne Danz, (303) 275-4706
Dynamet Technology, Inc. Contact:
Susan Abkowitz, (781) 272-5967

The grant will be used to produce a metal matrix composite material composed of Ti-6Al-4V and 10 wt% titanium carbide particulate. The titanium metal matrix composite offers both dramatically improved (400%) durability and reduced thermal conductivity (50% compared to steel) which will provide energy savings by reducing preheating energy consumption by 4-8%.

Keywords: Metal Matrix Composite, Titanium, Aluminum, Die Casting

64. **AN INSOLUBLE TITANIUM-LEAD ANODE FOR SULFATE ELECTROLYTES**
$200,000
DOE Contact: Roxanne Danz, (303) 275-4706
Materials and Electrochemical Research, (MER) Corporation Contact: Dr. R.O. Loutfy,
(520) 574-1980

The grant will be used to develop insoluble anodes for electrowinning of metals such as copper, zinc, nickel, cobalt, etc. and for electrolytic manganese dioxide production. The proposed anodes significantly reduce contamination of the products with lead and can be used at lower voltage and increased current density, resulting in higher productivity and energy savings up to 25%.

Keywords: Electrowinning, Anodes

65. **DEVELOPMENT OF AN INNOVATIVE ENERGY EFFICIENT HIGH TEMPERATURE NATURAL GAS FIRED FURNACE**
$199,361
DOE Contact: Jeff Hahn, (303) 275-4775
Procedyne Corp. Contact: Vijay Shroff, (732) 249-8347

The grant will be used to improve the efficiency of gas-fired furnaces used for heat-treating, metal recovery, and inorganic chemical production. Compared to current gas-fired heating mantles, the proposed furnace can save up to 70% of natural gas fuel and achieve a higher combustion efficiency for a given combustion gas discharge temperature.

Keywords: Heat Treating, Gas-fired Furnaces

66. **A NEW HIGH TEMPERATURE COATING FOR GAS TURBINES**
$200,000
DOE Contact: Jeff Hahn, (303) 275-4775
Turbine Coating, Inc. Contact: Maggie Zheng, (518) 348-0551

The grant will be used to develop a new coating with cracking resistance and enhanced oxidation protection for hot section components of gas turbines. Energy savings will be derived from reducing one of the two traditional coating steps and extending component life.

Keywords: Coatings, Gas Turbines

67. **TOUGH-COATED HARD POWDERS (TCHPs): A NEW PARADIGM IN MINING AND MACHINING TOOL MATERIALS**
$200,000
DOE Contact: Jeff Hahn, (303) 275-4775
EnDurAloy Corp. Contact: Rick Toth, (912) 598-1210

The grant will be used to demonstrate a new process to sinter tungsten carbide particles resulting in increased hardness, strength, and abrasion resistance with the potential to extend tool life 10-25 times.

Keywords: Tungsten Carbide, Wear Resistant Tools

68. **A NEW ENERGY SAVING METHOD OF MANUFACTURING CERAMIC PRODUCTS FROM WASTE GLASS**
$199,977
DOE Contact: Jeff Hahn, (303) 275-4775
Haun Labs Contact: Dr. Michael Haun, (707) 538-0584

The grant will be used to develop a new method to lower energy costs of manufacturing ceramic products. The process calls for the substitution of traditional raw materials with waste glass. Melting temperatures and associated energy consumption will decrease by 35% to 50% by sintering glass powder instead of using traditional ceramic materials.

Keywords: Cullet, Ceramic, Sintering Glass Powder

69. **DISTILLATION COLUMN FLOODING PREDICTOR**
$52,900
DOE Contact: Roxanne Danz, (303) 275-4706
Inventor Contact: George Dzyacky, (219) 365-8336

The grant will be used to develop a pattern recognition system that identifies patterns of instability in a petroleum refinery distillation tower prior to flooding. The technology is credited with de-bottlenecking refinery processes and increasing gasoline production by 5%-7%.

Keywords: Distillation Column Flooding, Petroleum Refinery

70. **ENERGY SAVING LIGHTWEIGHT REFRACTORY**
$158,041
DOE Contact: Jeff Hahn, (303) 275-4775
Silicon Carbide Products, Inc. Contact: David Witmer, (607) 562-7585

The grant will be used to develop a new manufacturing technique to produce a unique silicon carbide based material that has high strength, increased high temperature qualities, and will cost less to manufacture. In addition, the new material has shown great promise in molten aluminum applications.

Keywords: Refractory, Silicon Carbide

71. **HIGH INTENSITY SILICON VERTICAL MULTI-JUNCTION SOLAR CELLS**
$142,900
DOE Contact: Lizanna Pierce, (303) 275-4727
PhotoVolt, Inc. Contact: Bernard Sater, (440) 234-4081

The grant will be used to develop a low-cost, high-volume fabrication process for high intensity vertical multi-junction (VMJ) solar cells and demonstrate performance viability in solar concentrators. The unique features of the VMJ cell make it capable of more efficient operation at higher intensities than other silicon concentrator solar cell designs.

Keywords: Solar Cells, Solar Concentrators, Photovoltaic

72. **FABRICATION AND TESTING OF A PROTOTYPE CERAMIC FURNACE COIL**
$199,853
DOE Contact: Roxanne Danz, (303) 275-4706
FM Technologies, Inc. Contact:
Dr. Ralph Bruce, (703) 425-5111

The grant will be used to demonstrate a process for joining pairs of ceramic tubes to fabricate furnace coils for ethylene production plants. Ethylene has the greatest annual production of any organic chemical and is the number one consumer of energy in the petrochemical industry. Replacement of metal alloy coils with ceramic coils could increase ethylene production by up to 10% leading to substantial energy savings and increased productivity.

Keywords: Ceramic Tubes, Furnace Coils, Ethylene Production

73. **GERMANIUM COMPOUNDS AS HIGHLY SELECTIVE FLUORINATION CATALYSTS**
$40,000
DOE Contact: Roxanne Danz, (303) 275-4706
Starmet Corporation Contact:
Dr. Matthew Stephens, (978) 369-5410, Ext. 582

The grant will be used to demonstrate the concept for a new, highly selective catalyst for the fluorination of hydrocarbons. This catalyst will meet the needs of the fluorocarbon industry for process simplification, for reduction in capital costs, and for the elimination of energy intensive processing steps and separation processes.

Keywords: Germanium Compounds, Hydrocarbon Fluorination, Catalyst

74. **DEVELOPMENT OF PHOSPHORS FOR USE IN HIGH-EFFICIENCY LIGHTING AND DISPLAYS**
$40,000
DOE Contact: Andy Trenka, (303) 275-4745
Brilliant Technologies, Inc. Contact:
Douglas Kezler, (541) 737-6736

The grant will be used to develop new phosphors for use in high-efficiency, LED-activated lamps and displays, providing improved color rendering and significant energy savings. The phosphors will provide for the first time a means to produce true tri-chromatic white light under LED excitation.

Keywords: Phosphors, LED-activated Lamps, LED

75. **NOVEL CERAMIC COMPOSITION FOR HALL-HEROULT CELL ANODE APPLICATION**
$39,989
DOE Contact: Roxanne Danz, (303) 275-4706
Advanced Refractory Technologies, Inc. Contact:
Thomas Mroz, (716) 875-4091

The grant will be used to develop a replacement for traditional carbon anodes with non-consumable material that will reduce primary aluminum production costs, reduce energy consumption by up to 20%, and minimize environmental impact. The proposed project will evaluate ceramic material in anode-simulation conditions for corrosion and oxidation resistance, electrical properties, and cost efficiency compared to carbon anodes.

Keywords: Hall-Heroult, Anode, Aluminum Production

76. **FUNCTIONALLY GRADED MATERIALS FOR IMPROVED HIGH TEMPERATURE PERFORMANCE OF Nd-Fe-B-BASED PERMANENT MAGNETS**
$39,948
DOE Contact: Jeff Hahn, (303) 275-4775
Iowa State University Contact: Alan Russel, (515) 294-3204

The grant will be used to develop a processing method to produce a novel microstructure in Nd-Fe-B-type magnets by use of pulsed laser deposition. This method is projected to increase the useful operating temperature by 115°C and will substantially expand potential applications allowing Nd-Fe-B-type magnets to replace weaker magnets required for elevated temperature use. These magnets could reduce the weight of automobile starter motors by 14 lbs. resulting in improved overall gas mileage.

Keywords: Nd-Fe-B Based Magnets, Permanent Magnets, Pulse Laser Deposition

77. **IMPROVED ALKYLATION CONTACTOR**
$40,000
DOE Contact: Roxanne Danz, (303) 275-4706
VHP, Inc. Contact: Jim Vemich, (801) 397-1983

The grant will be used to develop a new type of contactor that will significantly increase the surface area between the hydrocarbon and acid catalyst phases while greatly reducing the mass transfer resistances by improved convection. Benefits from the new process include reducing acid consumption by at least 50%, improving the octane number of gasoline, eliminating the energy currently used to chill the reactants and acid below ambient temperature, and increasing the yield of high-octane gasoline.

Keywords: Alkylation, Petroleum Refining, Acid Catalyst

78. **LOW COST SYNTHESIS AND CONSOLIDATION OF TIC**
$40,000
DOE Contact: David Blanchfield, (303) 275-4797
The University of Idaho, Institute for Materials and Advanced Processes Contact: Dr. F.H. Froes, (208) 885-7989

The grant will be used to demonstrate a cost-affordable process for the synthesis of ultrafine titanium carbide (TiC) powder from low cost precursors by an ambient temperature mechanochemical process to form fine grained metal matrix composites. The proposed ambient temperature process will use less energy compared to other carbide manufacturing processes and the quality of the synthesized TiC is superior in purity and particle size to conventional products.

Keywords: Titanium Carbide Powder, Metal Matrix Composites

79. **DEVELOPMENT OF ALUMINUM IRON ALLOYS FOR MAGNETIC APPLICATIONS**
$40,000
DOE Contact: Roxanne Danz, (303) 275-4706
Magna-Tech P/M Labs Contact: Kenneth Moyer, (856) 786-9061

The grant will be used to develop a powder metallurgy process to admix aluminum powder with iron powder to form iron alloy magnets. Upon sintering, a liquid phase is formed with superior magnetic properties to wrought alloys. When utilized in motor applications, the weight of small motors used in today's automobile may be reduced by 15% and a 15-25% increase in motor efficiency may be realized.

Keywords: Powder Metallurgy, Aluminum Iron Alloys, Magnets

80. **NOVEL FREQUENCY-SELECTIVE SOLAR GLAZING SYSTEM**
$40,000
DOE Contact: Andy Trenka, (303) 275-4745
Orion Engineering, Inc. Contact: Thomas Regan, (978) 589-9850

The grant will be used to develop a novel frequency-selective glass material for use in automobile, building, or solar-thermal collector application. This material is capable of transmitting selective frequencies of light with almost no reflection while efficiently transmitting visible light. The glazing could be used to minimize direct solar heating, resulting in reduced heating and cooling requirements for buildings and automobiles.

Keywords: Glazing, Windows, Frequency-Selective Glass

81. **A CERAMIC COMPOSITE FOR METAL CASTING**
$40,000
DOE Contact: Roxanne Danz, (303) 275-4706
MER Corporation Contact: James Withers, (520) 574-1980

The grant will be used to demonstrate nitride/nitride-carbide ceramic composite casting dies. Ceramic composite materials offer complete stability to molten metals and are resistant to erosion, oxidation, thermal fatigue, and cracking. The potential life span of ceramic composite dies could be ten times that of coated steel dies.

Keywords: Die Casting, Ceramic Composite, Metal Casting

82. **ELECTROCHEMICAL METHOD FOR EXTRACTION OF OXYGEN FROM AIR**
$40,000
DOE Contact: Lizanna Pierce, (303) 275-4727
James Mulvihill and Associates Contact: James Mulvihill, (412) 221-2551

The grant will be used to develop a process to produce pure oxygen from air by combining the anode reaction of a water electrolysis cell and the cathode reaction of a fuel cell in a single unit. The combined cell requires less energy to produce pure oxygen compared with a standard water electrolysis cell.

Keywords: Water Electrolysis, Oxygen, Fuel Cell

83. **ENERGY SAVING METHOD FOR PRODUCING ETHYLENE GLYCOL AND PROPYLENE GLYCOL**
$40,000
DOE Contact: Roxanne Danz, (303) 275-4706
Gallatin Research Contact: Warren Miller, (541) 388-2198

The grant will be used to demonstrate a new process that could dramatically reduce the energy and water requirements in glycol production. Together, these two chemicals account for over 7 billion pounds of production consuming 33 trillion Btu and four billion gallons of water. The proposed process could reduce energy and water consumption by 20%.

Keywords: Glycol Production, Ethylene Glycol, Propylene Glycol

84. **IMPROVED REFRACTORIES USING ENGINEERED PARTICLES**
$40,000
DOE Contact: Jeff Hahn, (303) 275-4775
Powdermet, Inc. Contact: Andrew Sherman, (818) 768-6420

The grant will be used to determine the technical feasibility of producing a higher thermal shock resistant carbon-alumina refractory by producing and testing engineered alumina particles. The novel material has the potential to increase refractory durability by three to five fold.

Keywords: Refractory, Carbon-alumina, Thermal Shock

85. **ENABLING TOOL FOR INNOVATIVE GLASS APPLICATIONS**
$40,000
DOE Contact: Jeff Hahn, (303) 275-4775
Michigan Technological University, Institute of Materials Processing Contact: J. M. Gillis, (906) 487-1820

The grant will be used to develop an abrasive jet cutting system using glass as the abrasive media. Angular glass particles have been shown to be an acceptable alternative abrasive to garnet and at one-tenth the price of garnet, will allow for a wider array of glass products to be produced. Spent abrasive glass will be suitable for use as a plastic filler in a variety of polymers.

Keywords: Glass, Abrasive Jet Cutting System, Garnet

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

86. **DEMONSTRATION OF A THREE-PHASE ROTARY SEPARATOR TURBINE**
$519,326
DOE Contact: Julia Oliver, (510) 637-1952
Douglas Energy Co. Contact: Lance Hays, (714) 524-3338
CA Energy Commission Contact: Dennis Fukumoto, (916) 653-6222

Douglas Energy and the CA Energy Commission will demonstrate a newly developed compact separator for the petroleum industry which utilizes previously wasted process energy to generate power and separate gas, oil, and water. This technology, to be demonstrated at a Chevron 15,000 barrel per day facility, will substantially improve the efficiency and productivity of high pressure offshore oil and gas drilling operations.

Keywords: Oil and Gas Production, Hydrocarbon Separation, Petroleum

87. **CERAMIC TURBINE WHEEL TECHNOLOGY TO PROVIDE ECONOMIC, EFFICIENCY AND ENVIRONMENTAL ENHANCEMENTS TO MICROTURBINES**
$524,673
DOE Contact: Julia Oliver, (510) 637-1952
CA Energy Commission Contact: Dennis Fukumoto, (916) 653-6222
Honeywell Contact: Mark Skowronski, (310) 512-4178

Honeywell and the CA Energy Commission will commercially demonstrate the use of a ceramic wheel within a gas-powered turbine. Replacing a traditional metallic wheel with ceramic material allows turbines to run at substantially higher temperatures. This improves overall cost effectiveness by 15%, while reducing the use of fossil fuels. Several key industries, including glass, paper, chemicals, petroleum refining and metal casting could benefit from this technology.

Keywords: Ceramic, Turbine Wheel, Gas-powered Turbine

88. **PRECISION IRRIGATION TECHNOLOGIES FOR THE AGRICULTURAL INDUSTRY**
$455,000
DOE Contact: Gibson Asuquo, (303) 275-4841
CO Office of Energy Management Contact: Kevin Opp, (303) 620-4292
CO Corn Growers Admin. Committee Contact: Harold Smedley, (303) 674-5465

The CO Office of Energy Management and the Colorado Corn Administrative Committee will demonstrate and commercially validate a unique site specific technology called "Accu-Pulse". It includes a software-based data collection system that analyzes water, nutrients, vegetative material, and pests in individual sub-areas within a larger field so they can be effectively managed for maximum production and/or minimal inputs of water, fertilizers and pesticides. This will reduce waste, save water and energy, and enable farmers to remain economically competitive.

Keywords: Agriculture, Precision Irrigation

89. **ENERGY CONSERVING TOOL FOR COMBUSTION DEPENDENT INDUSTRIES**
$304,867
DOE Contact: Scott Hutchins, (617) 565-9765
CT Bureau of Waste Management Planning & Standards Division Contact: Lynn Stoddard, (860) 424-3236
AFR Contact: James Markham, (860) 528-9806

CT Bureau of Waste Management Planning & Standards Division and Advanced Fuel Research (AFR) will demonstrate a new, portable, low-cost, energy-efficient multi-gas analyzer for industries utilizing combustion boiler and turbine systems. This state-of-the-art combustion tuning tool saves substantial fuel, reduces emissions, and validates pollution abatement/control technology.

Keywords: Combustion Tuning, Multi-gas Analyzer, Boiler, Turbine System

90. **ENERGY-SAVING REGENERATION OF HYDROCHLORIC ACID PICKLING LIQUOR**
$472,231
DOE Contact: Scott Hutchins, (617) 565-9765
CT Bureau of Waste Management Planning & Standards Division Green Technology Contact: Doug Olsen, (914) 855-0331

CT Bureau of Waste Management Planning & Standards Division and Green Technology Group will demonstrate an innovative technology that regenerates spent hydrochloric acid from steel pickling, that results in 95% energy savings, 52% cost savings, and 91% reduction in CO_2 over conventional technologies. This process generates no wastewater or residual waste, and produces significant operating and capital cost savings in addition to major energy savings.

Keywords: Hydrochloric Acid Recovery, Pickle Liquor, Galvanizing

91. **SUPERCRITICAL FLUID PURIFICATION OF COMBI-CHEM LIBRARIES**
$500,000
DOE Contact: Maryanne Daniel, (215) 656-6964
DE Economic Development Office Contact: Cheryl Heiks, (302) 577-8487
Berger Instruments Contact: Ken Klein, (302) 266-8201

DE Economic Development Office and Berger Instruments will demonstrate an innovative Scale Supercritical Fluid Chromatograph (SFC) that purifies combinatorial chemistry compound libraries at 20 to 100 times the rate of current systems. This innovation makes it economically feasible for pharmaceutical companies to purify hundreds of thousands of compounds per year with 90% recovery and 95% purity, while reducing both energy consumption and solvent waste by more than 90%, compared to current methods. SFC has the industry-wide potential of saving 4 million gallons of chemical waste, and 590 megawatt-hours of electricity per year.

Keywords: Pharmaceuticals, Combinatorial Chemistry, Compound Purification

92. **FULL-SCALE 100 TON/HR DEMONSTRATION OF MAGNETIC ELUTRIATION TECHNOLOGY FOR CLEAN AND EFFICIENT PROCESSING OF IRON ORE**
$500,000
DOE Contact: Brian Olson, (312) 353-8579
MN Dept. Public Service Contact: Janet Streff, (651) 297-2545
5R Research Contact: John McGaa, (651) 730-4526

MN Dept. Public Service and 5R Research Inc. will demonstrate an improved mineral processing technology known as "magnetic elutriation" which increases selectivity when weakly-magnetic tailings are separated from magnetic iron ores. This patented process produces yields of 99% magnetic iron recovery, while eliminating the need for chemicals used in conventional separation practices. Industry wide, this innovation will reduce chemical use by 1700 tons and save 170 GWHrs of electrical energy each year.

Keywords: Mining, Magnetic Elutriation, Mineral Processing

93. **REDUCING FOUNDRY EMISSIONS AND GREEN SAND WASTE VIA INTEGRATED ADVANCED OXIDATION-UNDERWATER PLASMA PROCESSING**
$525,000
DOE Contact: Maryanne Daniel, (215) 656-6964
PA Dept. of Environmental Protection Contact:
Calvin Kirby, (717) 783-9981
Advanced Cast Productions, Inc. Contact:
William Franz, (814) 724 2600

The PA Dept. of Environmental Protection and Advanced Cast Productions, Inc. will demonstrate for commercialization an integrated Advanced Oxidation-Underwater Plasma (AO-UP) system that dramatically enhances the industrial competitiveness of green sand foundries. The technology decreases the amount of green sand consumables and solid wastes generated, while reducing direct energy costs by 1.5% and indirect costs by 9%, from avoidance of volatile organic compounds and hazardous air pollutants.

Keywords: Foundry Sand, Green Sand, Plasma Processing, Foundries

OFFICE OF TRANSPORTATION TECHNOLOGIES

	FY 1999
Office of Transportation Technologies - Grand Total	$39,832,101
Office of Advanced Automotive Technologies	$31,147,500
Transportation Materials Technology	$27,165,000
Propulsion Materials	$1,805,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$175,000
Material Support for Nonthermal Plasma Development	175,000
Technology Transfer and Management Coordination	$270,000
Technical Project Management	270,000
Device or Component Fabrication, Behavior or Testing	$1,360,000
Inorganic Proton Exchange Membrane Electrode/Support Development	60,000
Microstructural Membrane Electrode Assembly Characterization	25,000
Rapid Surface Modification of Aluminum Engine Block Bores by a High-Density, Infrared Process	300,000
Lead-Free Solders for Automotive Electronics	150,000
Mechanical Reliability Assessment of Electronic Ceramics and Electronic Ceramic Components	125,000
Composite Bipolar Plates	200,000
Metallic Bipolar Plates	50,000
Carbon Foam Thermal Management Materials for Electronic Packaging	175,000
Microwave Regenerated Diesel Exhaust Particulate Filter	200,000
Characterization of Intelligent Processing for Permanent Magnets	75,000
Lightweight Vehicle Materials	$25,360,000
Device or Component Fabrication, Behavior or Testing	$25,360,000
Low-Cost High-Performance Wrought Aluminum Components for Automotive Applications	3,275,000
Low-Cost High-Performance Cast Light Metals for Automotive Applications	2,050,000
Advanced Materials and Processes for Automotive Applications	1,770,000
Automotive-Related Graduate Fellowships	125,000
Materials and Processes for Propulsion System Applications	350,000
Technology Assessment and Evaluation	1,050,000
Reinforced Composite Materials—Joining, Durability, and Enabling Technologies	2,710,000
USAMP Cooperative Agreement	3,100,000
Development of Low-Cost Carbon Fiber	2,480,000
Development of Low-Cost Lightweight Metals and Alloys	925,000
Recycling	1,000,000
Structural Reliability of Lightweight Glazing Alternatives	400,000
High Rate Processing Technologies for Composite Materials	525,000
The High Temperature Materials Laboratory User Program	5,500,000
Automotive-Related Graduate Fellowships	100,000

OFFICE OF TRANSPORTATION TECHNOLOGIES (continued)

	FY 1999
Office of Advanced Automotive Technologies (continued)	
Electric Drive Vehicle Technologies	$3,982,500
Advanced Battery Materials	$3,582,500
Optimized Li-Ion System	$980,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$245,000
Optimization of Cathode Materials	127,000
Development of Novel Electrolytes	118,000
Materials Properties, Behavior, Characterization or Testing	$735,000
Reactivity and Safety Aspects of Carbonaceous Anodes	140,000
Optimized Lithium-ion Electrolyte and Binder	75,000
SEI Layer Formation on Carbon Anodes	75,000
Electrode Surface Layers	70,000
Carbon Electrochemistry	225,000
Corrosion of Current Collectors	150,000
High-Performance Non-Flammable Electrolytes	$225,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$225,000
Non-flammable Electrolytes	75,000
Development of Non-flammable Electrolytes	75,000
Non-flammable Electrolytes	75,000
Non-Carbonaceous Anode Materials	$155,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$155,000
Non-carbonaceous Anode Materials	125,000
Non-carbon Anodes	30,000
Novel Cathode Materials	$497,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$497,000
New Cathode Materials Based on Layered Structures	72,000
Novel Cathode Materials	100,000
Novel Cathode Structures	225,000
New Cathode Materials: Aerogels	100,000

OFFICE OF TRANSPORTATION TECHNOLOGIES (continued)

	FY 1999
Office of Advanced Automotive Technologies (continued)	
Electric Drive Vehicle Technologies (continued)	
Advanced Battery Materials (continued)	
Advanced Solid Polymer Electrolytes	$890,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$170,000
Composite Polymer Electrolytes	100,000
Highly Conductive Polyelectrolyte-Containing Rigid Polymers	70,000
Materials Properties, Behavior, Characterization or Testing	$645,000
Advanced Solid Polymer Electrolytes	275,000
Lithium-Polymer Electrolyte Interface	70,000
Advanced Solid Polymer Electrolytes	300,000
Materials Structure and Composition	$75,000
Modeling of Lithium/polymer Electrolytes	75,000
Advanced Diagnostic Methods	$200,000
Materials Structure and Composition	$200,000
Diagnostics: Electrode Surface Layers	120,000
Battery Materials: Structure and Characterization	80,000
Improved Electrochemical Models	$485,500
Materials Properties, Behavior, Characterization or Testing	$300,000
Improved Electrochemical Models	250,000
Thermal Modeling/Thermal Management	50,000
Materials Structure and Composition	$185,500
Microstructural Modeling of Highly Porous Fibrous and Particulate Electrodes	185,500
Novel Electrode Couples	$150,000
Device or Component Fabrication, Behavior or Testing	$150,000
New Couples: Lithium/Sulfur Cells	150,000

OFFICE OF TRANSPORTATION TECHNOLOGIES (continued)

	FY 1999
Office of Advanced Automotive Technologies (continued)	
Electric Drive Vehicle Technologies (continued)	
Fuel Cell Materials	$400,000
Materials Properties, Behavior, Characterization or Testing	$400,000
Electrode Kinetics and Electrocatalysis	400,000
Office of Heavy Vehicle Technologies	$8,684,601
Transportation Materials Program	$8,684,601
Heavy Vehicle Propulsion System Materials	$4,499,601
Materials Preparation, Synthesis, Deposition, Growth or Forming	$1,887,000
Cost-Effective Smart Materials for Diesel Engine Applications	400,000
Cost-Effective Sintering	147,000
Low-Cost, High-Toughness Ceramics	350,000
Intermetallic-Bonded Cermets	100,000
Diesel Particulate Trap Development	100,000
Insulating Structural Ceramics for High Efficiency, Low Emission Engines	100,000
Thick Thermal Barrier Coatings (TTBCs) for Low Emissions, High Efficiency Diesel Engine Components	100,000
Materials for Low Emissions, High Efficiency Diesel Engine Components	0
Materials for Low Emissions, High Efficiency Diesel Engine Components	0
R&D for Advanced Ceramics and Cermets	200,000
Development of Low-Cost, Cast Engine Materials with Enhanced Reliability	75,000
Carbon Foams from Coal for Heavy Vehicle Applications	215,000
Carbothermal Reduction Synthesis of Titanium Carbide Powders	50,000
Silicon Carbide Nanocoating of Fine Zirconia	50,000
Materials Properties, Behavior, Characterization or Testing	$1,445,000
Diesel Exhaust Catalyst Characterization	200,000
Life Prediction Verification	200,000
High Temperature Tensile Testing	250,000
Computed Tomography	120,000
International Exchange Agreement (IEA)	200,000
Standard Reference Materials	200,000
Mechanical Property Standardization	100,000
Reliable Joining Techniques for Advanced Diesel Engine Valves	50,000
Raman and Fluorescence Spectroscopic Characterization of Ceramic Materials: Stress, Phase, and Temperature	50,000
Oscillatory Pressing of Spray-Dried Ceramic Powders	75,000
Technology Transfer and Management Coordination	$440,000
Technical Project Management	440,000

OFFICE OF TRANSPORTATION TECHNOLOGIES (continued)

	FY 1999
Office of Heavy Vehicle Technologies (continued)	
Transportation Materials Program (continued)	
Heavy Vehicle Propulsion System Materials (continued)	
Device or Component Fabrication, Behavior or Testing	$727,601
Durability of Diesel Engine Component Materials	250,000
Advanced Machining/Manufacturing	225,000
Laser-Based NDE Methods	80,000
Cylindrical Wire Electrical Discharge Machining Process	60,000
Quantifying the Environmental Effects on the Mechanical Properties of Advanced Silicon Nitride Materials for Diesel Engine Applications	60,000
Development of Electrochemical Oxygen Compressor for Diesel Engines	52,601
High Strength Weight Reduction Materials	$4,185,000
Device or Component Fabrication, Behavior or Testing	$4,185,000
Design, Analysis and Development of Lightweight Frames for Truck and Bus Applications	680,000
Development of a Casting Process for Producing Ultra-Large Components	1,450,000
Development of Metal Compression Forming (MCF) for Production of High Integrity Truck Components	450,000
Technology Development for Lightweight Engines	200,000
Advanced Forming Technologies for Lightweight Alloys	530,000
Development of Carbon Monoliths for Safe, Low Pressure Adsorption Storage and Release of Natural Gas	275,000
Technology Assessment and Evaluation	600,000

OFFICE OF TRANSPORTATION TECHNOLOGIES

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

Within OAAT, the bulk of the materials R&D is carried out through the Transportation Materials Technologies program, with additional specialty materials R&D in the Electric Drive Vehicle Technologies program. The Transportation Materials Technologies program develops: (a) *Automotive Propulsion Materials* to enable advanced propulsion systems for hybrid vehicles, and (b) *Lightweight Vehicle Materials* to reduce vehicle weight and thereby decrease fuel consumption. The program seeks to develop advanced materials with the required properties and the processes needed to produce them at the costs and volumes needed by the automotive industries. Improved materials for body, chassis, and powertrain are critical to attaining the challenging performance standards for advanced automotive vehicles. The DOE contacts are Patrick Davis (202) 586-8061, for automotive propulsion materials and Joseph Carpenter, (202) 586-1022, for automotive lightweight vehicle materials. The Electric Vehicle R&D program includes the support of Advanced Battery Development for electric and hybrid vehicle applications. The DOE contact is Ray Satula, (202) 586-8064.

The Heavy Vehicle Materials Technology program focuses on two areas: (a) *Heavy Vehicle Propulsion System Materials,* and (b) *High Strength Weight Reduction Materials.* In collaboration with U.S. industry and universities, efforts in propulsion system materials focus on the materials technology critical to the development of the low 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 Sid Diamond, (202) 586-8032.

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 Sid Diamond, (202) 586-8032.

The Office of Transportation Technology also oversees the Northwest Alliance for Transportation Technologies (NATT). NATT is an initiative of Pacific Northwest National Laboratory (PNNL) 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 the goals of the Partnership for a New Generation of Vehicles (PNGV). NATT partners will use their resources to design new lightweight metals and processes and to lower materials costs.

OFFICE OF ADVANCED AUTOMOTIVE TECHNOLOGIES

TRANSPORTATION MATERIALS PROGRAM

The Office of Advanced Automotive Technologies (OAAT) is responsible for the research, development, and validation of light-duty vehicle technologies that will enable a dramatic reduction in the nation's dependence on petroleum. OAAT's programs will also help improve the quality of the air we breathe. The transportation sector is a major source of air pollution and greenhouse gases. The development of advanced automotive propulsion systems, as well as the increased use of alternative fuels, will help reduce emissions, especially in urban areas, and lead to an overall improvement in public health.

The focus of OAAT's efforts is on light-duty vehicles, which include cars, mini-vans, pickup trucks, and sport-utility vehicles. The office works to promote cooperation in close partnership with the auto industry, suppliers, universities, and Department of Energy (DOE) national laboratories. OAAT's approach emphasizes jointly funded partnerships with industry.

OAAT also plays a major role in the Partnership for a New Generation of Vehicles (PNGV), which brings together the resources of the automotive industry and government in a historic quest to triple the fuel efficiency of today's automobile by the year 2004.

DOE initiated the Ceramic Technology R&D in 1983 to develop reliable structural ceramics for advanced heat engines. The effort developed processing techniques which greatly improved the properties and reliability of ceramics, and recently shifted its focus to reducing the cost of ceramic components. Research and development activities for advanced automotive applications are ongoing in the areas of ceramic manufacturing, ceramic synthesis and processing, non-destructive evaluation (NDE) and inspection, corrosion resistant coatings and joining, alternative forming and densification processes, development of life prediction methodology and validation, and materials testing and standards. Efforts are closely coordinated with activities in the Office of Heavy Vehicle Technologies materials program.

Key elements of each program are organized and described briefly in the following. Patrick Davis is the DOE program manager, (202) 586-8061, and is responsible for overall coordination of projects in the Automotive Propulsion Materials Program.

PROPULSION MATERIALS

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

94. **MATERIAL SUPPORT FOR NONTHERMAL PLASMA DEVELOPMENT**
    $175,000
    DOE Contact: P. B. Davis, (202) 586-8061
    ORNL Contact: D. P. Stinton, (423) 574-4556
    ORNL Contact: S. D. Nunn, (423) 576-1668

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

Keywords: Diesel, Fabrication, Gelcasting

TECHNOLOGY TRANSFER AND MANAGEMENT COORDINATION

95. **TECHNICAL PROJECT MANAGEMENT**
    $270,000
    DOE Contact: P. B. Davis, (202) 586-8061
    ORNL Contact: D. P. Stinton, (423) 574-4556

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

Keywords: Advanced Heat Engines, Alloys, Automotive Applications, Carbon, Coordination, Metals, Management, Structural Ceramics

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

96. **INORGANIC PROTON EXCHANGE MEMBRANE ELECTRODE/SUPPORT DEVELOPMENT**
    $60,000
    DOE Contact: P. B. Davis, (202) 586-8061
    ORNL Contact: D. P. Stinton, (423) 574-4556
    ORNL Contact: M. A. Janney, (423) 574-4281

The goal of this effort is to develop electrically conducting electrodes/supports and catalytically active ceramic sandwich layers for use in ceramic electrolyte PEM membranes based on nanoparticles of TiO_2 and Al_2O_3. The materials developed in this project will be evaluated by Professor Marc Anderson at the University of Wisconsin who is working on microporous inorganic proton exchange membranes for fuel cells.

Keywords: Aluminum Oxide, Ceramics, Fuel Cells

97. **MICROSTRUCTURAL MEMBRANE ELECTRODE ASSEMBLY CHARACTERIZATION**
$25,000
DOE Contact: P. B. Davis, (202) 586-8061
ORNL Contact: D. P. Stinton, (423) 574-4556
ORNL Contact: T. A. Nolan, (423) 574-8422

One of the major impediments to rapid implementation of proton exchange membrane (PEM)-based electrical energy sources is the large amount of platinum needed to catalyze the fuel-air reaction at the low temperatures at which PEMs operate. The reduction of precious metal (PM) content without loss of efficiency (or better, improvement) is critical to the success of this technology. This project will apply the tools of microstructural characterization and microchemical analysis to achieve PM reduction, in an effort to duplicate the major accomplishments these tools have provided in the development of improved automotive and heavy vehicle emission calalysts.

Keywords: Catalysts, Characterization, Fuel Cells, Platinum

98. **RAPID SURFACE MODIFICATION OF ALUMINUM ENGINE BLOCK BORES BY A HIGH-DENSITY, INFRARED PROCESS**
$300,000
DOE Contact: P. B. Davis, (202) 586-8061
ORNL Contact: D. P. Stinton, (423) 574-4556
ORNL Contact: C. Blue, (423) 574-5112

An innovative, rapid, high density surface modification process is being used to develop a new, durability enhancing coating for aluminum automotive applications such as engine block cylinder bores, compressor housings, fuel pumps, and sealing surfaces. Treating the cylinder internal bores to enhance wear resistance and lower friction is intended to eliminate the need for heavy cast iron cylinder liners, or allow for utilization of machinable aluminum alloys such as 319, with use of 390 in high-wear areas.

Keywords: Aluminum, Cost Reduction, Engines, Wear

99. **LEAD-FREE SOLDERS FOR AUTOMOTIVE ELECTRONICS**
$150,000
DOE Contact: P. B. Davis, (202) 586-8061
ORNL Contact: D. P. Stinton, (423) 574-4556
ORNL Contact: M. L. Santella, (423) 574-4805

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

Keywords: Electronics, Joining/Welding, Testing

100. **MECHANICAL RELIABILITY ASSESSMENT OF ELECTRONIC CERAMICS AND ELECTRONIC CERAMIC COMPONENTS**
$125,000
DOE Contact: P. B. Davis, (202) 586-8061
ORNL Contact: D. P. Stinton, (423) 574-4556
ORNL Contact: A. A. Wereszczak, (423) 574-7601

The objectives of this task are to predict and assess the mechanical reliability of electronic ceramic devices with emphasis on those used for automotive power electronics (e.g., capacitors). This is accomplished through the combination and use of thermomechanical characterization of the electronic ceramics that comprise the devices; thermomechanical stress modeling using FEA; and probabilistic design and life prediction techniques specifically developed for ceramics.

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

101. **COMPOSITE BIPOLAR PLATES**
$200,000
DOE Contact: P. B. Davis, (202) 586-8061
ORNL Contact: D. P. Stinton, (423) 574-4556
ORNL Contact: T. M. Besmann, (423) 574-6852

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

Keywords: Carbon Products, Fuel Cells, Manufacturing

102. **METALLIC BIPOLAR PLATES**
$50,000
DOE Contact: P. B. Davis, (202) 586-8061
ORNL Contact: D. P. Stinton, (423) 574-4556
ORNL Contact: M. P. Brady, (423) 574-5153

The objective of this work is to demonstrate "proof of principle" for forming defect-free, corrosion-resistant nitride coatings via gas nitridation of metallic bipolar plates for PEM fuel cells.

Keywords: Coatings, Corrosion Resistance, Forming, Fuel Cells

103. **CARBON FOAM THERMAL MANAGEMENT MATERIALS FOR ELECTRONIC PACKAGING**
$175,000
DOE Contact: P. B. Davis, (202) 586-8061
ORNL Contact: D. P. Stinton, (423) 574-4556
ORNL Contact: J. W. Klett, (423) 574-5220

The purpose of this work is to develop thermal-management materials for electronic packaging utilizing high-thermal-conductivity carbon foam. The objective will be to design, build, and test heat exchangers for specific applications at the industrial collaborators, targeting heat flux/weight improvements of at least 30% of current designs. It is expected that a reduction in heat exchanger life-cycle costs of 20% can be achieved.

Keywords: Carbon Products, Electronics, Heat Exchangers, Heat Transfer

104. **MICROWAVE REGENERATED DIESEL EXHAUST PARTICULATE FILTER**
$200,000
DOE Contact: P. B. Davis, (202) 586-8061
ORNL Contact: D. P. Stinton, (423) 574-4556
Industrial Ceramic Solutions Contact: R. Nixdorf, (423) 482-7552

The first phase of this effort demonstrated the heating efficiency of the Microwave-Regenerated Diesel Particulate Filter in a bench-scale test, according to the specifications suggested by the PNGV 4SDI committee. In the second phase, a filter system designed for the Ford DIATA diesel engine was fabricated and tested in two separate campaigns at the Ford Scientific Laboratory in Dearborn, Michigan. The system surpassed the FY 1999 DOE PNGV milestone requirements for filtration efficiency and filter-regeneration efficiency.

Keywords: Automotive Applications, Diesel, Filters, Microwave Processing

105. **CHARACTERIZATION OF INTELLIGENT PROCESSING FOR PERMANENT MAGNETS**
$75,000
DOE Contact: P. B. Davis, (202) 586-8061
ORNL Contact: D. P. Stinton, (423) 574-4556
ORNL Contact: E. A. Payzant, (423) 574-4472

The purpose of this work is to quantify the relationship between processing parameters and the crystal chemistry and microstructure of NdFeB permanent magnets.

Keywords: Microscopy, Permanent Magnets, Processing, X-ray Diffraction

LIGHTWEIGHT VEHICLE MATERIALS

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

106. **LOW-COST HIGH-PERFORMANCE WROUGHT ALUMINUM COMPONENTS FOR AUTOMOTIVE APPLICATIONS**
$3,275,000
DOE Contact: Joseph Carpenter, (202) 586-1022
ORNL Contact: Phil Sklad, (865) 574-5069
PNNL Contact: Mark Smith, (509) 376-2847
Laboratory Partners: ORNL, LANL, INEEL, PNNL
Industry Partners: Alcoa, Erie Press Systems, Imageware, AutoDie International, Advanced Technology Associates, Reynolds Metals Company, Commonwealth Aluminum
University Partners: University of Michigan, Michigan Technological University (MTI), University of Stuttgart (IFU)

The objectives of this effort are : to evaluate and improve aluminum forming processes for automotive applications; to develop and implement low-cost continuous casting technologies for production of high-quality aluminum sheet; to develop numerical analysis tools that can be used to develop and optimize the forming process and predict distortions of multi-element structures (NATT),and to develop and optimize tailored blank fabrication and forming for high-volume, low-cost automotive panels and structures(NATT).

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

107. LOW-COST HIGH-PERFORMANCE CAST LIGHT METALS FOR AUTOMOTIVE APPLICATIONS
$2,050,000
DOE Contact: Joseph Carpenter, (202) 586-1022
ORNL Contact: Phil Sklad, (865) 574-5069
PNNL Contact: Ed Courtright, (509) 375-6926
Laboratory Partners: LLNL, ORNL, SNL, INEEL, PNNL, ANL
Industry Partners: USAMP (Ford, GM, Chrysler), LEP (Ford, GM, Chrysler), Thixomat

The objectives of this effort are: to optimize design knowledge and improve product capability for light-weight, high-strength, cast structural components; to improve the energy efficiency and cost effectiveness of large-scale automotive aluminum die castings by extending die life and reducing die wear (NATT); to develop magnesium die casting alloys with improved high temperature properties, and to demonstrate semi-solid molding methods for the production of high-temperature creep-resistant alloys (NATT).

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

108. ADVANCED MATERIALS AND PROCESSES FOR AUTOMOTIVE APPLICATIONS
$1,770,000
DOE Contact: Joseph Carpenter, (202) 586-1022
ORNL Contact: Phil Sklad, (865) 574-5069
PNNL Contact: Mark Smith, (509) 376-2847
Laboratory Partners: Ames Laboratory, PNNL, ORNL
University Partners: University of Wisconsin-Milwaukee
Industry Partners: USAMP (Ford, GM, Chrysler), The Electric Power Research Institute (EPRI), Alcoa, MC-21

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

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

109. AUTOMOTIVE-RELATED GRADUATE FELLOWSHIPS
$125,000
DOE Contact: Joseph Carpenter, (202) 586-1022
ORNL Contact: Arvid Pasto, (865) 574-5123

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

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

110. MATERIALS AND PROCESSES FOR PROPULSION SYSTEM APPLICATIONS
$350,000
DOE Contact: Joseph Carpenter, (202) 586-1022
ORNL Contact: Phil Sklad, (865) 574-5069
Laboratory Partners: SNL
Industry Partners: USAMP (Ford, GM, and Chrysler)

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

Keywords: Induction Hardening, Nondestructive Evaluation, Steel

111. **TECHNOLOGY ASSESSMENT AND EVALUATION**
$1,050,000
DOE Contact: Joseph Carpenter, (202) 586-1022
ORNL Contacts: Phil Sklad, (865) 574-5069, Dave Warren (865) 574-9693 and Dick Ziegler (865) 574-5149

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, Technical Management

112. **REINFORCED COMPOSITE MATERIALS—JOINING, DURABILITY, AND ENABLING TECHNOLOGIES**
$2,710,000
DOE Contact: Joseph Carpenter, (202)586-1022
ORNL Contact: Dave Warren (865) 574-9693
Laboratory Partners: LBNL, LLNL, ORNL
Industry Partners: USAMP/Automotive Composites Consortium, Oak Ridge Institute of Science and Technology, Goodrich, Baydur Adhesives, Michigan Materials and Processing Institute, Budd Company, Dow
University Partners: University of Texas-Austin, University of Tennessee, University of Tulsa, University of Michigan, University of California-Santa Barbara, University of Cincinnati, Wayne State University, Stanford University, University of Nottingham

The objective of this effort is to develop critical enabling technologies necessary for the implementation of advanced structural composite materials. In cooperation with the ACC Energy Management working group, develop material and component models for composite materials in high energy impacts for prediction of passenger safety and optimization of component designs. In cooperation with the ACC Materials and Joining Working Groups, develop long term durability test methodologies, durability driven design guidelines, adhesive test methods, non-destructive inspection techniques and material models which can be used in designing automotive components. Specific technology thrust areas include the development of Mode II, and Mixed Mode Fracture test methods, creep, fatigue, environmental durability tests 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. Develop and demonstrate reliable attachment technologies for use in lightweight composite structures for automotive applications. Develop NDE technology to evaluate bonded joint integrity of automotive assemblies, such as a body-in-white. Adhesive joint and composite research includes bulk material characterization, fracture, fatigue, creep, and creep fracture. This work also includes the development of NDE methods, advanced curing technologies and structural analysis model. Technology implementation is conducted through Automotive Composites Consortium (ACC) focal projects.

Keywords: Polymer, Composites, Joining, Fracture, Durability, Preforming, Automotive, Adhesives, Non-Destructive Inspection, Environmental Degradation, Carbon Fiber Preforming

113. **USAMP COOPERATIVE AGREEMENT**
$3,100,000
DOE Contact: Joseph Carpenter, (202) 586-1022
ORO Contact: Mary Rawlins (865) 576-0823
Industry Partner: US Automotive Materials Partnership (Daimler Chrysler, Ford, GM), Goodrich, Baydur Adhesives, Michigan Materials and Processing Institute, Budd Company, Dow, Georgia Tech, Westmoreland
University Partners: University of Tulsa, University of Michigan, University of Santa Barbara, University of Cincinnati, Wayne State University, Stanford University, University of Nottingham

The objectives of this project are to define and conduct vehicle related R&D in materials and materials processing. Projects include Design and Product Optimization for Cast Light Metals, Powder Metallurgy of Particle Reinforced Aluminum, Non-Toxic Free Machining Steel, 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

114. **DEVELOPMENT OF LOW-COST CARBON FIBER**
$2,480,000
DOE Contact: Joseph Carpenter, (202)586-1022
ORNL Contact: Dave Warren (865) 574-9693
Laboratory Partners: ORNL
Industry Partners: USAMP/Automotive Composites Consortium, Lambda Technologies, AKZO Fortafil Fibers, Amoco Cornerstone Technologies, Westvaco
University Partners: North Carolina State University

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 it's low strain to failure. Candidate resin systems are screened for potential of meeting automotive industry requirements.

Keywords: Polymer, Composites, Carbon Fiber, Durability, Low Cost Carbon Fiber, Precursor, Carbon Fiber Processing, Microwave Energy

115. **DEVELOPMENT OF LOW-COST LIGHTWEIGHT METALS AND ALLOYS**
$925,000
DOE Contact: Joseph Carpenter, (202)586-1022
ORNL Contact: Phil Sklad, (865) 574-5069
PNNL Contact: Russ Jones, (509) 376-4276
Laboratory Partners: PNNL
Industry Partners: Alcoa, EIMEx, LLC Santa Fe Alloys
University Partners: Boston University

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

Keywords: Primary Metal, Low Cost, Reduction Technologies, Magnesium, Titanium

116. **RECYCLING**
$1,000,000
DOE Contact: Joseph Carpenter, (202)586-1022
ORNL Contact: Phil Sklad, (865) 574-5069
ANL Contact: George Fenske, (630) 252-5190
Laboratory Partners: PNNL, ANL, Albany Research Laboratory
Industry Partners: Aluminum Association, Garfield Alloys, Alcoa

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

Keywords: Recycle, Scrap, Sorting

117. **STRUCTURAL RELIABILITY OF LIGHTWEIGHT GLAZING ALTERNATIVES**
$400,000
DOE Contact: Joseph Carpenter, (202)586-1022
ORNL Contact: Phil Sklad, (865) 574-5069
PNNL Contact: M. A. Khaleel, (509) 375-2438
Laboratory Partners: PNNL
Industry Partners: Visteon

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

Keywords: Glazing, Structural Reliability

118. **HIGH RATE PROCESSING TECHNOLOGIES FOR COMPOSITE MATERIALS**
$525,000
DOE Contact: Joseph Carpenter, (202)586-1022
ORNL Contact: Dave Warren (865) 574-9693
Laboratory Partners: ORNL, PNL
Industry Partners: USCAR (Daimler Chrysler, Ford, General Motors), Delphi MASCOTech

Develop technologies to cost effectively process composite materials into automotive components, integrate these technologies into demonstration projects that display cost effective use of composites that can be manufactured in automotive factories, develop advanced vehicle system designs based on composite materials to both define future research needs and demonstrate the technical and economic viability of developing technologies.

Keywords: Automotive, Composite, High Rate Processing

119. **THE HIGH TEMPERATURE MATERIALS LABORATORY USER PROGRAM**
$5,500,000
DOE Contact: Sidney Diamond, (202) 586-8032
ORNL Contact: Arvid Pasto, (865) 574-5123

The HTML (High Temperature Materials Laboratory) is a national user facility, offering opportunities for American industries, universities, and other federal agencies to perform in-depth characterization of advanced materials under the auspices of its User Program. Available are electron microscopy for microstructural and microchemical analysis, equipment for measurement of the thermophysical and mechanical properties of materials to elevated temperatures, X-ray and neutron diffraction for structure and residual stress analysis, high speed grinding machines, and measurement of component shape, tolerances, surface finish, and friction and wear properties.

Keywords: Materials Characterization, Ceramics, Composites, Alloys, Components

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

The fellowship program, administered by the High Temperature Materials Laboratory (HTML) of Oak Ridge National Laboratory through Oak Ridge Associated Universities (ORAU), has sponsored Master's and Ph.D. degree students who are U.S. citizens in pursuing a career in the area of lightweight materials for automotive applications. Projects are relevant to the Office of Advanced Automotive Technologies (OAAT), and have included characterization of ceramic-particle metal-matrix composites, and evaluation of the effects of equal channel extrusion on composite microstructure. Three students have completed their Ph.D. degrees, and a Master's degree student and the final Ph.D. student are nearing the completion of their studies.

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

ELECTRIC DRIVE VEHICLE TECHNOLOGIES PROGRAM

ADVANCED BATTERY MATERIALS

OPTIMIZED LI-ION SYSTEM

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

121. **OPTIMIZATION OF CATHODE MATERIALS**
$127,000
DOE Contact: Ray Sutula, (202) 586-8064
Oakland University Contact: T. Malinski, (248) 370-2339

The objective of this project is to develop a stable lithium nickelate cathode by systematic substitution of multiple cations that prevent phase and domain segregation in the oxide slabs. Ti, Mg and Al were identified as elements that effectively stabilize the structure of cathode materials. A mechano-milling process was successfully developed to prepare single-phase multidoped cathode materials.

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

122. **DEVELOPMENT OF NOVEL ELECTROLYTES**
$118,000
DOE Contact: Ray Sutula, (202) 586-8064
University of Delaware Contact: K. A. Wheeler, (302) 739-4934

The objective of this project is to develop improved electrolytes for Li-ion batteries, e.g., arylsulfones and cross-linked PEG sulfones. Synthesis of improved electrolytes is underway and a series of six aryl sulfones will be evaluated.

Keywords: Intercalation Electrodes, Rechargeable Batteries

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

123. **REACTIVITY AND SAFETY ASPECTS OF CARBONACEOUS ANODES**
$140,000
DOE Contact: Ray Sutula, (202) 586-8064
University of Michigan Contact: G. A. Nazri, (810) 986-0737

The objective of this project is to investigate the chemical and electrochemical and safety aspects of carbonaceous anodes used in Li-ion batteries and to identify the reaction products that form during charge/discharge cycling of Li-ion cells. The SEI layer was determined to thermally decompose at around 150°C. Treatment of carbon surfaces with trimethyl chlorosilane leads to a reduction of gas evolution by a factor of 10 or more.

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

124. **OPTIMIZED LITHIUM-ION ELECTROLYTE AND BINDER**
$75,000
DOE Contact: Ray Sutula, (202) 586-8064
University of Windsor Contact: R. Aroca, (519) 253-4232

The objective of this project is to develop a multi-component electrolyte and non-flammable binder with high conductivity and thermal stability in a wide temperature range for application in Li-ion high-power batteries. A unique set-up for purification of solvents and salt for reliable and reproducible conductivity measurements was identified. The highest conductivity with a 2/1 mole ratio of EC/DMC was achieved, which showed a minimum in ion pairing and less structural ordering. Li^+-ion solvation energy was calculated in various electrolyte blends and preferential solvation was observed.

Keywords: Batteries, Solid-State Cells, Electric Vehicles, Electrolyte

125. **SEI LAYER FORMATION ON CARBON ANODES**
$75,000
DOE Contact: Ray Sutula, (202) 586-8064
Lawrence Berkeley National Laboratory Contact: P. N. Ross, (510) 486-6226

The objective of this project is to study the physical and electrochemical properties of the passive film formed on carbon anodes using *in-situ* spectroscopic techniques. A study of the chemistry of Li intercalation into highly oriented pyrolytic graphite (HOPG) by evaporation and annealing in UHV was completed. The surface chemistry of UHV cleaved LiC_6(0001) was determined and a full *ab initio* computational study of the electrochemical reduction of solvents for Li-ion batteries was completed.

Keywords: Batteries, Solid-State Cells, Electric Vehicles, Surface Layer

126. **ELECTRODE SURFACE LAYERS**
$70,000
DOE Contact: Ray Sutula, (202) 586-8064
Lawrence Berkeley National Laboratory Contact: F. R. McLarnon, (510) 486-4636

The objectives of this project are to characterize the passive films formed on carbonaceous anodes using *in situ* spectroscopy techniques and to investigate surface treatment of current collectors for improved adhesion, conductivity and lifetime. It was found that the thickness of the surface layer formed on carbon electrodes is weakly dependent on the type of carbon material.

Keywords: Batteries, Solid-State Cells, Electric Vehicles, Surface Layer

127. **CARBON ELECTROCHEMISTRY**
$225,000
DOE Contact: Ray Sutula, (202) 586-8064
Lawrence Berkeley National Laboratory Contact: K. Kinoshita, (510) 486-7389

The objectives of this project are to identify the critical parameters that control the reversible intercalation of Li in carbonaceous materials and to determine the maximum Li intercalation/storage capacity of carbonaceous materials in nonaqueous electrolytes. Studies suggest that there is a strong correlation between the irreversible capacity loss (formation of SEI layer) and the relative fraction of edge sites associated with graphitized carbons. *In situ* ellipsometry/ electrochemistry studies on graphite indicated that SEI formation was strongly influenced by the type of Li salt. This study was conducted in collaboration with Hydro-Quebec.

Keywords: Carbon Electrode, Rechargeable Batteries

128. **CORROSION OF CURRENT COLLECTORS**
$150,000
DOE Contact: Ray Sutula, (202) 586-8064
University of California, Berkeley Contact:
J. W. Evans, (510) 642-3807

The objective of this project is to investigate the behavior of current collectors for rechargeable Li batteries. The studies indicate that carbon coatings protect Al current collectors from corrosion in a typical baseline electrolyte, $LiPF_6$/EC+DMC, used in Li-ion cells.

Keywords: Current Collector, Rechargeable Batteries

HIGH-PERFORMANCE NON-FLAMMABLE ELECTROLYTES

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

129. **NON-FLAMMABLE ELECTROLYTES**
$75,000
DOE Contact: Ray Sutula, (202) 586-8064
Lawrence Berkeley National Laboratory Contact:
K. Kinoshita, (510) 486-7389

The objectives of this project are to develop non-flammable electrolytes (NFEs) that have flash points >100°, high ionic conductivity (>10^{-3} S/cm at 20°C), a wide electrochemical voltage window (0-5 V), and are compatible with other cell components, environmentally friendly and can pass abuse tolerance testing in Li-ion batteries. The catalytic influence of PF_5 on the thermal stability of NFEs at elevated temperatures was determined.

Keywords: Non-flammable Electrolyte, Rechargeable Batteries

130. **DEVELOPMENT OF NON-FLAMMABLE ELECTROLYTES**
$75,000
DOE Contact: Ray Sutula, (202) 586-8064
Illinois Institute of Technology Contact:
J. Prakash, (312) 567-3639

The objective of this program is to develop nonflammable electrolytes with high flash point (>100°C), ionic conductivity (10^{-3} S/cm), and wider voltage window (0-5 V *vs.* Li) in an effort to provide better thermal stability and fire safety. A flame retardant material, hexa-methoxy-tri-aza-phosphazene ($N_3P_3[OCH_2\,CH_3]_6$), was discovered that provides improved thermal stability to the electrolyte. A provisional patent on "Nonflammable electrolytes for batteries" has been filed by IIT.

Keywords: Non-flammable Electrolyte, Rechargeable Batteries

131. **NON-FLAMMABLE ELECTROLYTES**
$75,000
DOE Contact: Ray Sutula, (202) 586-8064
Covalent Associates, Inc. Contact: A. B. McEwen, (781) 938-1140

The objective of this program is to develop non-flammable electrolytes for Li-ion batteries that meet the goals for high-power and thermal abuse tolerance for transportation applications. Synthesis of improved electrolytes is underway. Ethyl trifluoroacetate (ETFA), $CF_3COO_2H_5$, was prepared and shows encouraging cycling behavior with $LiPF_6$ and $LiC(SO_2\,CF_3)_3$ - containing solutions.

Keywords: Non-flammable Electrolyte, Rechargeable Batteries

NON-CARBONACEOUS ANODE MATERIALS

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

132. **NON-CARBONACEOUS ANODE MATERIALS**
$125,000
DOE Contact: Ray Sutula, (202) 586-8064
Argonne National Laboratory Contact:
M. M. Thackeray, (630) 252-9183

The overall objective of this task is to develop and characterize non-carbonaceous anode materials for high-energy rechargeable Li batteries for Electric Vehicles (EVs) and hybrid EVs. The specific objective of the research effort will be to identify materials that are inherently safer than carbon-based electrodes (particularly when subjected to overcharge conditions at elevated temperature) without compromising capacity, rate capability and cycle life. The search for new inexpensive materials focused on alloy/intermetallic systems and metal oxides that provide potentials above metallic Li and with capacities >400 mAh/g, or >1000 mAh/ml. Studies were initiated that demonstrated that Li could be inserted into h¢-Cu_6Sn_5, a NiAs-type structure.

Experiments are underway to verify its electrochemical stability by studies with Li_2CuSn.

Keywords: Non-carbon Electrodes, Rechargeable Batteries

133. **NON-CARBON ANODES**
$30,000
DOE Contact: Ray Sutula, (202) 586-8064
State University of New York Binghamton Contact:
M. S. Whittingham, (607) 777-4623

The objective of this project is to investigate the formation of some manganese/vanadium oxides and simple alloys such as modified Li/Al. Studies observed that layered manganese oxides doped with Co, Fe or Ni showed enhanced capacity on cycling. The doped materials also show enhanced electronic conductivity.

Keywords: Non-carbon Electrodes, Rechargeable Batteries

NOVEL CATHODE MATERIALS

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

134. **NEW CATHODE MATERIALS BASED ON LAYERED STRUCTURES**
$72,000
DOE Contact: Ray Sutula, (202) 586-8064
State University of New York Binghamton Contact:
M. S. Whittingham, (607) 777-4623

The objective of this project is to investigate the formation of stabilized manganese oxides, to characterize them structurally and in electrochemical cells. Hydrothermally formed Co-, Fe- and Ni-substituted manganese oxides exhibited enhanced conductivity and electrochemical behavior. The cycling rate was found to be a critical factor in stability of the layered phase. Vanadium-pillared manganese oxides were recognized as possible cathode materials.

Keywords: Intercalation Electrodes, Rechargeable Batteries

135. **NOVEL CATHODE MATERIALS**
$100,000
DOE Contact: Ray Sutula, (202) 586-8064
Argonne National Laboratory Contact:
M. M. Thackeray, (630) 252-9183

The objective of this project is to find lower-cost and higher-capacity cathodes for rechargeable Li EV batteries than the presently available $LiCoO_2$, while retaining its positive attributes of high cycle life, good electronic conductivity and structural stability. The specific objective of this research will be to identify new transition metal oxide cathode materials, particularly those based on Mn, that offer enhanced behavior in Li-ion and Li/polymer cells. A major focus will be on stabilizing Mn oxide structures against conversion to the spinel phase; to this end a range of Mn oxide structures were investigated. Studies observed that composite $Li_x MnO_2$ structures derived from orthorhombic and layered $LiMnO_2$ are more stable than standard $LiMn_2O_4$ spinel when cycled over both the 3 and 4 V plateaus.

Keywords: Intercalation Electrodes, Rechargeable Batteries

136. **NOVEL CATHODE STRUCTURES**
$225,000
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 examine tunnel-containing MnO_2s based on the $Na_{0.44}MnO_2$ structure for potential use in Li and Li ion cells. $Li_xTi_yMn_{1-y}O_2$ compounds (y = 0.11, 0.22, 0.33, 0.44 and 0.55) were synthesized that showed encouraging cycling performance in Li/polymer cells.

Keywords: Intercalation Electrodes, Rechargeable Batteries

137. **NEW CATHODE MATERIALS: AEROGELS**
$100,000
DOE Contact: Ray Sutula, (202) 586-8064
Lawrence Berkeley National Laboratory Contact:
E. J. Cairns, (510) 486-5028

The objectives of this project are to synthesize high-surface-area aerogel materials and characterize aerogel-derived electrodes and evaluate cell performance. Novel lithium metal oxide "hexagel" materials were prepared with specific capacities up to 138 mAh/g. Initial capacity fade rates were reduced from 8% per cycle to 3% per cycle through improvements in cathode fabrication.

Keywords: Intercalation Electrodes, Rechargeable Batteries

ADVANCED SOLID POLYMER ELECTROLYTES

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

138. COMPOSITE POLYMER ELECTROLYTES
$100,000
DOE Contact: Ray Sutula, (202) 586-8064
North Carolina State University/Michigan State University Contacts: S. A. Khan, 919) 515-4519/
G.L. Baker, (517) 355-9715

The objectives of this project are to develop solid composite electrolytes utilizing synthesized fumed silica fillers with tailored surface chemistries and to investigate the electrochemical and rheological characteristics of these novel composite polymer electrolytes. Studies showed that the interfacial resistance of polymer electrolytes increases by an order of magnitude without the fumed silica but only by a factor of four in the presence of fumed silica. It is concluded that the fumed silica stabilizes the Li-electrolyte interface.

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

139. HIGHLY CONDUCTIVE POLYELECTROLYTE-CONTAINING RIGID POLYMERS
$70,000
DOE Contact: Ray Sutula, (202) 586-8064
Northwestern University Contact: D. F. Shriver, (847) 491-5655

The objective of this project is to synthesize and test a new class of rigid polymer electrolytes for rechargeable Li and Li-ion batteries. The rigid polymer electrolyte, poly(1,3-dioxolan-2-one-4,5-diyl oxalate) (PVICOX), with ionic conductivity of the polymer-lithium triflate (1:1) complex of »10^{-4} Scm^{-1} at room temperature, was synthesized. Tests were conducted of symmetrical Li/polymer/Li and cathode/polymer/cathode cells, which indicated the formation of resistive interface(s) in the cells.

Keywords: Batteries, Solid-State Cells, Electric Vehicles, Polymer Electrolyte

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

140. ADVANCED SOLID POLYMER ELECTROLYTES
$275,000
DOE Contact: Ray Sutula, (202) 586-8064
Lawrence Berkeley National Laboratory Contact: J. B. Kerr, (510) 486-6279

The objectives of this project are to determine by a combination of directed polymer synthesis, theoretical calculations, and transport measurements, the upper limits of conductivity of binary salt and single-ion "dry" polymer electrolytes; and how the polymer architectures and salt structures influence the mechanical strength and processability of the polymer electrolyte membranes. Methods for *in situ* curing or cross-linking of polymer membranes that have excellent mechanical strength, good electrode adhesion, acceptable ion-transport properties and minimal reactivity toward Li were developed. A method of grafting anions on to comb-branch polymers to provide single-ion conductors was evaluated. Transport properties of a linear polymer, oxymethylene-linked polyethylene glycol 400 (PEMO), with lithium trifluoromethanesulfonate and lithium bis(trifluoromethanesulfonyl)imide at 40, 60 and 85°C, were determined.

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

141. LITHIUM-POLYMER ELECTROLYTE INTERFACE
$70,000
DOE Contact: Ray Sutula, (202) 586-8064
Lawrence Berkeley National Laboratory Contact: P. N. Ross, (510) 486-6226

The objectives of this project are to study Li/oligoether interfacial reaction products as a simulated Li/PEO SEI layer and to investigate Li/PEO SEI layer stability with FTIR. Completed a study of Li/oligoether interfacial reactions products by PES in UHV for the homologous series of glymes, $CH_3(OCH_2CH_2)_nOCH_3$, n=1,2 etc was completed. Large n values correspond to polyethylene glycol dimethyl ether (PEGDME). Spontaneous polymerization is a proposed reaction for monoglyme/diglyme, but the character of the polymer is unclear. A full *ab initio* computational study of the electrochemical reduction of ethereal solvents for Li batteries was also completed.

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

142. **ADVANCED SOLID POLYMER ELECTROLYTES**
$300,000
DOE Contact: Ray Sutula, (202) 586-8064
Los Alamos National Laboratory Contact:
T. Zawodzinski, (505) 667-0925

The objective of this project is to determine the transport properties in Li-conducting electrolytes. ^{19}F ENMR was implemented and it demonstrated greatly improved sensitivity and response to measure anion and cation transference numbers.

Keywords: Intercalation Electrodes, Rechargeable Batteries, Polymer Electrolyte

MATERIALS STRUCTURE AND COMPOSITION

143. **MODELING OF LITHIUM/POLYMER ELECTROLYTES**
$75,000
DOE Contact: Ray Sutula, (202) 586-8064
Northwestern University Contact: M. A. Ratner, (847) 491-5652

The objective of this project is to apply molecular dynamics and Monte Carlo simulation to analyze polymer electrolytes, thus developing a microscopic understanding of their stability, structure and conduction properties. Theoretical studies on the effect of aluminate and aluminosilicate in polymer electrolytes indicated that the ability of the silicon atom to reduce the local basicity was key to increasing the number of mobile Li ions and the ionic conductivity.

Keywords: Batteries, Solid-State Cells, Electric Vehicles, Polymer Electrolyte

ADVANCED DIAGNOSTIC METHODS

MATERIALS STRUCTURE AND COMPOSITION

144. **DIAGNOSTICS: ELECTRODE SURFACE LAYERS**
$120,000
DOE Contact: Ray Sutula, (202) 586-8064
Lawrence Berkeley National Laboratory Contact:
F. R. McLarnon, (510) 486-4636

The objectives of this project are to characterize the morphology, structure, composition and surface layers on Li anodes and metal oxide cathodes and to modify electrode surface layers to improve cell performance. A spin-coating technique was developed to prepare thin-film $LiMn_2O_4$ electrode. X-ray and Raman spectroscopies revealed a polycrystalline structure was obtained, and cycling in $LiPF_6$/EC+DMC indicated electrochemical behavior nearly identical to that for $LiMn_2O_4$ electrodes prepared from commercially available cathode material powders.

Keywords: Thin Films, Surface Studies

145. **BATTERY MATERIALS: STRUCTURE AND CHARACTERIZATION**
$80,000
DOE Contact: Ray Sutula, (202) 586-8064
Brookhaven National Laboratory Contact:
J. McBreen, (516) 344-4513

The objectives of this project are to elucidate the molecular aspects of battery materials and processes by *in situ* synchrotron X-ray techniques and to provide fundamental information needed to improve the design and performance of advanced rechargeable batteries. *In situ* XRD of $Li_xMn_2O_4$ cycled on both the 4.1 V and 3.0 V plateaus were conducted to investigate the crystallographic stability. Cycling to the 3.0 V plateau causes the formation of the tetragonal phase, which is due to the generation of lattice defects.

Keywords: X-ray Studies, Electrode Materials

IMPROVED ELECTROCHEMICAL MODELS

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

146. **IMPROVED ELECTROCHEMICAL MODELS**
$250,000
DOE Contact: Ray Sutula, (202) 586-8064
University of California, Berkeley Contact:
J. Newman, (510) 642-4063

The objectives of this project are to report important parameters crucial in the operation of advanced secondary electrochemical power systems; to determine transport and other properties for electrochemical applications; and to improve the performance of electrochemical cells by identifying the controlling phenomena. A computational study evaluated the use of two separator types, ionomer and polymer, with liquid electrolyte in Li batteries. The analysis showed that the optimized specific energies of presently available ionomer and polymer systems are similar (24 Wh/kg and 23 Wh/kg), and significantly below the USABC goal of 100 Wh/kg. Batteries with ion exchange and polymer separators showed peak powers of 8 W/kg and 20 W/kg, again far below USABC objectives—60 W/kg and 90 W/kg.

Keywords: Electrochemical Phenomena, Solid-State Cells, Electric Vehicles

147. **THERMAL MODELING/THERMAL MANAGEMENT**
$50,000
DOE Contact: Ray Sutula, (202) 586-8064
University of California, Berkeley Contact: J. W. Evans, (510) 642-3807

The objective of this project is to study heat generation, heat transfer and thermal management of large-scale batteries for EV applications. Measurements of important unknown thermal conductivities of electrolytes and composite cathodes used in Li/polymer batteries were completed. Heat generation rates were measured for various Li/ polymer cells under various discharge/charge rates. A mathematical model coupling thermal and electrochemical phenomena was developed and it predicted electrical and thermal behavior of large batteries.

Keywords: Thermal Management, Rechargeable Batteries

MATERIALS STRUCTURE AND COMPOSITION

148. **MICROSTRUCTURAL MODELING OF HIGHLY POROUS FIBROUS AND PARTICULATE ELECTRODES**
$185,500
DOE Contact: Ray Sutula, (202) 586-8064
University of Michigan Contact: A. M. Sastry, (734) 764-3061

The objectives of this project are to develop stochastic geometry models for key morphologies of Li-ion electrode materials, to map connectivity of these microstructures over useful ranges of manufactured materials. Modeling studies of conduction and mechanics in porous substrates were completed. Mechanics simulations were completed and validated for failure mechanisms of porous Ni electrodes in metal hydride batteries.

Keywords: Modeling Microstructural Characterization

NOVEL ELECTRODE COUPLES

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

149. **NEW COUPLES: LITHIUM/SULFUR CELLS**
$150,000
DOE Contact: Ray Sutula, (202) 586-8064
Lawrence Berkeley National Laboratory Contact: E. J. Cairns, (510) 486-5028

The objectives of this project are to identify mechanisms responsible for rapid capacity face of Li/polymer/S cells and to develop improved electrode and electrolyte formulations. Studies of composite fumed-silica polymer electrolytes in Li/S cells have been completed. One cell achieved 20 cycles at room temperature with at least 150 mAh/g of electrode.

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

FUEL CELL MATERIALS

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

150. **ELECTRODE KINETICS AND ELECTROCATALYSIS**
$400,000
DOE Contact: JoAnn Milliken, (202) 586-2480
Lawrence Berkeley National Laboratory Contact: P. N. Ross, (510) 486-6226

Research is conducted on the kinetics and mechanisms of the electrode reactions in low temperature polymer electrolyte membrane (PEM) fuel cells. Based on these results new electrocatalysts are being developed using a material-by-design approach. Multimetallic catalysts are synthesized under carefully controlled conditions producing tailor-made surfaces. Surface composition and structure is determined using a combination of surface analytical techniques, Low Energy Electron Diffraction (LEED), Low Energy Ion Scattering (LEIS) and Auger Electron Spectroscopy (AES). The ultimate goal of this work is to develop catalysts having increased activity and improved CO-tolerance for use in PEM fuel cells operating on reformed hydrocarbon fuels. Recent accomplishments include the discovery that a Pd-Au alloy exhibits 3-4 times higher catalytic activity than state-of-the-art Pt-Ru, and significantly higher tolerance to CO.

Keywords: Spectrographic Analysis, Electrocatalysts, Electrooxidation

OFFICE OF HEAVY VEHICLE TECHNOLOGIES

TRANSPORTATION MATERIALS PROGRAM

HEAVY VEHICLE PROPULSION SYSTEM MATERIALS

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

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

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

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

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

151. **COST-EFFECTIVE SMART MATERIALS FOR DIESEL ENGINE APPLICATIONS**
$400,000
DOE Contact: Sidney Diamond, (202) 586-8032
ORNL Contact: D. R. Johnson, (865) 576-6832
ORNL Contact: J. O. Kiggans, Jr., (865) 574-8863

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

Keywords: Cost Effective Ceramics, Sensors, Smart Materials

152. **COST-EFFECTIVE SINTERING**
$147,000
DOE Contact: Sidney Diamond, (202) 586-8032
ORNL Contact: T. N. Tiegs, (865) 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 and intermetallic bonded carbides through the development of continuous sintering techniques.

Keywords: Composites, Cost Effective Ceramics, Intermetallics, Silicon Nitride, Sintering

153. **LOW-COST, HIGH-TOUGHNESS CERAMICS**
$350,000
DOE Contact: Sidney Diamond, (202) 586-8032
ORNL Contact: D. R. Johnson, (865) 576-6832
ORNL Contact: T. N. Tiegs, (865) 574-5173

Significant improvements in the reliability of structural ceramics for advanced diesel engine applications could be attained if the critical fracture toughness, (K_{1c}), were increased without strength degradation. Currently, studies on toughening of ceramics by two methods, microstructure development in oxide-based ceramics, and incorporation of ductile intermetallic phases, are being initiated.

Keywords: Composites, Intermetallics, Nickel Aluminide, Toughened Ceramics

154. **INTERMETALLIC-BONDED CERMETS**
$100,000
DOE Contact: Sidney Diamond, (202) 586-8032
ORNL Contact: D. R. Johnson, (865) 576-6832
ORNL Contact: P. F. Becher, (865) 574-5157

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

Keywords: Cermets, Composites, Diesel, Intermetallics

155. **DIESEL PARTICULATE TRAP DEVELOPMENT**
$100,000
DOE Contact: Sidney Diamond, (202) 586-8032
ORNL Contact: D. R. Johnson, (865) 576-6832
ORNL Contact: R. A. Lowden, (865) 576-2769

Traps and filters are being developed to effectively control diesel particulate emissions from large trucks and other heavy vehicles. The particulate traps are necessary to comply with impending regulations and to alleviate public concerns over particulate emissions. A candidate particulate removal system, conceived by Industrial Ceramic Solutions and Microwave Technologies, utilizes a microwave regenerated ceramic filter system. Although initial results have been promising, the composition of the filter media, i.e., quality of SiC fiber, and thickness and chemistry of the SiC coating, has not been optimized. It is the purpose of this task to optimize the composition and structure of the filter material for strength, coupling, uniformity and efficiency of heating, and filtration.

Keywords: Diesel, Filters, Microwave Processing, Silicon Carbide

156. **INSULATING STRUCTURAL CERAMICS FOR HIGH EFFICIENCY, LOW EMISSION ENGINES**
$100,000
DOE Contact: Sidney Diamond, (202) 586-8032
ORNL Contact: D. R. Johnson, (865) 576-6832
Caterpillar Contact: M. C. Long, (309) 578-8672

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

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

157. **THICK THERMAL BARRIER COATINGS (TTBCS) FOR LOW EMISSIONS, HIGH EFFICIENCY DIESEL ENGINE COMPONENTS**
$100,000
DOE Contact: Sidney Diamond, (202) 586-8032
ORNL Contact: D. R. Johnson, (865) 576-6832
Caterpillar Contact: M. Brad Beardsley, (309) 578-8514

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

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

158. **MATERIALS FOR LOW EMISSIONS, HIGH EFFICIENCY DIESEL ENGINE COMPONENTS**
$0
DOE Contact: Sidney Diamond, (202) 586-8032
ORNL Contact: D. R. Johnson, (865) 576-6832
Cummins Contact: Paul Becker, (812) 377-4701

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

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

159. **MATERIALS FOR LOW EMISSIONS, HIGH EFFICIENCY DIESEL ENGINE COMPONENTS**
$0
DOE Contact: Sidney Diamond, (202) 586-8032
ORNL Contact: D. R. Johnson, (865) 576-6832
Detroit Diesel Contact: Yuri Kalish, (313) 592-7825

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

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

160. **R&D FOR ADVANCED CERAMICS AND CERMETS**
$200,000
DOE Contact: Sidney Diamond, (202) 586-8032
ORNL Contact: D. R. Johnson, (865) 576-6832
Cummins Contact: Thomas Yonushonis, (812) 377-7078

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

Keywords: Cermets, Components, Corrosion Resistance, Diesel, Engines, Fracture Toughness, Strength, Wear

161. **DEVELOPMENT OF LOW-COST, CAST ENGINE MATERIALS WITH ENHANCED RELIABILITY**
$75,000
DOE Contact: Sidney Diamond, (202) 586-8032
ORNL Contact: D. R. Johnson, (865) 576-6832
ORNL Contact: P. J. Maziasz, (865) 574-5082

The goals of this work are to: (1) build upon the successful ATS stainless steel foil development program to develop cast austenitic stainless steel compositions and/or processes that provide improved resistance to creep, fatigue, and oxidation in gas turbine and diesel engine operating environments, and (2) develop data and methodologies required for high-confidence life prediction for new and existing cast alloys.

Keywords: Alloys, Casting, Creep, Diesel, Fatigue, Gas Turbines, Oxidation, Reliability, Stainless Steel

162. **CARBON FOAMS FROM COAL FOR HEAVY VEHICLE APPLICATIONS**
$215,000
DOE Contact: Sidney Diamond, (202) 586-8032
ORNL Contact: D. R. Johnson, (865) 576-6832
West Virginia University Contact: A. H. Stiller, (304) 293-2111, ext. 408

The goals of this work are to: (1) to evaluate the properties of carbon foam as structural material in heavy vehicle manufacturing including its potential for energy absorption applications, and (2) to prepare coal-derived pitch precursors for fibers that will be activated and used for low-pressure gas storage. The first objective will be pursued by preparing and evaluating samples of coal-based carbon foam and laminated, coal-based carbon foams that could be suitable candidates for heavy vehicle applications. The second objective will be done in conjunction with Oak Ridge National Laboratory.

Keywords: Applications, Carbon Products

163. **CARBOTHERMAL REDUCTION SYNTHESIS OF TITANIUM CARBIDE POWDERS**
$50,000
DOE Contact: Sidney Diamond, (202) 586-8032
ORNL Contact: D. R. Johnson, (865) 576-6832
University of Colorado Contact: A. W. Weimer, (303) 492-3759

Little work has been done to optimize the synthesis of titanium carbide (TiC) powders by carbothermal reduction. Better control is needed over the starting precursor sources, the precursor composition, and the synthesis processing in order to produce a high-purity, fine, submicron powder. The goal of this work is to explore the synthesis of TiC by carbothermal reduction using a two-step process similar to that developed for the synthesis of submicron, high-purity tungsten carbide powders, which are also oxygen sensitive. Analytical characterization will include composition analysis (C, O, residual metals), microscopy, and X-ray diffraction.

Keywords: Powder Synthesis, Processing, Titanium Carbide

164. **SILICON CARBIDE NANOCOATING OF FINE ZIRCONIA**
$50,000
DOE Contact: Sidney Diamond, (202) 586-8032
ORNL Contact: D. R. Johnson, (865) 576-6832
University of Colorado Contact: A. W. Weimer, (303) 492-3759

Many potential applications for structural ceramics (e.g., ZrO_2) require that these materials be joined to similar or different ceramics or to metallic alloys (e.g., NiAl). Unfortunately, conventional filler metals do not wet most oxide ceramics. It is believed that this problem can be overcome by precoating the ceramic oxide surface with a suitable carbide material to form an interfacial layer that can be wetted by the bulk of the filler metal or metallic alloy. The objective of this work will be to explore coating of ZrO_2 with an ultra-thin SiC layer to improve the metallic wettability of zirconia.

Keywords: Coatings, Joining, Silicon Carbide, Zirconia

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

165. **DIESEL EXHAUST CATALYST CHARACTERIZATION**
$200,000
DOE Contact: Sidney Diamond, (202) 586-8032
ORNL Contact: D. R. Johnson, (865) 576-6832
ORNL Contact: L. F. Allard, (865) 574-4981

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

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

166. **LIFE PREDICTION VERIFICATION**
$200,000
DOE Contact: Sidney Diamond, (202) 586-8032
ORNL Contact: D. R. Johnson, (865) 576-6832
ORNL Contact: C. R. Brinkman, (865) 574-5106

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

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

167. **HIGH TEMPERATURE TENSILE TESTING**
$250,000
DOE Contact: Sidney Diamond, (202) 586-8032
ORNL Contact: D. R. Johnson, (865) 576-6832
North Carolina A&T State University Contact: J. Sankar, (919) 334-7620

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

Keywords: Advanced Materials, Creep, Diesel, Fracture, Microscopy, Silicon Nitride, Tensile Testing

168. **COMPUTED TOMOGRAPHY**
$120,000
DOE Contact: Sidney Diamond, (202) 586-8032
ORNL Contact: D. R. Johnson, (865) 576-6832
Argonne National Lab Contact: W. A. Ellingson, (312) 972-5068

The objective of this project has shifted towards diesel engines with a focus on fuel injector nozzles and other critical fuel delivery components relative to development of advanced characterization methods which could be useful as part of new, lower-cost manufacturing technologies. One example of advanced manufacturing technology is the use of a new femto-second laser for drilling hole patterns in fuel injectors. Work with Caterpillar, Cummins, and Deere and Company is in progress.

Keywords: Components, Computed Tomography, Cost Effective, Diesel, Engine, Manufacturing, Nondestructive Evaluation

169. **INTERNATIONAL EXCHANGE AGREEMENT (IEA)**
$200,000
DOE Contact: Sidney Diamond, (202) 586-8032
ORNL Contact: D. R. Johnson, (865) 576-6832
ORNL Contact: M. K. Ferber, (865) 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 completion of Subtask 9, Thermal Shock, and Subtask 10, Ceramic Powder Characterization.

Keywords: IEA, Powder Characterization

170. **STANDARD REFERENCE MATERIALS**
$200,000
DOE Contact: Sidney Diamond, (202) 586-8032
ORNL Contact: D. R. Johnson, (865) 576-6832
NIST Contact: S. Jahanmir, (301) 975-3671

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

171. **MECHANICAL PROPERTY STANDARDIZATION**
$100,000
DOE Contact: Sidney Diamond, (202) 586-8032
ORNL Contact: D. R. Johnson, (865) 576-6832
NIST Contact: G. Quinn, (301) 975-5765

The purpose of this effort is to develop mechanical test standards in support of the Propulsion System Materials Program.

Keywords: Mechanical Properties, Test Procedures

172. **RELIABLE JOINING TECHNIQUES FOR ADVANCED DIESEL ENGINE VALVES**
$50,000
DOE Contact: Sidney Diamond, (202) 586-8032
ORNL Contact: D. R. Johnson, (865) 576-6832
Caterpillar Contact: E. A. Ott, (309) 578-6133

The objective of this program is to investigate the feasibility of producing cost-effective engine valves that are capable of more severe engine operating environments and longer usable lifetimes. This effort will explore low-cost techniques for joining of high-performance titanium aluminide engine valve heads to more-cost-effective valve stem materials.

Keywords: Components, Corrosion, Cost Reduction, Intermetallics, Joining

173. **RAMAN AND FLUORESCENCE SPECTROSCOPIC CHARACTERIZATION OF CERAMIC MATERIALS: STRESS, PHASE, AND TEMPERATURE**
$50,000
DOE Contact: Sidney Diamond, (202) 586-8032
ORNL Contact: D. R. Johnson, (865) 576-6832
ORNL Contact: M. Lance, (865) 241-4536

The purpose of this effort is to investigate two relatively novel techniques in the field of materials science, Raman and fluorescence spectroscopy. These techniques have recently been applied to measuring local stresses and phases in ceramics with a high degree of success. Both techniques utilize the same equipment and have a spatial resolution of approximately 2 micrometers, far exceeding the resolution of standard X-ray techniques.

Keywords: Ceramics, Microscopy, Stress Analysis

174. **OSCILLATORY PRESSING OF SPRAY-DRIED CERAMIC POWDERS**
$75,000
DOE Contact: Sidney Diamond, (202) 586-8032
ORNL Contact: D. R. Johnson, (865) 576-6832
ORNL Contact: M. A. Janney, (865) 574-4281

Spray-dried alumina and zirconia powders were tested under static conditions (conventional) and oscillatory uniaxial pressing conditions. The static tests followed conventional behavior with both the permanent compaction, and the elastic springback and recompaction, following the critical-state soil mechanics model. The vibratory compaction tests (i.e., repeated application and removal of the stress) also showed behavior that generally followed critical-state model prediction. However, for a given applied peak stress, repeated release and reapplication of that stress (i.e., vibratory loading) resulted in additional compaction of the powder relative to that achieved during the initial application of the stress. When the compacting stress was raised to a new, higher-compacting stress, the response of the compact returned to the original permanent compaction path.

Keywords: Behavior, Powders, Processing

TECHNOLOGY TRANSFER AND MANAGEMENT COORDINATION

175. TECHNICAL PROJECT MANAGEMENT

$440,000
DOE Contact: Sidney Diamond, (202) 586-8032
ORNL Contact: D. R. Johnson, (865) 576-6832

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

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

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

176. DURABILITY OF DIESEL ENGINE COMPONENT MATERIALS

$250,000
DOE Contact: Sidney Diamond, (202) 586-8032
ORNL Contact: D. R. Johnson, (865) 576-6832
ORNL Contact: P. J. Blau, (865) 574-5377

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

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

177. ADVANCED MACHINING/MANUFACTURING

$225,000
DOE Contact: Sidney Diamond, (202) 586-8032
ORNL Contact: D. R. Johnson, (865) 576-6832
ORNL Contact: S. B. McSpadden, Jr., (865) 574-5444

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

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

178. LASER-BASED NDE METHODS

$80,000
DOE Contact: Sidney Diamond, (202) 586-8032
ORNL Contact: D. R. Johnson, (865) 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

179. CYLINDRICAL WIRE ELECTRON DISCHARGE MACHINING PROCESS

$60,000
DOE Contact: Sidney Diamond, (202) 586-8032
ORNL Contact: D. R. Johnson, (865) 576-6832
North Carolina State University Contact: A. J. Shih, (919) 515-5260

The primary objective of this new program is to prove a new concept called cylindrical wire electrical discharge machining process. The new concept proposed is to add a rotary work-holding device to a conventional 2-axis wire EDM machine to enable the generation of intricate cylindrical form on difficult-to-machine materials. Applications of this cylindrical wire EDM process include the diesel injection plunger, engine valve, turbocharger shaft, hydraulic pump actuator, miniature parts, etc.

Keywords: Components, Machining, Structural Ceramics

180. **QUANTIFYING THE ENVIRONMENTAL EFFECTS ON THE MECHANICAL PROPERTIES OF ADVANCED SILICON NITRIDE MATERIALS FOR DIESEL ENGINE APPLICATIONS**
$60,000
DOE Contact: Sidney Diamond, (202) 586-8032
ORNL Contact: D. R. Johnson, (865) 576-6832
Pacific Northwest National Laboratory Contact: C. A. Lewinsohn, (509) 372-0268

The primary challenge facing the incorporation of silicon nitride components in the high-end diesel and natural gas (NG) market is the ability of materials engineers to guarantee the lifetime of the component. Currently, there is a lack of information concerning failure mechanisms and their rates, under conditions expected in diesel and NG engine applications. The overall objective of this new effort is to quantify crack growth phenomena in a variety of commercial silicon nitride materials in diesel and natural gas environments.

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

181. **DEVELOPMENT OF ELECTROCHEMICAL OXYGEN COMPRESSOR FOR DIESEL ENGINES**
$52,601
DOE Contact: Sidney Diamond, (202) 586-8032
ORNL Contact: D. R. Johnson, (865) 576-6832
LoTEC Contact: S. Limaye, (801) 972-6868

The overall objective of this new program is to develop a commercially viable, highly efficient electrochemical air composition management system for heavy duty diesel engines. In order to accomplish this objective, plans are to develop an electrochemical oxygen compressor which will subsequently be integrated with the thermal management system.

Keywords: Characterization, Components, Electrochemistry, Fabrication

HIGH STRENGTH WEIGHT REDUCTION MATERIALS

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

182. **DESIGN, ANALYSIS AND DEVELOPMENT OF LIGHTWEIGHT FRAMES FOR TRUCK AND BUS APPLICATIONS**
$680,000
DOE Contact: Sid Diamond, (202) 586-8032
ORNL Contact: Phil Sklad, (865) 574-5069
Laboratory Partners: ORNL
Industry Partners: Autokinetics, Daimler Chrysler, Ford, Budd Company, Alcan, Alcoa, Tower Automotive

The objective of this project is to develop concepts for lightweight frames for Class 1 and 2 trucks and buses, develop and implement low-cost manufacturing technologies, and validate concepts on full size vehicles. Materials under consideration include aluminum, high strength steels, Metal Matrix Composites (MMCs), and polymer matrix composites.

Keywords: Frames, Manufacturing, Lightweight, Trucks, Buses

183. **DEVELOPMENT OF A CASTING PROCESS FOR PRODUCING ULTRA-LARGE COMPONENTS**
$1,450,000
DOE Contact: Sid Diamond, (202) 586-8032
ORNL Contact: Phil Sklad (865) 574-5069
Laboratory Partner: ORNL
Industry Partner: Alcoa

The objective of this project is to develop a low cost process to produce very large thin wall castings (3m X 1.7m X 0.4m), to impact economics by part consolidation and reduced assembly requirements, and to validate the technology by producing 50 full size minivan liftgates.

Keywords: Ultra-large Casting, Low Cost Casting Process, Thin Wall Casting

184. DEVELOPMENT OF METAL COMPRESSION FORMING (MCF) FOR PRODUCTION OF HIGH INTEGRITY TRUCK COMPONENTS
$450,000
DOE Contact: Sid Diamond, (202) 586-8032
ORNL Contact: Phil Sklad (865) 574-5069
Laboratory Partners: ORNL
Industry Partners: Thompson Aluminum Casting, Tennessee Tool and Engineering-Die Casting

The objective of this project is to develop and integrate the necessary hardware and production procedures to take the MCF process from proof-of-concept to a level capable of producing high-integrity A356 aluminum alloy parts at rates and volumes necessary for truck and automotive applications.

Keywords: Metal Compression Forming, Aluminum Alloy, Casting, Truck and Automotive

185. TECHNOLOGY DEVELOPMENT FOR LIGHTWEIGHT ENGINES
$200,000
DOE Contact: Sid Diamond, (202) 586-8032
ORNL Contact: Phil Sklad (865) 574-5069
Laboratory Partners: ORNL
Industry Partners: Cummins Engine Company

The objective of this project is to develop effective strategies for improving the ability of lightweight aluminum engines to withstand high stresses at elevated temperatures, to evaluate various techniques for achieving these required strengthening, to validate the various approaches by producing test articles for characterization and validation testing.

Keywords: Lightweight Engines, Aluminum

186. ADVANCED FORMING TECHNOLOGIES FOR LIGHTWEIGHT ALLOYS
$530,000
DOE Contact: Sid Diamond, (202) 586-8032
ORNL Contact: Phil Sklad (865) 574-5069
Laboratory Partners: LANL, PNNL, INEEL

The objective of this project is to evaluate new forming technologies for processing lightweight alloys, to use the new process to achieve improved microstructure, properties, performance, and control in the production of components for heavy vehicles.

Keywords: Extrusion, Lightweight Alloys, Forming

187. DEVELOPMENT OF CARBON MONOLITHS FOR SAFE, LOW PRESSURE ADSORPTION STORAGE AND RELEASE OF NATURAL GAS
$275,000
DOE Contact: Sid Diamond, (202) 586-8032
ORNL Contact: Phil Sklad (865) 574-5069
Laboratory Partners: ORNL

The objective of this project is to develop and test monolithic carbon adsorbent materials for the storage of natural gas in heavy vehicles. The goal is to develop the ability to safely store and release sufficient natural gas at low pressure (<500psi) to power an urban multi-stop delivery van for 80 miles.

Keywords: Natural Gas Storage, Carbon Monolith

188. TECHNOLOGY ASSESSMENT AND EVALUATION
$600,000
DOE Contact: Sid Diamond (202) 586-8032
ORNL Contact: Phil Sklad, (865) 574-5069
Laboratory Partners: ORNL

The objective of these activities is: to provide assessment of various technologies, to conduct workshops to assess technology needs for the trucking industry, to develop multi-year program plans, and to provide guidance to program management as to appropriate investments for R&D funding.

Keywords: Cost, Planning, Workshops, Technical Management

OFFICE OF POWER TECHNOLOGIES

	FY 1999
Office of Power Technologies - Grand Total	$56,996,000
Office of Solar Energy Technologies	$24,033,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$16,027,000
Amorphous Silicon for Solar Cells	4,809,000
Polycrystalline Thin-film Materials for Solar Cells	10,149,000
Deposition of III-V Semiconductors for High-efficiency Solar Cells	1,069,000
Materials Properties, Behavior, Characterization or Testing	$4,150,000
Materials and Device Characterization	4,150,000
Device or Component Fabrication, Behavior or Testing	$3,856,000
High-efficiency Crystalline Silicon Solar Cells	3,856,000
Office of Geothermal Technologies	$863,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$175,000
Thermally Conductive Composites for Heat Exchangers	175,000
Materials Properties, Behavior, Characterization or Testing	$688,000
Advanced High Temperature Geothermal Well Cements	95,000
Advanced Coating Materials	155,000
Geothermal Heat Pump Grouting Materials	135,000
Clad and Thermal Sprayed Ni-Base Alloys	100,000
Microbiological Attack of Concrete in Cooling Towers	88,000
Cements for Remediation of Deformed Well Casing	115,000
Office of Energy Management	$32,100,000
Advanced Utility Concepts Division	$32,100,000
High Temperature Superconductivity for Electric Systems	$32,100,000
Device or Component Fabrication, Behavior or Testing	$32,100,000
The Superconductivity Partnership Initiative	14,000,000
The 2nd Generation Wire Initiative	8,000,000
Strategic Research	10,100,000

OFFICE OF POWER TECHNOLOGIES

OFFICE OF SOLAR ENERGY TECHNOLOGIES

The National Photovoltaics program sponsors high-risk high-payoff research and development in photovoltaic technology from which private enterprise can choose options for further development and competitive application in U.S. electric power 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 spectral response and quantum efficiency of the cell's semiconductor material and the effectiveness of charge carrier separation and collection. The practical efficiency is limited by the fraction of incoming light that is transmitted into the cell, the presence of parasitic resistances (series resistance in the metallization and contacts, and shunt resistance through the thickness of the cell), and material imperfections that support dark recombination of excess photogenerated carriers. Cost is affected by the expense of semiconductor material growth, the complexity of cell fabrication, and fabrication requirements of final module assembly.

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

189. **AMORPHOUS SILICON FOR SOLAR CELLS**
$4,809,000
DOE Contact: Jeffrey Mazer, (202) 586-2455
NREL Contact: Bolko von Roedern, (303) 384-6480

This project performs applied research on the deposition and characterization of amorphous silicon thin films to improve solar cell properties. Efficient conversion is hindered by unintended impurities or undesired structure in the deposited films and by poor uniformity of the films over large ($4000cm^2$) areas. The films are deposited by plasma enhanced chemical vapor deposition (glow discharge), thermal chemical vapor deposition, and sputtering. The long term goal is to develop technology for 15 percent efficient (stabilized) photovoltaic modules with cost under $\$50/m^2$ and with 30-year lifetime. This will allow system lifetime energy cost under $0.06/kWh, and subsequent wide competition of amorphous Si-based PV in large-scale distributed power scenarios.

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

190. **POLYCRYSTALLINE THIN-FILM MATERIALS FOR SOLAR CELLS**
$10,149,000
DOE Contact: Jeffrey Mazer, (202) 586-2455
NREL Contact: Harin Ullal, (303) 384-6486

This project performs applied research on the deposition of $CuInSe_2$ (CIS) and CdTe thin films, and also on crystalline silicon films, for solar cells. Research is focused on improving conversion efficiency by depositing more nearly stoichiometric CIS and CdTe films, by controlling interlayer diffusion and lattice matching in heterojunction structures, and by controlling the uniformity of deposition over large ($4000cm^2$) areas. The films are deposited by chemical and physical vapor deposition, electrodeposition, sputtering, and recrystallization. The long term goal is to develop technology for 15 percent efficient photovoltaic modules with cost under $\$50/m^2$ and with 30-year lifetime. This will allow system lifetime energy cost under $0.06/kWh, and subsequent wide competition of polycrystalline film-based PV in large-scale distributed power scenarios.

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

191. **DEPOSITION OF III-V SEMICONDUCTORS FOR HIGH-EFFICIENCY SOLAR CELLS**
$1,069,000
DOE Contact: Jeffrey Mazer, (202) 586-2455
NREL Contact: Sarah Kurtz, (303) 384-6475

This project performs applied research on deposition of III-V semiconductors for super high efficiency concentrator solar cells. Research is focused on depositing layers precisely controlled in terms of composition, thickness, and uniformity, and studying the interfaces between the layers. The materials are deposited by metal organic chemical vapor deposition, liquid phase epitaxy, and molecular beam epitaxy. The long-term goal is to develop three- and four-junction III-V-based cells that will attain 38 percent efficiency under high concentration.

Keywords: Semiconductors, Chemical Vapor Deposition, Solar Cells

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

192. **MATERIALS AND DEVICE CHARACTERIZATION**
$4,150,000
DOE Contact: Jeffrey Mazer, (202) 586-2455
NREL Contact: Angelo Mascarenhas, (303) 384-6608

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

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

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

193. **HIGH-EFFICIENCY CRYSTALLINE SILICON SOLAR CELLS**
$3,856,000
DOE Contact: Jeffrey Mazer, (202) 586-2455
NREL Contact: John Benner, (303) 384-6496
SNL Contact: James Gee, (505) 844-7812

This project performs applied research on crystalline silicon devices to improve conversion efficiency. The project employs new and improved dopant profiles, advanced back-surface fields, and silicon nitride and other bulk passivation treatments to reduce electron-hole recombination at cell surfaces and in the bulk. Control of point defects in crystalline silicon is studied by a variety of techniques, and is thoroughly discussed at the NREL-sponsored Silicon Devices and Materials Conference held in Colorado each August. 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 materials research and development.

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

194. **THERMALLY CONDUCTIVE COMPOSITES FOR HEAT EXCHANGERS**
$175,000
DOE Contact: R. LaSala, (202) 586-4198
BNL Contact: M. L. Berndt, (631) 344-3060

This project is investigating thin thermally conductive polymer-based composites for use as corrosion and scale-resistant liner materials on carbon steel tubing used in shell and tube heat exchangers in binary geothermal processes or for bottoming cycles in multi-stage flash plants. Corrosion and scaling on the brine side of carbon steel tubing in shell and tube heat exchangers have been major problems in the operation of geothermal processes. Compared to the cost of high alloy steels, a considerable economic benefit could result from the utilization of a proven corrosion resistant composite material if sufficient heat transfer and anti-fouling properties can be achieved. The work consists of determination of the effects of compositional and processing variables on the thermal and fouling properties of the composite and measurements of the physical and mechanical properties after exposure to hot brine in the laboratory and in plant operations. The effects of antioxidant, SiC fillers and low surface energy additives on the fouling coefficient and scale adhesion are also being evaluated.

Field tests with flowing hypersaline brine under heat exchange conditions in conjunction with NREL were performed to evaluate coatings consisting of SiC-filled polyphenylene sulfide polytetrafluoroethylene (PPS)/zinc phosphate and SiC-filled polytetrafluoroethylene (PTFE)/PPS/zinc phosphate. After five months of testing the coatings failed. Current research is examining highly crystallized rigid PPS and PTFE-blended PPS composites containing varying amounts of a very hard polysulfone powder with a melting point of >450°C and an ultra fine, packed zinc phosphate crystal primer.

Keywords: Thermally Conductive Composites, Polymers, Corrosion, Heat Transfer, Heat Exchanger Tubes, Scale Resistance

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

195. ADVANCED HIGH TEMPERATURE GEOTHERMAL WELL CEMENTS

$95,000
DOE Contact: R. LaSala, (202) 586-4198
BNL Contact: M. L. Berndt, (631) 344-3060

Well cements that are chemically and thermally resistant to geothermal brines containing high concentrations of CO_2 are vital to ensuring well integrity and durability. This task focuses on formulating and testing calcium phosphate-based (CaP) cements to withstand high temperature, high CO_2 and acidic conditions. Emphasis is being placed on phase chemistry, and the mechanical, physical, and chemical resistance properties of the cured materials. Cements have been subjected to long-term exposure and the changes in binding phases analyzed. Addition of latex to the cements has been investigated as a means of improving acid resistance.

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

196. ADVANCED COATING MATERIALS

$155,000
DOE Contact: R. LaSala, (202) 586-4198
BNL Contact: M. L. Berndt, (631) 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. 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. Polyphenylene sulfide (PPS) based coatings are of particular interest in geothermal systems. However, hydrothermal oxidation under high temperature and low pH conditions needs to be addressed. The usefulness of antioxidants in improving the performance of PPS was investigated.

Keywords: Corrosion Protection, Polymers, Coatings, Antioxidants, Polyphenylene Sulfide

197. GEOTHERMAL HEAT PUMP GROUTING MATERIALS

$135,000
DOE Contact: R. LaSala, (202) 586-4198
BNL Contacts: M. L. Berndt, (631) 344-3060 and A. J. Philippacopoulos, (631) 344-6090

Ground heat exchangers used with geothermal heat pumps (GHPs) rely on a grouting material to provide heat transfer between the polyethylene U-loop and the surrounding formation. Research focused on formulating and characterizing economic superplasticized cement-silica sand grouts to meet the property requirements for backfilling GHP boreholes. The optimized grout formulation (Mix 111) had a thermal conductivity up to three times higher than that of bentonite and neat cement grout thus permitting substantial reductions in required length of the heat exchanger. Mechanical and hydraulic properties, shrinkage resistance, bond strength to U-loop and durability were also better than neat cement grouts. In particular, the grout exhibited superior borehole sealing capabilities. Heat transfer and thermal stress analysis were conducted to investigate the response of the grouted borehole and surrounding formation to different thermal loading conditions. The investigations were based on finite element modeling of the complete system, i.e., the polyethylene pipes, the grout and the surrounding formation. Both pipes were incorporated into the model. Using these models, several heat transfer analyses were performed considering heating and cooling modes of operation as well as a parametric variation of the materials involved.

Field tests conducted at Oklahoma State University and Sandia National Laboratories on 250 ft deep boreholes verified the improved performance conferred by Mix 111. Thermal resistance was reduced up to 35% compared with high solids bentonite grout and 16% compared with thermally enhanced bentonite. The grout has been approved by the New Jersey Department of Environmental Protection and used successfully on several commercial projects throughout the US.

Keywords: Geothermal Heat Pumps, Cementitious Grouts, Ground Heat Exchanger, Thermal Conductivity, Coefficient of Permeability, Infiltration Rate, Heat Transfer Analysis, Thermal Stresses

198. **CLAD AND THERMAL SPRAYED NI-BASE ALLOYS**
$100,000
DOE Contact: R. LaSala, (202) 586-4198
BNL Contact: M. L. Berndt, (631) 344-3060

Clad and thermal sprayed corrosion resistant alloys have the potential to provide more economic corrosion protection than wrought materials. The objectives of this project are to characterize and compare the corrosion characteristics of clad, thermal sprayed and wrought Ni-base materials for corrosion protection in geothermal brine and steam transportation systems. The laboratory and field data obtained in this project could be used to develop service life models that will support more detailed life cycle cost analysis as well as improve understanding of the factors controlling performance of the clad and thermal sprayed materials.

The alloys investigated included Inconel 625, Incoloy 825, Hastelloy C-276 and C-22. The clad materials were roll bonded to carbon steel substrates. The thermal sprayed coatings were produced by the HVOF process to reduce porosity and enhance protective properties. Cyclic polarization tests were performed to investigate the pitting and repassivation potentials. It was found that Inconel 625 and Hastelloy C-276 gave the best corrosion protection for the synthetic brine chemistry and experimental conditions used to date. This generally correlates with prior experimental studies involving weight loss and pit depth measurements and field tests in brines with similar chemistry. Slight differences in pitting and repassivation potentials for the clad and wrought alloys were measured. The in-situ corrosion resistance of the clad Inconel 625 and Hastelloy C-276 is predicted to be comparable to that in wrought form. The thermal sprayed coatings exhibited passivity which was encouraging and suggests that the coatings are suitable for field testing. The clad and thermal sprayed materials exhibited some variability in corrosion characteristics between test specimens, although the basic performance was similar.

Keywords: Corrosion, Clad Materials, Thermal Sprayed Coatings, Ni-base Alloys

199. **MICROBIOLOGICAL ATTACK OF CONCRETE IN COOLING TOWERS**
$88,000
DOE Contact: R. LaSala, (202) 586-4198
BNL Contact: M. L. Berndt, (631) 344-3060

The overall objective of this project is to evaluate strategies and materials for repair and prevention of microbiological attack of concrete in cooling towers in geothermal power plants and thereby reduce maintenance costs and extend service life.

Commercially available concrete repair and protection materials have been selected for performance comparison. To date these have included three epoxy coatings, an epoxy sealant and an epoxy-modified cement mortar. In addition, a latex-modified mortar prepared in house and representative of the type commonly used in concrete repair was evaluated. The materials have been assessed for bond strength, acid resistance and resistance to microbiologically influenced corrosion. Coated concrete panels were exposed to sulphur oxidizing bacteria (*Thiobacillus ferrooxidans*) at 40°C for a period of 60 days. The coatings and mortars were then evaluated for degradation due to acid attack in the form of etching, softening or decrease in bond strength. Of the materials tested, the epoxy coatings gave the best overall performance. It is planned to perform long-term field testing in collaboration with geothermal power plant operators on materials delineated from the laboratory tests as having the best potential. The experimental and field work is combined with development of recommendations and guidelines for repair and protection of concrete structures with the tested materials. The project is being extended to incorporate calcium aluminate mortars that have been used with success in concrete sewers and to consider how durability can potentially be improved through concrete mix design.

Keywords: Microbiologically Influenced Corrosion, Concrete, Epoxy Coatings, Repair, Mortars, Cooling Towers, Bond Strength, Durability

200. **CEMENTS FOR REMEDIATION OF DEFORMED WELL CASING**
$115,000
DOE Contact: R. LaSala, (202) 586-4198
BNL Contacts: M. L. Berndt, (631) 344-3060
and A. J. Philippacopoulos, (631) 344- 6090

Under certain circumstances geothermal wells can experience excessive deformation. Formation movement, which in turn, is associated the long-term response of the site due to tectonic or other loads such as those related to subsidence are suspected to be among the main causes of casing damage. Remediation of geothermal wells is a cost effective alternative to plugging and abandonment. A remediation procedure has been developed. It involves: (a) plugging of the geothermal well temporarily using an isolation packer, (b) milling the deformed area and finally (c) patching the area using a casing patch. The casing patch essentially consists of a liner cemented into place. The objective of this project is to develop and analyze optimum cement formulations for use in geothermal well casing remediation projects. Cement formulations are systematically tested to obtain material properties and their range of applicability. The influence of additives and fiber reinforcement on pertinent properties at elevated temperatures is under investigation. At the same time, numerical modeling is performed to investigate the patch/formation interaction. Laboratory testing and finite element analysis are carried out interactively to achieve optimization. Failure analysis of the cement patch as well as yield surface characterization of the cement materials is being carried out.

Keywords: Geothermal Wells, Casing Deformation, Casing Remediation, Cements, Material Testing, High-Temperature Properties, Structural Analysis

OFFICE OF ENERGY MANAGEMENT

ADVANCED UTILITY CONCEPTS DIVISION

HIGH TEMPERATURE SUPERCONDUCTIVITY FOR ELECTRIC SYSTEMS

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

201. **THE SUPERCONDUCTIVITY PARTNERSHIP INITIATIVE**
$14,000,000
DOE Contact: Jim Daley, (202) 586-1165

The Superconductivity Partnership Initiative (SPI) is an industry-led venture between the Department of Energy (DOE) and industrial consortia intended to accelerate the use of high temperature superconductivity (HTS) in energy applications. Each SPI team includes a vertical integration of non-competing companies that represent the entire spectrum of the research and development (R&D) cycle. That is, the teams include the ultimate user of the technology (an electric power company), as well as a major manufacturing company and a supplier of superconducting components. Each team also includes one or more national laboratories who perform specific tasks defined by the team. The SPI goal is to design cost-effective HTS systems for electricity generation, delivery and use. The funding amount includes DOE's share of the SPI design activities, as well as parallel HTS technology development that directly supports the SPI teams. All of these projects incorporate high-temperature superconducting wire into a utility electric application.

Project subtasks are as follows:

A. Current Controller

The Current Controller project, led by General Atomics, completed its field evaluation testing at a Southern California Edison substation. Current controllers can be used on transmission and distribution systems to protect system components from damaging power surges caused by ground faults. Compared to conventional devices, HTS current controllers offer better protection and improved system flexibility, reliability and performance. The testing was completed in July, and the unit has been relocated to Los Alamos National Laboratory (LANL) for further analysis.

LANL Contact: Dean Peterson, (505) 665-3030

B. 1,000 hp and 5,000 hp Motors

The project, led by Rockwell Automation, advanced toward the demonstration of a 1,000 horsepower (hp) motor in 2000 and a 5,000 hp motor in 2001. The rotor for the 1,000 hp unit was assembled and balanced, and thermal testing on the stator got underway. Design analysis and preliminary system component testing for the 5,000 hp unit also began. Superconducting motors can have a large impact on electrical energy utilization through reduced losses and size compared to conventional iron core motors. These reduced losses and the smaller size will be the driving force for the commercial introduction of superconducting motors in industrial applications.

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

C. Superconducting Transmission Cable

Southwire Company and Oak Ridge National Laboratory (ORNL) completed construction of a 30 meter, three-phase HTS cable to feed electricity to a Southwire production plant. This effort included conductor fabrication, cable assembly including terminations and vacuum-insulated pipe, and the construction of a control building and switchyard. This cable was tested at full current and voltage as well as at off-design conditions. After extensive testing, the cable was dedicated and began delivering power in early 2000.

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

D. Superconducting Transmission Cable

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

Pirelli Contact: Nathan Kelley, (803) 356-7762

E. Flywheel Electricity System

In 1999, work began on two new additions to the portfolio of SPI project partnerships, one of which involves the development and demonstration of a 10 kWh Flywheel Electricity System. High Temperature Superconducting bearings are an enabling technology for the flywheel design. The bearings will allow the flywheel to store electricity for longer lengths of time with increased efficiency. Scientists at Boeing and Argonne National Laboratory succeeded in developing a preliminary design, which will undergo modeling and testing.

Boeing Contact: Mike Strasik, (425) 237-7176

F. Reciprocating Magnetic Separator

The second new SPI project partnership to result from a competitive award in 1998 teams DuPont with the National High-Magnetic Field Laboratory to develop a reciprocating magnetic separator. These devices are used in the materials field and are traditionally large consumers of utility electricity. In 1999, a conceptual design was finalized and construction of a demonstration unit began. Strategic separator research centered on determining the effects of new HTS coated conductors on selected power applications and a study of magnetic flux trapping and superconductor normalization phenomena.

DuPont Contact: Chris Rey, (302) 695-9470

Keywords: Motor, Current Controller, Transmission Cable, Flywheel, Separator

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

The 2nd generation Wire Initiative capitalizes on two processing breakthroughs announced in 1995 and 1996: the Ion-Beam Assisted Deposition (IBAD) process refined by LANL and the Rolling Assisted Biaxial Texturing (RABiTS) technique pioneered by ORNL. Since then, industry-led consortia have evolved to develop these techniques into viable commercial processes for making HTS wire. In FY 1999, this initiative funded collaborative research and development between the national laboratories and industry partners, and strategic research and development at the laboratories with a focus on improving the understanding of substrate preparation as well as buffer layer and superconductor deposition. Project subtasks are as follows:

A. Collaborative R&D Projects

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

Thick HTS Films - Teams made significant progress in 1999 in the development of thick HTS films. The films will be deposited on flexible tapes containing oxide buffer layers deposited by IBAD. Continuing coated conductor efforts focused on studying novel buffers and improvements in the superconductor deposition.

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

IBAD Research - Program partners were completing the first phase of research on the IBAD approach. Electron beam evaporation is 3M's selected method of deposition of all the layers. ORNL worked to characterize bare, textured nickel and films grown by a variety of techniques, and to develop buffer layer and superconductor deposition technology. ORNL continued pursuing a promising alternative to in-situ formation of the YBCO film, by electron beam co-evaporation of Y, Ba, and Cu. ORNL scientists worked on determining the thickness limits of epitaxial film formation, and assessing the feasibility of rapid precursor depositions for the ex-situ precursor reaction process.

YBCO/RABiTS - Development and demonstration of the fabrication of lengths of YBCO/RABiTS using MOCVD technology continued. Mechanical and processing conditions needed to develop the desired surface texture and smoothness of the bare nickel were analyzed. In addition to providing samples of short and long-length RABiTS, program researchers continued to characterize products for uniformity of texture and electrical and mechanical properties.

B. Strategic 2nd Generation Wire Projects

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

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

C. Wire Characterization

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

Oxide buffer layer research - Work on developing sol-gel derived oxide buffer layer systems continued in 1999. A variety of deposition and processing strategies were being investigated to develop a fundamental understanding of this deposition approach and to optimize film properties. Additionally, Sandia scientists worked on developing high-quality, solution-derived, 123-type superconducting films for coated conductor applications.

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

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

D. Process Technology

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

E. UTSI

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

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

203. **STRATEGIC RESEARCH**
$10,100,000
DOE Contact: Jim Daley, (202) 586-1165
Argonne National Laboratory Contact:
U. Balachandran, (630) 252-4250
Brookhaven National Laboratory Contact:
David Welch, (516) 282-3517
Los Alamos National Laboratory Contact:
Dean Peterson, (505) 665-3030
National Renewable Energy Laboratory
Contact: Richard Blaugher, (303) 384-6518
Oak Ridge National Laboratory Contact:
Robert Hawsey, (615) 574-8057
Oxford Superconducting Technology
Contact: Seung Hong, (732) 541-1300
University of Wisconsin Contact:
David C. Larbalestier, (608) 263-2194

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

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

Project subtasks are as follows:

A. Fundamental Studies

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

B. Wire Development

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

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

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

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

BSCCO research - Efforts to develop BSCCO tapes with improved critical current densities, particularly at high magnetic fields and temperatures, were continued. Activities included AC loss characterization research at Brookhaven National Laboratory and extensive research on phase relationship, production processes and architecture at Argonne National Laboratory, as well as several other ongoing Lab efforts.

ORNL funded three university research and development projects in FY 1999. Researchers at Stanford University began investigating ion-beam assisted deposition of buffer layers and in-situ deposition of YBCO by electron beam evaporation. The University of Wisconsin initiated research efforts on BSCCO critical currents and microstructures, YBCO coated conductor microstructure, and pulse tube cryocooler technology. Finally, researchers at the University of Houston began research into high-rate photon-assisted metallo-organic chemical vapor deposition for YBCO onto buffered, textured metallic substrates.

C. Device Development

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

AC loss characterization - Attempts to characterize ac losses in HTS tapes, under conditions which simulate the electromagnetic conditions in utility devices, continued. Program participants worked to design a cable configured to minimize AC losses.

In FY 1999, work was continued toward producing long lengths of YBCO conductors. The objective of this project is to develop YBCO wires and coils that will lead to greater understanding of the quench behavior of these new wires, and to produce a small demonstration motor for educational use.

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

OFFICE OF SCIENCE

	FY 1999
Office of Science - Grand Total	$461,957, 625
Office of Basic Energy Sciences	$419,258,600
Division of Materials Sciences	$407,636,000
Division of Chemical Sciences	$5,000,000
Division of Engineering and Geosciences	$6,622,600
Engineering Sciences Research	$3,137,800
Materials Preparation, Synthesis, Deposition, Growth or Forming	$932,000
Fundamentals of Thermal Plasma Processing	500,000
Metal Transfer in Gas-Metal Arc Welding	155,000
Thermal Plasma Chemical Vapor Deposition of Advanced Materials	165,000
Research on Combustion-Driven HVOF Thermal Sprays	112,000
Materials Properties, Behavior, Characterization or Testing	$ 2,205,800
An Investigation of History-Dependent Damage in Time-Dependent Fracture Mechanics	100,000
Intelligent Control of Thermal Processes	500,000
Elastic-Plastic Fracture Analysis: Emphasis on Surface Flaws	500,000
Modeling and Analysis of Surface Cracks	200,000
Development of Measurement Capabilities for the Thermophysical Properties of Energy-Related Fluids	490,000
High-T_c Superconductor-Semiconductor Integration and Contact Technology	130,800
Transport Properties of Disordered Porous Media From the Microstructure	135,000
Stress and Stability Analysis of Surface Morphology of Elastic and Piezoelectric Materials	150,000
Geosciences Research	$ 3,484,800
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 360,900
Solution-Reprecipitation of Calcite and Partitioning of Divalent Metals	0
Transition Metal Catalysis in the Generation of Petroleum and Natural Gas	110,900
Mineral Dissolution and Precipitation Kinetics: A Combined Atomic Scale and Macro-Scale Investigation	125,000
Surface Chemistry of Pyrite and Isostructural Analogs: A Combined Surface Science and Aqueous Geochemical Investigation	125,000
Materials Structure and Composition	$810,000
Reaction Mechanisms of Clay Minerals and Organic Diagenesis: an HRTEM/AEM Study	0
Infrared Spectroscopy and Hydrogen Isotope Geochemistry of Hydrous Silicate Glasses	150,000
Biomineralization: Systematics of Organic-Directed Controls on Carbonate Growth Morphologies and Kinetics Determined by *In situ* Atomic Force Microscopy	215,000
Reactions and Transport of Toxic Meals in Rock-Forming Silicates at 25°C	225,000
Development of an Experimental Database and Theories for Prediction of Thermodynamic Properties of Aqueous Electrolytes of Geochemical Significance at Supercritical Temperatures and Pressures	220,000

OFFICE OF SCIENCE (continued)

	FY 1999
Office of Basic Energy Sciences (continued)	
Division of Materials Sciences (continued)	
Division of Chemical Sciences (continued)	
Division of Engineering and Geosciences (continued)	
Geosciences Research (continued)	
Materials Properties, Behavior, Characterization or Testing	$2,313,900
Dynamic Nonlinear Elastic Response of Earth Materials	250,000
Structure and Reactivity of Ferric Oxide and Oxyhydroxide Surfaces: Quantum Chemistry and Molecular Dynamics	240,000
Cation Diffusion Rates in Selected Minerals	200,000
Grain Boundary Transport and Related Processes in Natural Fine-Grained Aggregates	0
Thermodynamics of Minerals Stable Near the Earth's Surface	150,000
New Method for Determining Thermodynamic Properties of Carbonate Solid-Solution Minerals	0
Theoretical Studies of Metal Species in Solution and on Mineral Surfaces	48,100
Micromechanics of Failure in Brittle Geomaterials	270,800
Three-Dimensional Imaging of Drill Core Samples Using Synchrotron-Computed Microtomography	195,000
Shear Strain Localization and Fracture Evolution in Rocks	370,900
Dissolution Rates and Surface Chemistry of Feldspar Glass and Crystal	142,000
Transport Phenomena in Fluid-Bearing Rocks	178,800
Cation Chemisorption at Oxide Surfaces and Oxide-Water Interfaces: X-ray Spectroscopic Studies and Modeling	268,300
Office of Advanced Scientific Computing Research	$5,240,000
Division of Technology Research	$5,240,000
Laboratory Technology Research Program	$5,240,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$3,172,000
High Performance Tailored Materials for Levitation and Permanent Magnet Technologies (ANL 97-02)	250,000
Atomic Scale Structure of Ultrathin Magnetic Multilayers and Correlation With Resistance, Giant Magnetoresistance, and Spin-Dependent Tunneling (ORL 97-03)	250,000
Improved Materials for Semiconductor Devices (PNL 98-17)	125,000
Development of High-Temperature Superconducting Wire Using RABiTS Coated Conductor Technologies (ORL 97-02)	250,000
Development of Bismuth-Based Superconducting Wire with Improved Current Carrying and Flux Pinning Properties	125,000
Light Emission Processes and Dopants in Solid State Light Sources (LBL 97-13)	250,000
Development of Buffer Layers Suitable for Deposition of Thick Superconducting $YBa_2Cu_3O_7$ Layers by Post-Deposition Annealing Process (BNL 98-05)	250,000
Interplay Between Interfacial and Dielectric and Ferroelectric Behaviors of Barium Strontium Titanate Thin Films (PNL 99-08)	125,000

OFFICE OF SCIENCE (continued)

	FY 1999
Office of Advanced Scientific Computing Research (continued)	
Division of Technology Research (continued)	
Laboratory Technology Research Program (continued)	
Materials Preparation, Synthesis, Deposition, Growth or Forming (continued)	
Combinatorial Discovery and Optimization of Novel Materials for Advanced Electro Optical Devices (LBL 97-18)	250,000
Advanced Computational Models and Experiments for Deformation of Aluminum Alloys - Prospects for Design (PNL 99-07)	125,000
Near-Frictionless Carbon Coatings (ANL 98-03)	250,000
Smooth Diamond Films for Friction and Wear Applications and Chemically Protective Coatings (ANL 97-05)	250,000
Nanometer Characterization and Design of Molecular Lubrication for the Head-Disk Interface (LBL 98-10)	153,000
An Advanced Hard Carbon Plasma Deposition System with Application to the Magnetic Storage Industry (LBL 98-16)	175,000
A Facility for Studying Micromagnetic Structures (LBL 95-12)	94,000
Interfacial Properties of Electron Beam Cured Composites (ORNL 99-08)	125,000
Photocatalytic Metal Deposition for Nanolithography (ANL 99-13)	125,000
Device or Component Fabrication, Behavior or Testing	$955,000
Ionically Conductive Membranes for Oxygen Separation (LBL 97-03)	150,000
Advanced Separations Technology for Efficient and Economical Recovery and Purification of Hydrogen Peroxide (ANL 98-07)	250,000
Synthesis and Crystal Chemistry of Technologically Important Ceramic Membranes (ANL 97-06)	195,000
Catalytic Production of Organic Chemicals Based on New Homogeneously Catalyzed Ionic Hydrogenation Technology (BNL 97-05)	235,000
Highly Dispersed Solid Acid Catalysts on Mesoporous Silica (PNL 97-28)	125,000
Enabling Materials and Processing Technologies	$1,113,000
Development of a High-Efficiency Rotary Magnetocaloric Refrigerator Prototype (AL 99-02)	125,000
Rapid Prototyping for Bioceramics (ANL 95-08)	42,000
Direct Casting of Titanium Alloy Wire for Low-Cost Aerospace and Automotive Fasteners (PNL 99-02)	125,000
Controlled Nonisothermal Hot Forging Using Infrared for Microstructural Control (ORL 98-08)	225,000
Nonconsumable Metal Anodes for Primary Magnesium Production (ANL 98-05)	220,000
Development of Electrolyte and Electrode Materials for Rechargeable Lithium Batteries (BNL 98-04)	250,000
Optimized Catalysts for the Cracking of Heavier Petroleum Feedstocks (LBL 99-01)	126,000

OFFICE OF SCIENCE (continued)

	FY 1999
Office of Advanced Scientific Computing Research (continued)	
Small Business Innovation Research Program	$25,583,729
Device or Component Fabrication, Behavior or Testing	$10,262,277
Phase I	$4,080,850
High-Temperature Oscillator and Digital Clock	97,762
A Novel Potentiometric Pressure Sensor with a Temperature-Independent Signal for Geothermal Drilling	99,958
Capacitors for Extreme Temperature Applications	100,000
A High Temperature MEMS Inclination Sensor for Geothermal Drilling	100,000
High Temperature Micromachined Sensor for Industrial Gas Streams	100,000
Thermoelectric Quantum Well Devices	100,000
N Type Quantum Well Films and Devices	100,000
Economical Fabrication of Large Micro-Impingement Cooling Panels	99,806
Helium Cooled Refractory Metal Divertor Panel	99,990
Fast Repetitive Arc Free Current Limiting Circuit Breaker	99,893
Nitride-based Cold Cathodes for Miniature and Rugged Electron Sources	99,877
RF Pulse Compression Using a Diamond Switch	99,938
Development of a High Current Density Nb_3Sn Conductor With Ga and Mg Dopants for High Field Application	100,000
A High Current Very Low Cost Nb_3SnTi Doped Conductor Utilizing a Novel Internal Tin Process, with Separate Stabilizing Elements Scalable to Modern Niobium Titanium Production Economics	99,500
Automated Diamond Turning Lathe for the Production of Copper Accelerator Cells	100,000
High Power Switch	99,515
Adiabatic Forming of Copper Accelerator Cells for the NLC	100,000
Pulse Capacitors for Next Generation Linear Colliders	100,000
Carbon-Carbon Composite Closeout Frames for Space Qualified, Stable High Thermal Conductivity Detector Support Structures	99,469
Low Cost Support Structures, With New Advanced Composite Materials Tailored for Ultra-Stable Particle Tracking Detectors	99,985
New Fullerene-Based Resistor Technology for Use in Low Noise Instrumentation	100,000
SQUID Susceptometers for Read Out of Magnetic Microcalorimeters	100,000
Large Volume Detectors from New CdZnTe Growth Process	100,000
Fabrication of Seamless Niobium Superconducting Accelerating Cavities Using Directed Light Fabrication	100,000
Electromagnetically Forming a Seamless Niobium Radio Frequency (RF) Superconducting Cavity	88,968
Development of High Power RF Windows for Next-Generation Superconducting and Normal Conducting Accelerators	99,981
A 200-kW Average Power Microwave Window for L-Band Applications	98,000
Mercury Cadmium Telluride Detectors for Near Infrared Applications	99,806
Development of III-Nitride UV Detectors	99,910
Low Temperature, High Altitude Humidity Sensor	100,000
Low Cost Optical Moisture Sensor for Weather Balloons	100,000
A Diode Laser Sensor for High Precision Measurement of Terrestrial CO_2 Sources and Sinks	99,996
Low-Cost, High Resolution and High-Sensitivity PET Detector Modules	100,000
A Generic Approach to Improved Semi-Solid Forming of Metals	99,102

OFFICE OF SCIENCE (continued)

	FY 1999
Office of Advanced Scientific Computing Research (continued)	
Small Business Innovation Research Program (continued)	
Device or Component Fabrication, Behavior or Testing (continued)	
Phase I (continued)	
High-Strain-Rate Superplastic Forging of Aluminum Alloys	100,000
Semi-Solid Metal Freeform Fabrication	99,400
Supersmooth Neutron Optical Surfaces by Gas Cluster Ion Beam Processing	100,000
Three Dimensional Si Imaging Array For Cold Neutrons	100,000
Solid-State Neutron Detection Materials	100,000
Fluorescence Chemical Sensor for Chemical Warfare	99,999
Chemosensor Array for Detecting the Proliferation of Weapons of Mass Destruction	99,995
Phase II (First Year)	$3,603,132
Ultra-High-Speed Photonic Add-Drop Multiplexers for Wave-Division-Multiplexed Networking	374,953
An Improved Membrane Module Tubesheet for Industrial Separations	375,000
Sharp Bandpass AlGaN p-i-n Photodiode Detectors for Ultraviolet B Irradiance Measurements	374,983
Robust Micromachined Silicon Carbide Environmental Sensors	374,749
Hand-Held Monitor for On-Site Detection of Heavy Metals in Water Using Microfabricated Detector Chips	249,996
A Photocatalytic $Ti0_2$ Anode and Membrane Reactor for the Enhanced Destruction of Chloro-Organic Compounds in Water	375,000
A Novel UV Photodetector Array	374,955
Large Area, Low cost APDs Using Planar Processing	375,000
Gallium Arsenide P-I-N Detectors for High-sensitivity Imaging of Thermal Neutrons	375,000
Development of High Speed Mercury Cadmium Telluride Detector Arrays with Integral Readouts	353,496
Phase II (Second Year)	$2,578,295
Shaft Weld Replacement with a Ceramic Locking Assembly Joint	344,578
Development of Economical Procedures for Producing and Processing Fine Grained SSM Feedstock via Mechanical Stirring	359,140
Corrosion Resistant Bipolar Plates for PEM Fuel Cells	375,000
High Brightness LEDs based on the (Al,Ga,In)N Materials System	374,577
Development of High Power RF Windows and Waveguide Components for the Next Linear Collider	375,000
Electrical Discharge Machining Application to the Development of mm-wave Accelerating Structures	375,000
Beryllium and Tungsten Brush Armor for Plasma Facing Components	375,000

OFFICE OF SCIENCE (continued)

	FY 1999
Office of Advanced Scientific Computing Research (continued)	
Small Business Innovation Research Program (continued)	
Materials Properties, Behavior, Characterization or Testing	$1,568,108
Phase I	$1,193,108
Intercalated Phosphonate-Clay Composites as Latent Heat Storage Materials for Masonry	100,000
Fiber Reinforced Polymer Composite Building Panels Capable of Energy Storage Through High Enthalpy Solid-State Phase Transition	100,000
SunGuard: A Roofing Tile for Natural Cooling	100,000
Evaluation of Integrated Wall Systems Incorporating Electrochromic Windows	100,000
Development of a High Resolution X-Ray Imaging-Spectrometer	100,000
Enabling Materials for Magnetic Fusion Energy	99,996
Low Cost Dispersion Strengthened Ferritic Steels	99,969
Hg-Ba-Ca-Cu-O HTS Current Leads for High Energy Physics Applications at High Magnetic Field and Temperature	99,922
High Performance Nb_3Sn (Ta) Wires by Tin Enrichment and Increased Filament Content	99,933
Microwave Absorbing Materials for Accelerators in Cryogenic Environments	100,000
An Advanced Avalanche-Photodiode Based Spectroscopic Radiation Imager	100,000
Novel Solid State Electochemical Sensor	93,288
Phase II (Second Year)	$375,000
High Current Density High Repetition Rate Ferroelectric Cathode	375,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$13,753,344
Phase I	$3,099,186
Ion-Conducting Oxide Ceramic Materials for Solid-Oxide Fuel Cells Using Novel Low Cost Combustion Chemical Vapor Deposition	100,000
Cathode-Supported Thin-Film Solid Oxide Cells with Low Operating Temperatures	100,000
Thermally Stable Catalysts for Methane Combustion	100,000
Improved Carbon Molecular Sieve Membranes for Oxygen-Nitrogen Separation	99,993
Improved Precursors for Oxygen-Selective Membranes in Practical Devices for Methane Conversion	100,000
Supported Flat Plate Thin Films for Oxygen Separation	99,998
Mixed-Conducting Oxide Ceramic Membranes for Oxygen Separation Using Novel Low Cost Combustion Chemical Vapor Deposition	100,000
A New Radiation Resistant Epoxy Resin System for Liquid Impregnation Fabrication of Composite Insulation	99,997
Advanced Heat Sink Materials for Fusion Energy Devices	100,000
Robust Ceramic Coatings for Vanadium Alloys to Use in Lithium Cooled usion Systems	100,000
Hybrid 3-D SiC/C High Thermal Conductivity Composites	100,000

OFFICE OF SCIENCE (continued)

	FY 1999
Office of Advanced Scientific Computing Research (continued)	
Small Business Innovation Research Program (continued)	
Materials Preparation, Synthesis, Deposition, Growth or Forming (continued)	
Phase I (continued)	
A Novel Process for the Fabrication of Advanced High Temperature Superconductors	100,000
Co-Processed Ceramic Insulation for High Field Accelerator Magnets	100,000
Improvement of High Field Performance and Reliability of Nb3Sn Conductor by PIT Method	100,000
Ultra Low Loss RF Window Materials	99,999
Ultra-Hard Diamond-Like Nanocomposite Coatings for Wear Applications	99,975
Application of the Combinatorial Synthesis and LHPG Techniques to the Development of New Scintillator Materials	99,915
Ultra-hard Nanolayered Coatings for Wear-resistant Applications	100,000
Functionally Graded, Nanocrystalline, Multiphase, Boron-and-Carbon-Based Superhard Coatings	99,923
Large Area Filtered Arc Deposition of Carbon and Boron Based Hard Coatings	99,839
Ultrahard Nanostructured Diamond Thin Films Using Inductively Coupled Plasma	99,607
High Current Density in Bi2223 Tape and Low AC Loss Wire	100,000
Low Cost Bi-2223 Conductors for HTS Transformers	100,000
Meter Length YBCO Coated Conductor Development	100,000
Non-Vacuum, Reel-to-Reel Processing of High-Temperature Superconducting Coated Conductors	100,000
Novel Catalyst for CH_4-CO Conversion	100,000
Hydrophobic Ionic Liquid Biphase Catalysis	99,953
SiC-Based Hydrogen Selective Membranes for Catalytic Membrane Reactor Applications	99,987
Novel Non-Flammable Electrolytes for Lithium Batteries	100,000
Flame Retardant Electrolytes for Li-Ion Batteries	100,000
Nonflammable Lithium-Ion Battery Electrolytes	100,000
Phase II (First Year)	$3,299,919
Carbon Nanostructures from Coal-Derived Liquid Feedstocks	375,000
Adherent and Reliable Alumina Coating Development	375,000
Synthesis of Mesoporous Tin Oxide for Chemical Gas Sensors	375,000
Polyurethane-Clay Nanocomposite and Microcellular Foaming	375,000
Nanostructured Manganese Dioxides for Li-Ion Batteries	375,000
Combustion Chemical Vapor Deposition of High Temperature Ceramic Insulator Coatings on Superconductor Wire	300,000
An Improved Reaction-Bonded Silicon Carbide Process for SiC/SiC Composites	375,000
The Application of Plasma Assisted Chemical Vapor Deposition (PACVD) Coatings for Die Casting Dies	375,000
Hard, Wear Resistant Coatings for Die-Casting Dies by an Advanced Filtered Cathodic Arc Deposition Process	374,919

OFFICE OF SCIENCE (continued)

	FY 1999
Office of Advanced Scientific Computing Research (continued)	
Small Business Innovation Research Program (continued)	
Materials, Preparation, Synthesis, Deposition, Growth or Forming (continued)	
Phase II (Second Year)	$7,354,239
A Novel Reactive Joining Compound for High Temperature Applications	274,331
Development of Novel Boron-Based Multilayer Thin-Film	375,000
Advanced Plasma Surface Modification System	375,000
High-Flux, Low Energy Ion Source for High Rate Ion-Assisted Deposition of Hard Coatings	375,000
Semi-Solid Thermal Transformation to Produce Semi-Solid Formable Alloys	375,000
A Simple Process to Manufacture Grain Aligned Permanent Magnets	375,000
A Novel Technique for the Enhancement of Coercivity in High Energy Permanent Magnets	375,000
Stabilization of Nitride Magnet Material via Sol-Gel Route	375,000
A Combinatorial Approach to the Synthesis and Characterization of Novel Anode Materials For Direct Methanol Fuel Cells	375,000
Low Cost Deposition of Buffer Layers for Manufacturable YBCO HTS Conductors	375,000
Buffer Layers on Textured Nickel Using Commercially Viable CCVD Processing	375,000
Development of Efficient and Practical Passive Solar Building Systems with High Recycled Content Using the Preplaced Aggregate Concrete Technology	375,000
Heterogeneous Hydroformylation of Alkenes with Syngas	375,000
Tubular SOFC with Deposited Nano-Scale YSZ Electrolyte	374,972
High Speed Long Wavelength Infrared Detector Array/Preamplifier Development	375,000
Development of Cadmium Germanium Arsenide Crystals	375,000
An Easily Dispersed Reactive Coating for Surface Decontamination	368,056
Rapid Quench Nb_3Al for High Field Accelerator Applications	375,000
Ultra-Lightweight Carbon-Carbon Cooling Structure For Pixel and Silicon Strip Detectors	336,880
Development of Scintillators and Waveshifters for Detection of Ionizing Radiation	375,000
Small Business Technology Transfer Research Program	$1,995,296
Device Component Fabrication, Behavior or Testing	$997,168
Phase I	$497,222
Thin-Film Fiber Optic Sensors for Power Control and Fault Detection	99,930
Novel Carbon Monoxide Sensor for PEM Fuel Cell Systems	100,000
Electrochemical Sensors for Volatile Nitrogen Compounds in Air	98,536
Organic Diodes Using ISAM Polymers	99,942
Ink-Jet Printing for Fabrication of Full-Color Polymer LED Displays	98,814
Phase II (First Year)	$250,000
High Energy and Power Ultracapacitors Utilizing Novel Type III Polymers and Non-Aqueous Electrolytes	250,000

OFFICE OF SCIENCE (continued)

	FY 1999
Office of Advanced Scientific Computing Research (continued)	
Small Business Technology Transfer Research Program (continued)	
Device or Component Fabrication, Behavior or Testing (continued)	
Phase II (Second Year)	$499,696
Novel Thin Film Scintillator for Intermediate Energy Photons Detection and Imaging	249,696
Advanced Ceramic Hot Gas Filters	250,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$748,378
Phase II (First Year)	$248,848
Boron Carbide Coatings for Enhanced Performance of Radio-Frequency Antennas in Magnetic Fusion Devices	248,848
Phase II (Second Year)	$499,530
New High-Performance GaSb-Based Thermophotovoltaic (TPV) Devices	249,530
High Efficiency Magnet Refrigerators as Alternate Environmentally Safe Commercial Refrigeration Devices	250,000
Office of Fusion Energy Sciences	$9,880,000
Materials Properties, Behavior, Characterization or Testing	$9,880,000
Structural Materials Development	720,000
Modeling Irradiation Effects in Solids	50,000
Fusion Systems Materials	3,679,000
Structural Materials for Fusion Systems	1,270,000
Development of Radiation-hardened Ceramic Composites for Fusion Applications	94,000
Mechanisms of Plastic and Fracture Instability for Alloy Development of Fusion Materials	285,000
Damage Analysis and Fundamental Studies for Fusion Reactor Materials Development	502,000
Materials Development for Plasma Facing Components	2,800,000
Structural Materials Development for the Conduit of ITER Cable-in-conduit-conductors	100,000
Development and Testing of Insulating Coatings	310,000
Identification and Evaluation of Insulating Coatings	70,000

OFFICE OF SCIENCE

The Office of Science (SC) 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 Science is responsible for six major outlay programs: Basic Energy Sciences, Fusion Energy Sciences, Biological and Environmental Research, High Energy and Nuclear Physics and Advanced Scientific Computing 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 Science 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 Advanced Scientific Computing Research - Division of Technology Research

Office of Biological and Environmental Research - Medical Sciences Division

Office of Fusion Energy Sciences - Division of Advanced Physics and Technology

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

OFFICE OF BASIC ENERGY SCIENCES

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

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

DIVISION OF MATERIALS SCIENCES

The Division of Materials Sciences conducts a broad program of materials research to increase the understanding of phenomena and properties important to materials behavior that will contribute to meeting the needs of present and future energy technologies. The Division supports fundamental research in materials at DOE national laboratories and plans, constructs, and operates national scientific user facilities needed for materials research. In addition, the Division funds over 230 grants, mostly with universities, on a wide range of topics in materials research.

Fundamental materials research is carried out at twelve DOE laboratories: Ames Laboratory at Iowa State University, Argonne National Laboratory, Brookhaven National Laboratory, Idaho National Environmental and 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 the University of Illinois Frederick Seitz Materials Research Laboratory.

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

Specific information on the Materials Sciences sub-program is contained in the DOE publication DOE/SC-0011 Materials Sciences Programs FY 1998 (published July 1999). This 190-page publication contains program descriptions for 517 research programs that were funded in Fiscal Year 1998 by the Division of Materials Sciences. Five cross-cutting indices identify all 517 programs according to Principal Investigator(s), Materials, Techniques, Phenomena and Environment. Other contents include identification of the Division of Materials Sciences Staff structure and expertise; a bibliographical listing of 48 scientific workshop reports on select topics that identify materials sciences research needs and opportunities; a descriptive summary of the DOE Center of Excellence for the Synthesis and Processing of Advanced Materials; a descriptive summary and access information on 15 National Research User Facilities including synchrotron light sources, neutron beam sources, electron beam microcharacterization instruments, materials preparation and combustion research; and an analytical summary of research funding levels. Limited copies may be obtained by calling (301) 903-3427 and requesting DOE publication DOE/SC-0011. Project summaries are also available under the Division's home page on the Worldwide Web (www.sc.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 1999 for materials-related programs was approximately $5 M in heterogeneous catalysis, electrochemical energy storage and conversion research and materials precursor chemistry.

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

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

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

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

For information about specific programs the DOE contact is William S. Millman, (301) 903-3285. The reader also is referred to the Worldwide Web for the publication Summaries of FY 1998 Research in the Chemical Sciences (www.er.doe.gov/production/bes/chmhome.html) for summaries of all funded programs and descriptions of major user and other special facilities.

DIVISION OF ENGINEERING AND GEOSCIENCES

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

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

The broad goals of the BES Engineering Research Program are: (1) to extend the body of knowledge underlying the current engineering practice so as to create new options for enhancing energy savings and production, for prolonging useful equipment life, and for reducing costs without degradation of industrial production and performance quality; and (2) to broaden the technical and conceptual base for solving future engineering problems in the energy technologies. The DOE contact for this program is Robert E. Price, (301) 903-3428.

ENGINEERING SCIENCES RESEARCH

A brief description of Engineering Sciences supported programs is found in DOE/SC-0135, Summaries of FY 1997 Engineering Research, which was published in June 1998. Limited copies may be obtained by calling (301) 903-3428.

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

204. **FUNDAMENTALS OF THERMAL PLASMA PROCESSING**
$500,000
DOE Contact: Robert E. Price, (301) 903-3428
INEEL National Engineering Laboratory Contact: J. R. Fincke, (208) 526-2031

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

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

Keywords: Plasma Processing; Functionally Gradient Materials

205. **METAL TRANSFER IN GAS-METAL ARC WELDING**
$155,000
DOE Contact: Robert E. Price, (301) 903-3428
MIT Contacts: T. W. Eagar and J. Lang, (617) 253-3229

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

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

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

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

Keywords: Gas-Metal Arc, Welding

206. **THERMAL PLASMA CHEMICAL VAPOR DEPOSITION OF ADVANCED MATERIALS**
$165,000
DOE Contact: Robert E. Price, (301) 903-3428
University of Minnesota Contact: J. Heberlein, (612) 625-4538

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 INEEL.

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

207. **RESEARCH ON COMBUSTION- DRIVEN HVOF THERMAL SPRAYS**
$112,000
DOE Contact: Robert E. Price, (301) 903-3428
Pennsylvania State University Contact: G. Settles, (814) 863-1504

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

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

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

Keywords: Combustion, Oxy-Fuel

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

208. **AN INVESTIGATION OF HISTORY-DEPENDENT DAMAGE IN TIME-DEPENDENT FRACTURE MECHANICS**
$100,000
DOE Contact: Robert E. Price, (301) 903-3428
Battelle Memorial Institute Contact: F. Brust, (614) 424-5034

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

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

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

Keywords: Damage, Fracture Mechanics

209. **INTELLIGENT CONTROL OF THERMAL PROCESSES**
$500,000
DOE Contact: Robert E. Price, (301) 903-3428
INEEL Contact: H. Smartt, (208) 526-8333

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

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

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

Keywords: Fuzzy Logic, Neural Networks

210. **ELASTIC-PLASTIC FRACTURE ANALYSIS: EMPHASIS ON SURFACE FLAWS**
$500,000
DOE Contact: Robert E. Price, (301) 903-3428
INEEL Contacts: W. G. Reuter, J. Epstein and 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. Moir, 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

211. **MODELING AND ANALYSIS OF SURFACE CRACKS**
$200,000
DOE Contact: Robert E. Price, (301) 903-3428
MIT Contacts: David M. Parks, (617) 253-0033
and F. A. McClintock, (617) 253-2219

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

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

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

Keywords: Fracture Mechanics, Welding

212. **DEVELOPMENT OF MEASUREMENT CAPABILITIES FOR THE THERMOPHYSICAL PROPERTIES OF ENERGY-RELATED FLUIDS**
$490,000
DOE Contact: Robert E. Price, (301) 903-3428
National Institute of Standards and Technology
Contacts: R. Kayser and W. Haynes,
(301) 975-2583

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

Keywords: Thermophysical Properties, Fluid

213. **HIGH-Tc SUPERCONDUCTOR-SEMICONDUCTOR INTEGRATION AND CONTACT TECHNOLOGY**
$130,800
DOE Contact: Robert E. Price, (301) 903-3428
National Institute of Standards and Technology
Contacts: J. W. Elkin, (303) 497-5448

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

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

Keywords: High T_c Superconductors, Contacts

214. **TRANSPORT PROPERTIES OF DISORDERED POROUS MEDIA FROM THE MICROSTRUCTURE**
$135,000
DOE Contact: Robert E. Price, (301) 903-3428
Princeton University Contact: S. Torquato, (609) 258-4600

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

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

Keywords: Porous Media, Transport Properties

215. **STRESS AND STABILITY ANALYSIS OF SURFACE MORPHOLOGY OF ELASTIC AND PIEZOELECTRIC MATERIALS**
$150,000
DOE Contact: Robert E. Price, (301) 903-3428
Stanford University Contacts: H. Gao and D. Barnett, (415) 725-2560

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

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

Keywords: Surfaces, Interfaces, Stress Analysis, Piezoelectrics

GEOSCIENCES RESEARCH

The BES Geosciences Research Program supports fundamental research of long-term relevance to multiple Department of Energy mission areas such as energy technology, national security, energy conservation, environmental quality, or safety. It seeks understanding of the processes and properties in the earth that will affect the success of DOE's efforts in its several business lines as well as contribute to broad scientific progress. In particular, individual research efforts supported by this program provide foundational support to both the Energy Resources and Environmental Quality efforts. The DOE contact for this Program is Nicholas B. Woodward (301) 903-5802.

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

216. **SOLUTION-REPRECIPITATION OF CALCITE AND PARTITIONING OF DIVALENT METALS**
$0
DOE Contact: N. B. Woodward, (301) 903-5802
University of Chicago Contact: Frank M. Richter, (773) 702-8118

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

Keywords: Carbonate Minerals, Dissolution and Precipitation Mechanisms

217. **TRANSITION METAL CATALYSIS IN THE GENERATION OF PETROLEUM AND NATURAL GAS**
$110,900
DOE Contact: N. B. Woodward, (301) 903-5802
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

218. **MINERAL DISSOLUTION AND PRECIPITATION KINETICS: A COMBINED ATOMIC-SCALE AND MACRO-SCALE INVESTIGATION**
$125,000
DOE Contact: N. B. Woodward, (301) 903-5802
University of Wyoming Contact: Carrick M. Eggleston, (307) 766-6769
LLNL Contact: Kevin G. Knauss, (510) 422-1372

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

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

219. **SURFACE CHEMISTRY OF PYRITE AND ISOSTRUCTURAL ANALOGS: A COMBINED SURFACE SCIENCE AND AQUEOUS GEOCHEMICAL INVESTIGATION**
$125,000
DOE Contact: Nicholas B. Woodward, (301) 903-5802
Temple University Contact: Dr. Daniel Strongin, (215) 204-7119
State University of New York at Stony Brook Contact: Dr. Martin Schoonen, (516) 632-8007

The research is to investigate the surface chemistry of pyrite and other major sulfide minerals at the molecular and microscopic level. Its objective is to understand basic aspects of the surfaces such as charge development, reactivity, surface stoichiometry, surface structure and interaction(s) with dissolved species. The work expands from initial pyrite investigations to include isostructural disulfides to develop a more thorough understanding of disulfide behavior in general. Identical experiments will be made on natural pyrite single crystals and on multi-faceted powders to determine the effect of different surface morphologies. Specific objectives include: 1) pyrite oxidation mechanisms, and the effects of adsorbates on the oxidation rate will be determined; and, 2) fundamental reactions that control surface charge development on pyrite surfaces will be identified.

Keywords: Surface Chemistry, Sulfide Mineralogy, Mineral Chemistry

MATERIALS STRUCTURE AND COMPOSITION

220. **REACTION MECHANISMS OF CLAY MINERALS AND ORGANIC DIAGENESIS: AN HRTEM/AEM STUDY**
$0
DOE Contact: N. B. Woodward, (301) 903-5802
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

221. **INFRARED SPECTROSCOPY AND HYDROGEN ISOTOPE GEOCHEMISTRY OF HYDROUS SILICATE GLASSES**
$150,000
DOE Contact: N. B. Woodward, (301) 903-5802
California Institute of Technology Contacts: S. Epstein, (818) 356-6100 and E. Stolper, (818) 356-6504

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

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

222. **BIOMINERALIZATION: SYSTEMATICS OF ORGANIC-DIRECTED CONTROLS ON CARBONATE GROWTH MORPHOLOGIES AND KINETICS DETERMINED BY *IN SITU* ATOMIC FORCE MICROSCOPY**
$215,000
DOE Contact: N.B. Woodward, (301) 903-5802
Virginia Polytechnic Institute and State University Contact: P. Dove, (540) 231-2444
LLNL Contact: James DeYoreo, (510) 423-4240

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

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

223. **REACTIONS AND TRANSPORT OF TOXIC METALS IN ROCK-FORMING SILICATES AT 25°C**
$225,000
DOE Contact: N. B. Woodward, (301) 903-5802
Johns Hopkins University Contact: D. R. Veblen, (410) 516-8487
Lehigh University Contact: E. Ilton, (610) 758-5834

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

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

224. **DEVELOPMENT OF AN EXPERIMENTAL DATA BASE AND THEORIES FOR PREDICTION OF THERMODYNAMIC PROPERTIES OF AQUEOUS ELECTROLYTES AND NONELECTROLYTES OF GEOCHEMICAL SIGNIFICANCE AT SUPERCRITICAL TEMPERATURES AND PRESSURES**
$220,000
DOE Contact: Nicholas B. Woodward, (301) 903-5802
Washington University Contact: Everett L. Shock, (314) 726-4258
University of Delaware Contact: Robert H. Wood, (302) 831-2941

The proposed research is to investigate the thermodynamic properties of aqueous electrolyte and non-electrolyte solutions at temperatures and pressures relevant to the Earth's crust. It will investigate thermodynamic properties of aqueous organic species that are important for understanding and quantitative prediction of interactions of geologic fluids with crustal rocks. Proposed experiments to measure volumes and heat capacities will provide critical data necessary for testing theoretical methods and predictions of thermodynamic properties based on both empirical and first-principles approaches, and to extend the compositional and temperature ranges of their calibration. The thermodynamic analysis involves parallel approaches, to extend the calibration basis of the empirical, broadly predictive, and widely used Helgeson-Kirkham-Flowers equations of state, at the same time as developing more accurate equations of state based on first-principles methods. The research will provide a comprehensive basis for evaluating the thermodynamics of organic transformations in sedimentary basins, including geochemical processes associated with the generation, migration, and emplacement of hydrocarbon resources.

Keywords: Thermodynamics, Electrolytes, Organic Geochemistry

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

225. **DYNAMIC NONLINEAR ELASTIC RESPONSE OF EARTH MATERIALS**
$250,000
DOE Contact: Nicholas B. Woodward, (301) 903-5802
LANL Contact: Dr. Paul A. Johnson, (505) 667-8936

The research is to investigate the mechanisms responsible for nonlinear elastic behavior and hysteresis in rock. The proposed work is developing an experimental program to explore mechanism causing nonlinear behavior. It will also develop theory and methodology for extracting the nonlinear properties of rock from resonance measurements. Finally the project will examine the microphysics associated with fluid-related hysteresis in rocks. The experiments are focused on resonance measurements in which the strain levels and frequency content of the driving waves can be carefully controlled.

Keywords: Elastic Behavior, Hysteresis, Non-Destructive Testing

226. **STRUCTURE AND REACTIVITY OF FERRIC OXIDE AND OXYHYDROXIDE SURFACES: QUANTUM CHEMISTRY AND MOLECULAR DYNAMICS**
$240,000
DOE Contact: N. B. Woodward, (301) 903-5802
PNNL Contacts: Jim Rustad and Andrew Felmy, (509) 376-1134

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

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

227. **CATION DIFFUSION RATES IN SELECTED MINERALS**
$200,000
DOE Contact: N. B. Woodward, (301) 903-5802
SNL Contacts: Randall T. Cygan, H. R. Westrich and Diana Fisler, (505) 844-7216

Objectives of this research are to determine experimental cation diffusion coefficients for pyroxene and carbonate minerals at temperatures less than 1000°C for evaluating disequilibrium behavior in geological, nuclear waste, energy, and materials applications. A new thin-film technique for preparation of diffusion couples was used to measure the relative slow diffusion of Mg^{2+}, Mn^{2+}, and Ca^{2+} in pyroxenes and carbonates. Depth profiles of tracer isotopes are then evaluated using an ion microprobe. Comparison of the diffusion coefficients determined under various oxygen fugacities provides information about the diffusion mechanism and the defect structure of the mineral sample. The experimental work has been complemented by atomistic simulations of calcium self-diffusion in calcite. Lattice energy, defect formation energies, and activation energy for a cation vacancy migration have been calculated, providing the mechanism and favored direction of migration of cations in the calcite structure. Results suggest that relaxation of atomic sites in the vicinity of a cation vacancy is a significant contribution to the energy for the migration of cations.

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

228. **THERMODYNAMICS OF MINERALS STABLE NEAR THE EARTH'S SURFACE**
$150,000
DOE Contact: N. B. Woodward, (301) 903-5802
University of California, Davis Contact: A. Navrotsky, (916) 752-9307

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

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

229. **NEW METHOD FOR DETERMINING THERMODYNAMIC PROPERTIES OF CARBONATE SOLID-SOLUTION MINERALS**
$0
DOE Contact: N. B. Woodward, (301) 803-5802
University of California, Davis Contacts:
P. A. Rock and W. E. Casey, (916) 752-0940

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

Keywords: Carbonate Minerals, Solubility, Electrochemical Cell

230. **THEORETICAL STUDIES OF METAL SPECIES IN SOLUTION AND ON MINERAL SURFACES**
$48,100
DOE Contact: N. B. Woodward, (301) 903-5802
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

231. **MICROMECHANICS OF FAILURE IN BRITTLE GEOMATERIALS**
$270,800
DOE Contact: N.B. Woodward, (301) 903-5802
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

232. **THREE-DIMENSIONAL IMAGING OF DRILL CORE SAMPLES USING SYNCHROTRON-COMPUTED MICROTOMOGRAPHY**
$195,000
DOE Contact: N. B. Woodward, (301) 903-5802
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

233. **SHEAR STRAIN LOCALIZATION AND FRACTURE EVOLUTION IN ROCKS**
$370,900
DOE Contact: N. B. Woodward, (301) 903-5802
Northwestern University Contact: J .W. Rudnicki, (708) 491-3411
SNL Contact: W. Olsson, 505-844-7344

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

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

234. **DISSOLUTION RATES AND SURFACE CHEMISTRY OF FELDSPAR GLASS AND CRYSTAL**
$142,000
DOE Contact: N. B. Woodward, (301) 903-5802
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

235. **TRANSPORT PHENOMENA IN FLUID-BEARING ROCKS**
$178,800
DOE Contact: N. B. Woodward, (301) 903-5802
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

236. **CATION CHEMISORPTION AT OXIDE SURFACES AND OXIDE-WATER INTERFACES: X-RAY SPECTROSCOPIC STUDIES AND MODELING**
$268,300
DOE Contact: N. B. Woodward, (301) 903-5802
Stanford University Contacts: G. E. Brown and G. A. Parks, (415) 723-9168

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

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

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237. **HIGH PERFORMANCE TAILORED MATERIALS FOR LEVITATION AND PERMANENT MAGNET TECHNOLOGIES (ANL 97-02)**
$250,000
DOE Contact: Walter M. Polansky, (301) 903-5995
ANL Contact: George W. Crabtree, (630) 252-5509

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

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

238. ATOMIC SCALE STRUCTURE OF ULTRATHIN MAGNETIC MULTILAYERS AND CORRELATION WITH RESISTANCE, GIANT MAGNETORESISTANCE, AND SPIN-DEPENDENT TUNNELING (ORL 97-03)
$250,000
DOE Contact: Walter M. Polansky, (301) 903-5995
ORNL Contact: William H. Butler, (423) 574-4845

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

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

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

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

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

240. **DEVELOPMENT OF HIGH-TEMPERATURE SUPERCONDUCTING WIRE USING RABITS COATED CONDUCTOR TECHNOLOGIES (ORL 97-02)**
$250,000
DOE Contact: Walter M. Polansky, (301) 903-5995
ORNL Contact: David K. Christen, (423) 574-6269

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

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

241. **DEVELOPMENT OF BISMUTH-BASED SUPERCONDUCTING WIRE WITH IMPROVED CURRENT CARRYING AND FLUX PINNING PROPERTIES (ANL99-15)**
$125,000
DOE Contact: Walter M. Polansky, (301) 903-5995
ANL Contact: Victor Maroni, (630) 252-4547

Progress in the commercialization of electric power equipment fabricated with high temperature superconducting materials has been limited by performance issues associated with the maximum achievable engineering critical current density, J_e, in long-length composite conductor. One of the most advanced conductors available today for such applications is the silver-clad $(Bi,Pb)_2Sr_2Ca_2Cu_3O_y$ (called Ag/Bi-2223) composite in multifilament form. However, the J_e of Ag/Bi-2223 at 77 K in magnetic fields of 1 Tesla or more is not presently adequate for most types of motors, generators, transformers, current limiters, and related power system components. Research is aimed at investigating two new pathways to fabricate the next generation of improved bismuth-based superconducting wire. One pathway is focused on the controlled growth of strong flux pinning centers in Ag/Bi-2223 filaments by the implementation of special heat treatment procedures. These create a transient thermodynamic state that promotes the growth of selected second phase nanocrystallites having the correct size, shape, and spatial distribution to induce strong inter- and intra-granular flux pinning. The second pathway involves reducing the c-axis blocking layer gap (between CuO_2 planes) in layered bismuth cuprates by demonstrating fabrication of the silver-clad $(Bi,Pb,Cd)_1Sr_2Ca_1Cu_2O$ (M-1212) along lines that have been developed for Ag/Bi-2223. The "in-principle" advantage of M-1212 over Bi-2223 stems from the shorter (by ~4 D) blocking gap in M-1212 due to fewer atomic layers in the c-axis repeat unit. From preliminary work, there are existing laboratory scale indications that both pathways can lead to significant improvement in the performance of bismuth-based high temperature composite conductors. The project extends DOE commitments in characterization and design of advanced materials for the acceleration of superconducting technologies to US markets.

Keywords: Superconducting Materials, Silver-Clad $(Bi,Pb)_2Sr_2Ca_2Cu_3Oy$

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

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

Keywords: Light Emitting Diodes, Red and Infrared, Hetero Epitaxial, Blue and Green LEDS, GaN

243. DEVELOPMENT OF BUFFER LAYERS SUITABLE FOR DEPOSITION OF THICK SUPERCONDUCTING $YBa_2Cu_3O_7$ LAYERS BY POST-DEPOSITION ANNEALING PROCESS (BNL 98-05)
$250,000
DOE Contact: Walter M. Polansky, (301) 903-5995
BNL Contact: M. Suenaga, (516) 344-3518

The goal of this project is to develop a textured buffer layer on top of a metallic substrate, e.g., a textured Ni, which is compatible with the Brookhaven National Laboratory method of fabricating thick $YBa_2Cu_3O_7$ films, a post-deposition annealing method. In order to accomplish this, the project has started: (1) the purchase and installation of a textured measurement attachment to an existing X-ray apparatus (This makes it possible to determine the degree of the texture of the buffer layer as well as the substrate and $YBa_2Cu_3O_7$ layers.), and (2) testing of the chemical compatibility of CeO_2 with $YBa_2Cu_3O_7$ layers at the high temperature required for the formation of $YBa_2Cu_3O_7$ layers. A texture measuring attachment to a X-ray diffractometer was purchased and was installed such that a texture analysis of the rolled tapes, the buffer, or the superconducting films can be determined. This unit has been delivered and installed, and the process of a final acceptance of the unit is being performed. Since the post-deposition annealing process for growing thick (>5 µm) $YBa_2Cu_3O_7$ involves heat treating $YBa_2Cu_3O_7$ precursor films in a moist atmosphere at high temperatures (>725° C), it is important to select a buffer layer material which does not interfere with the growth of $YBa_2Cu_3O_7$. In order to study this, the project has initially deposited a $YBa_2Cu_3O_7$ precursor film on a CeO_2 buffered single crystalline $LaAl0_3$ and heat treated it to form a $YBa_2Cu_3O_7$ layer on top of the CeO_2. Note that CeO_2 is a well-known buffer layer which is used in conjunction with pulsed laser deposition of $YBa_2Cu_3O_7$. Although a significant reaction takes place between the $YBa_2Cu_3O_7$ and CeO_2 layers if they are heat-treated above 750°C, the reaction appears to be sufficiently minimized by keeping the reaction temperature below 735°C. A further study is being conducted to see the extent of the reaction, and other possible candidates for the buffer materials are being examined. If this project is successful, the superconducting tapes will be used in electrical utility systems, greatly increasing the efficiency of power transmission. This project supports DOE's mission through increased energy efficiency.

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

244. INTERPLAY BETWEEN INTERFACIAL AND DIELECTRIC AND FERROELECTRIC BEHAVIORS OF BARIUM STRONTIUM TITANATE THIN FILMS (PNL99-08)

$125,000
DOE Contact: Walter M. Polansky, (301) 903-5995
PNL Contact: Young Liang, (510) 376-8565

Barium strontium titanate (BST) and related materials are entering commercial use for integrated circuit manufacture as conventional materials reach their fundamental limits. BST films have capacitance, leakage, and related electrical properties that surpass integrated circuit device requirements. One of the most important steps towards understanding the interplay between interfacial properties and dielectric and ferroelectric behaviors of BST ($Ba_{1-x}Sr_xTiO_3$) is the growth of high quality BST films on Si substrates. Successful epitaxial growth of crystalline BST on Si(001) is thought to require the formation of a two-dimensional interfacial silicide layer involving either Ba or Sr as the initial step. Bulk thermodynamics suggests that this thin silicide layer is required to stabilize the interface. The goal of the project is to address two specific issues of significant concern in BST thin-film technology: (1) the effect of interfacial chemistry and stress on the dielectric and ferroelectric properties of BST thin films, and (2) ferroelectric behavior at the nano-scale level. Research is focused on preparation, isolation, and characterization of an ultrathin silicide layer using Sr as the alkaline earth metal. Si(001)-(2x1) surfaces were prepared in ultra high vacuum (UHV) by rapid desorption of the native oxide layer. These surfaces were exposed to Sr from an effusion cell in an oxide MBE chamber as a function of evaporation rate, substrate temperature, and total dose. The resulting interfaces were characterized during growth with reflection high-energy electron diffraction (RHEED), and after growth with low-energy electron diffraction (LEED), x-ray photoemission (XPS), and x-ray photoelectron diffraction (XPD). Additionally, the team is initiating STM investigations to further elucidate this interface structure. Physical and electrical testing of these structures have been performed to determine interface roughness, interface layer formation, interface state density, dielectric properties (permittivity, leakage, etc.), and stability vs. post-growth processing. This project supports DOE's commitment to basic energy sciences in fostering the synthesis, processing, and characterization of advanced materials.

Keywords: BST Thin Films, Dielectric, Ferroelectric Materials, Interfacial Chemistry

245. COMBINATORIAL DISCOVERY AND OPTIMIZATION OF NOVEL MATERIALS FOR ADVANCED ELECTRO OPTICAL DEVICES (LBL 97-18)

$250,000
DOE Contact: Walter M. Polansky, (301) 903-5995
LBNL Contact: Xiao-Dong Xiang, (510) 486-4864

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

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

246. **ADVANCED COMPUTATIONAL MODELS AND EXPERIMENTS FOR DEFORMATION OF ALUMINUM ALLOYS - PROSPECTS FOR DESIGN (PNL99-07)**
$125,000
DOE Contact: Walter M. Polansky, (301) 903-5995
PNL Contact: M.A. Khaleel (509) 375-2438

Dislocations are the basic lattice line defects in crystalline materials, with defect densities as high as $10^{15}/m^2$. This project aims at understanding their collective and complex nonlinear dynamical behavior by merging a set of highly sophisticated experiments, using computer aided, massive numerical analyses, and experimental data. The project impacts future computational and experimental advances in dislocation theory and elevates prospects for predictive alloy properties control. One motivation for this work is to characterize fabrication and durability characteristics of aluminum tailor welded blanks in order to demonstrate their viability for high volume, low cost stamped automotive panels and structures. Finite Element Modeling is being used to formulate accurate constitutive relations to allow complete description of material response during manufacture. Application of this research to manufacture and design of existing and new lightweight Al materials supports DOE's initiatives in high performance computing.

Keywords: Aluminum Alloys, Dislocation Phenomena, Predictive Properties Control

247. **NEAR-FRICTIONLESS CARBON COATINGS (ANL 98-03)**
$250,000
DOE Contact: Walter M. Polansky, (301) 903-5995
ANL Contact: Ali Erdemir, (630) 252-6571

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

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

248. **SMOOTH DIAMOND FILMS FOR FRICTION AND WEAR APPLICATIONS AND CHEMICALLY PROTECTIVE COATINGS (ANL 97-05)**
$250,000
DOE Contact: Walter M. Polansky, (301) 903-5995
ANL Contact: Alan Krauss, (630) 252-3520

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

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

249. **NANOMETER CHARACTERIZATION AND DESIGN OF MOLECULAR LUBRICATION FOR THE HEAD-DISK INTERFACE (LBL 98-10)**
$153,000
DOE Contact: Walter M. Polansky, (301) 903-5995
LBNL Contact: Miquel Salmeron, (510) 486-6704

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

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

250. **AN ADVANCED HARD CARBON PLASMA DEPOSITION SYSTEM WITH APPLICATION TO THE MAGNETIC STORAGE INDUSTRY (LBL 98-16)**
$175,000
DOE Contact: Walter M. Polansky, (301) 903-5995
LBNL Contact: Andre Anders, (510) 486-6745

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

U.S. computer industry. Many of the top names in the magnetic storage industry have voiced their support for a filtered cathodic arc system for advanced carbon coating. The project supports the DOE mission in advanced materials, specifically synthesis and processing by ions and plasmas.

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

251. **A FACILITY FOR STUDYING MICROMAGNETIC STRUCTURES (LBL 95-12)**
$94,000
DOE Contact: Walter M. Polansky, (301) 903-5995
LBNL Contact: Howard Padmore, (510) 486-5787

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

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

252. **INTERFACIAL PROPERTIES OF ELECTRON BEAM CURED COMPOSITES (ORNL99-08)**
$125,000
DOE Contact: Walter M. Polansky, (301) 903-5995
ORNL Contact: Christopher Janke, (423) 574-9247

Electron Beam curing of composites and adhesives is a nonthermal, nonautoclave curing process which offers substantially reduced manufacturing costs and curing times, improvements in part quality and performance, reduced environmental and health concerns, and improvements in material handling, as compared to conventional thermal curing. As satisfactory properties of electron beam cured composites are achieved, U.S. industry expects rapid implementation of these materials for making better, less expensive, and lightweight airplanes, spacecraft, and automobiles. Previous research on electron beam cured composites has shown that interface dependent properties, such as composite interlaminar shear strength, are generally lower than those of high performance, autoclave cured composites. A primary objective of this project is to determine the chemical, physical, and/or mechanical mechanisms responsible for poor adhesion between carbon fibers and epoxy resins subjected to electron beam processing. Another important objective is to optimize electron beam compatible carbon fiber surface treatments, chemical agents, modified radiation curable epoxy resin systems, and improved fabrication and processing methods for producing electron beam cured composites having excellent interfacial properties. Currently, work is focused on characterization of the carbon fiber-epoxy resin interface and identification of the critical radiation processing parameters that influence the properties of electron beam cured composites. Additionally, various chemical agents, including coupling agents and reactive finishes, which are specifically designed to improve the fiber-resin adhesion properties, are being evaluated. The project complements DOE investments in advanced materials research, and research on energy efficiency and environmental stewardship.

Keywords: Electron Beam Processing, Electron Beam Cured Composites and Adhesives

253. **PHOTOCATALYTIC METAL DEPOSITION FOR NANOLITHOGRAPHY (ANL99-13)**
$125,000
DOE Contact: Walter M. Polansky, (301) 903-5995
ANL Contact: Tijana Rajh, (630) 252-3542

A major technical impediment for the development of mesoscopic scale electronic devices is obtaining molecular scale conducting patterns. Based on the parameters that are optimized in highly efficient photochemical energy conversion in natural photosynthesis, Argonne National Laboratory has developed a new mask-less photoelectrochemical method for depositing conductive metal patterns with nanometer scale precision. This technology will enable the rapid prototyping and manufacturing of mesoscopic electronics and offers the potential of low-cost small batch manufacturing and unparalleled levels of electronic integration. This new technology is being used to fabricate miniaturized (ultimate resolution limit of 1 nm) and rugged electrical interconnects and biomolecular electronic devices on any surface or in solution. This project will enable the 3-D integration of passive and active components of mesoscopic integrated conformal electronics. In addition, the technology provides a unique advantage compared to other electronic technologies, because the semiconductor substrate (precursor) can also perform active function in the bioelectronic device. Conductor precursors, semiconductor metal oxide nanoparticles modified with chelating agents, that bind metal cations (copper, silver, and gold), will be synthesized. Biological templates will be used to self-assemble conductor precursors in order to achieve spacial resolution via photocatalysis. The fast photoresponse of semiconductor nanodots also provides high time resolution. Based on a fundamental understanding of electron transfer reactions in this biomimetic approach, precursor formulations will be developed and characterized for photoelectrochemical response, redox stability, and mechanical properties. Precursors will be deposited on a range of substrates (silicon, glass, plastic, metals, ceramics, etc.) or in solution. Conductive patterns formed by catalytic semiconductor assisted solid state deposition of copper, silver, or gold will be studied as a function of nanoparticle size, reduction technique, and nanoparticle-chelate association complex. Interconnects and biomolecular assemblies will be studied to ascertain morphology, function, and 3-D characterization as a function of processing methodology. The technology developed in this project is an extension of DOE's efforts to promote characterization of materials useful to nanotechnology.

Keywords: Metal Deposition, Nanolithography, Self Assembly, Photocatalysis

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

254. **IONICALLY CONDUCTIVE MEMBRANES FOR OXYGEN SEPARATION (LBL 97-03)**
$150,000
DOE Contact: Walter M. Polansky, (301) 903-5995
LBNL Contact: Steven J. Visco, (510) 486-5821

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

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

255. **ADVANCED SEPARATIONS TECHNOLOGY FOR EFFICIENT AND ECONOMICAL RECOVERY AND PURIFICATION OF HYDROGEN PEROXIDE (ANL 98-07)**
$250,000
DOE Contact: Walter M. Polansky, (301) 903-5995
ANL Contact: Edward J. St. Martin, (630) 252-5784

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

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

256. **SYNTHESIS AND CRYSTAL CHEMISTRY OF TECHNOLOGICALLY IMPORTANT CERAMIC MEMBRANES (ANL97-06)**
$195,000
DOE Contact: Walter M. Polansky, (301) 903-5995
ANL Contact: James D. Jorgensen, (630) 252-5513

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

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

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

This project will focus on the development of new technology for the production of organic chemicals of commercial interest, based on fundamental research at BNL exploring the reactivity of transition metal hydride complexes. The scientific objectives are to explore the feasibility, scope, and selectivity of catalytic ionic hydrogenation technology. In these reactions, H_2 is added to an organic chemical sequentially, in the form of a proton (H^+) followed by hydride (H^-). The project plans to discover transition metal complexes that can carry out these functions catalytically, with hydrogen (H_2) being the ultimate source of both the proton and hydride.

Homogeneously catalyzed ionic hydrogenations offer the possibility of enabling efficient and selective hydrogenation processes for organic transformations that are difficult to achieve by conventional methods. Initial work will focus on attempts to develop prototype metal systems capable of catalytic hydrogenation of ketones. Tungsten systems with weakly coordinating counterions will be investigated first, since preliminary results have indicated that such systems have the requisite ability to form cationic tungsten dihydride complexes upon reaction with H_2. A key issue to be addressed will be the relative binding strength of different ligands to the metal, and measurements of this type may require high pressure nuclear magnetic resonance experiments at DuPont. When a successfully functioning catalytic system is developed, optimization will be attempted by systematic variation of ligands and the metal. Further elaborations will later attempt to utilize these methods in asymmetric hydrogenations to produce commercially viable processes. This project supports the fundamental DOE mission in understanding the mechanisms for catalysis and the chemical conversion of materials from biomass.

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

258. **HIGHLY DISPERSED SOLID ACID CATALYSTS ON MESOPOROUS SILICA (PNL 97-28)**
$125,000
DOE Contact: Walter M. Polansky, (301) 903-5995
PNNL Contact: Charles Peden, (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 super-acidic properties of tungstophosphoric acid and sulfated zirconia. The surface of mesoporous silica will be functionalized to accommodate the dispersion of tungstophosphoric acid and sulfated zirconia. This approach should produce a new class of highly active, shape selective, and robust solid superacid materials. The novel catalysts will be tested with the alkylation and isomerization reactions in the bench and pilot scale testing unit. The goal is to exceed the performance characteristics of existing solid superacid catalysts, thereby enabling the chemical and petrochemical industries to replace homogeneous acid catalysts. This will contribute to DOE's mission to reduce environmental impacts in the energy sector. Homogeneous acid catalysts such as sulfuric acid and aluminum chloride are currently used to catalyze many industrially important reactions. Although these homogeneous acid catalysts are efficient, they are not environmentally benign and create many operational problems. These problems can be mitigated with solid acid catalysts. Tungstophosphoric acid and sulfated zirconia are two solid acid catalysts with super acidity. Low catalytic efficiency is the common problem with these two catalysts. In addition, it is difficult to disperse tungstophosphoric acid on supports due to its large cluster size,, and sulfated zirconia generally suffers rapid deactivation. These problems can be minimized with the superior characteristics of mesoporous silica. This work will enhance understanding of how the mesoporous support properties and acid grafting strategy influence reactivity, yields, selectivity, thermal stability, coking, and regeneration of the solid acid catalysts. In FY 1998, efforts were conducted to define the specific catalyst properties of interest. Synthesis and functionalization of the mesoporous silica supports was also initiated.

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

259. **DEVELOPMENT OF A HIGH-EFFICIENCY ROTARY MAGNETOCALORIC REFRIGERATOR PROTOTYPE (AL99-02)**
$125,000
DOE Contact: Walter M. Polansky, (301) 903-5995
AL Contact: K. A. Gschneidner, Jr., (515) 294-7931

Magnetic refrigeration is based on the magnetocaloric effect—the ability of some materials to heat up when magnetized and cool when removed from the magnetic field. Using these materials as refrigerants would provide an environmentally friendly alternative to the volatile liquid chemicals, such as chlorofluorocarbons and hydrochlorofluorocarbons, used in traditional vapor-cycle cooling systems. The new materials, have two advantages over existing magnetic coolants: they exhibit a giant magnetocaloric effect, and their operating temperature can be tuned from about 30K (-400°F) to about 290K (65°F) by adjusting the ratio of silicon to germanium—the more germanium, the lower the temperature. The efficiency of the new materials make magnetic refrigeration even more competitive with conventional gas-compression technology by replacing complex and costly superconducting magnets with permanent magnets in refrigerator designs. The elimination of superconducting magnets may also open the way for small-scale applications of this technology, such as climate control in cars and homes, and in home refrigerators and freezers. In addition, G. Schneidner says, "the discovery may also launch totally new applications for efficient refrigerators at very low refrigeration powers since gas compression technology cannot be scaled down to such low cooling powers and since thermoelectric cooling is very inefficient (30 times less than magnetic refrigerants)." The first gadolinium-based magnetic refrigerator has been demonstrated. The refrigerator has been operating for over six months, which far exceeds the few hours or days of operation recorded by similar units. In addition, the unit has achieved cooling power 20 to 1,000 times greater than previous units. Currently, the team is working to find practical means of processing the new materials to construct and test a variety of magnetic refrigerators, which span temperatures from 20K (-425°F) to 300K (80°F) and have cooling powers ranging from one watt to 50,000 watts. The project transfers DOE's investments in materials research to research in energy efficiency through reduction in operating costs in air conditioning and refrigeration.

Keywords: Magnetocaloric Effect, Magnetocaloric Refrigeration, Gadolinium-based Magnetic Materials

260. **RAPID PROTOTYPING FOR BIOCERAMICS (ANL95-08)**
$42,000
DOE Contact: Walter M. Polansky, (301) 903-5995
ANL Contact: William Ellingson, (630) 252-5068

Solid Freeform Fabrication (SFF), also commonly called Rapid Prototyping, to direct fabrication of bioceramic materials with a focus on reducing costs for bone segment replacements or small orthopedic implants. Two technology areas are being coupled together: reverse engineering using high resolution 3D x-ray computed tomographic imaging (commonly called CAT scans in medical applications), and the new SFF technology using bioceramics. Recently, use of Tricalcium Phosphate (TCP) powder with new polymers has allowed the fabrication, debinding, and sintering of bioceramic orthopaedic implants which yielded sufficient properties for application. The fabrication was made possible by a new SFF feed system, which allows improved delivery of the bioceramic powder/polymer mix. This high-pressure extruder allows higher ceramic powder solids loading, thus reducing shrinkage. In addition, use of laser machining for the as-produced SFF bioceramics has also been demonstrated. The use of laser machining allows for a fast method to provide an appropriate surface finish. Extensive analysis of these materials is now in progress.

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

261. **DIRECT CASTING OF TITANIUM ALLOY WIRE FOR LOW-COST AEROSPACE AND AUTOMOTIVE FASTENERS (PNL99-02)**
$125,000
DOE Contact: Walter M. Polansky, (301) 903-5995
PNNL Contact: Mark Smith, (509) 376-2847

Current wire production methods require large ingots to undergo multiple reduction steps until a diameter of 7mm or less is obtained. The reduction steps are energy intensive, require expensive equipment, and result in the generation of scrap materials and undesirable etchant and lubricant waste. Economic analysis indicates that direct casting of a titanium wire to a diameter slightly larger than the desired final product, followed by relatively small final reduction steps, will result in significant savings to the aerospace industry and other titanium wire/rod users.

The direct casting process involves the use of a titanium core wire to serve as the carrier substrate onto which titanium will be cast and solidified at high feed rates. The objectives of the project include the development of unique atmosphere-controlled casting equipment, the application of thermal models to optimize the design and operation of the casting process, and extensive materials testing and characterization to establish the capability of the process to match properties produced by conventional processing. The project extends DOE investments in materials characterization to develop process technologies which further reduction of industrial waste emissions.

Keywords: Titanium Alloy Wire, Casting Processes

262. **CONTROLLED NONISOTHERMAL HOT FORGING USING INFRARED FOR MICROSTRUCTURAL CONTROL (ORL 98-08)**
$225,000
DOE Contact: Walter M. Polansky, (301) 903-5995
ORNL Contacts: Craig A. Blue, (423) 574-4357

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

Keywords: Hot Forging, Infrared Heating, Energy Savings

263. **NONCONSUMABLE METAL ANODES FOR PRIMARY MAGNESIUM PRODUCTION (ANL 98-05)**
$220,000
DOE Contact: Walter M. Polansky, (301) 903-5995
ANL Contact: Michael J. Pellin, (630) 252-3510

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

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

264. DEVELOPMENT OF ELECTROLYTE AND ELECTRODE MATERIALS FOR RECHARGEABLE LITHIUM BATTERIES (BNL98-04)
$250,000
DOE Contact: Walter M. Polansky, (301) 903-5995
BNL Contact: Xiao-Qing Yang, (516) 344-3663

Enhancing performance, reducing cost, and replacing toxic materials by environmentally benign materials are strategic goals of DOE in lithium battery research. Development of new electrolyte materials, aza and boron based anion receptors as additives, organic lithium salts, and plasticizers is aimed at enhancing the conductivity and lithium transference number of lithium battery electrolytes and reducing the use of toxic salts in these electrolytes. The objective of the project is to develop these electrolyte and cathode materials for rechargeable lithium batteries, especially for lithium ion and lithium polymer batteries. The research targets optimization of boron-compound-based composite electrolytes, and synthesis of new lithium salts and plasticizers for polymer and polymer gel electrolytes. Characterization of cathode materials will be carried out utilizing the National Synchrotron Light Source. In-situ x-ray absorption and x-ray diffraction techniques, developed at BNL, will be used to probe the relationship between performance and the electronic and structural characteristics of intercalation compounds such as $LiNiO_2$, $LiCoO_2$, and $LiMn_2O_4$ spinel. New cathode materials, such as $LiNi_{0.8}Co_{0.2}O_2$, $LiNi_{0.8}Co_{0.2-z}Al_zO_2$, and $LiNi_{0.7}Mg_{0.125}Ti_{0.125}O_2$, have also been studied. These results will be used to guide new material selection and quality control procedures. Successful research will result in the development of less expensive and more environmental friendly lithium battery materials for commercial applications.

The project marshals DOE's investment in basic materials research to promote economically and environmentally desirable new processes and materials for energy use.

Keywords: Lithium Based Materials, Lithium Batteries

265. OPTIMIZED CATALYSTS FOR THE CRACKING OF HEAVIER PETROLEUM FEEDSTOCKS (LBL99-01)
$126,000
DOE Contact: Walter M. Polansky, (301) 903-5995
LBL Contact: Gabor Somorjai, (510) 486-4831

Catalysts lower the energy required for chemical reactions to proceed and are widely used in petroleum refining and chemical manufacturing. The useful lifetime and, thus, the value of an industrial catalyst are limited by a process known as deactivation in which the efficiency of the catalyst declines over time. Understanding the deactivation process is essential for developing new catalysts with longer useful lifetimes. There are two industrially important catalytic systems under study at present. In the first study, zeolite-based catalysts are being developed to remove undesired sulfur compounds from gasoline. The goal of this project is to evaluate the mechanism by which sulfur is adsorbed on the catalyst. Of particular interest is the identification of catalyst "active sites" that actually interact with the sulfur. This is done by spectroscopically monitoring the identity of the surface species under reaction conditions. The second system under study is the "reforming" reactions of n-hexane and n-heptane with hydrogen that produce high octane gasoline by converting the reactants to benzene and toluene. Deactivation in these catalysts proceeds via "coking," the buildup and polymerization of carbonaceous reaction byproducts on the surface of the catalyst. The vibrational spectra of these byproducts will be obtained by UV-Raman spectroscopy for identification purposes. Ultraviolet excitation is required in this case to avoid interference from black body radiation from the hot catalyst material. Identification of problematic surface species will allow determination of the precise mechanism by which deactivation occurs in this system. These improvements will have a major impact on the efficiency of petroleum refining and gasoline production. The new surface science tools under development will have applicability to general studies in catalysis and surface science and support the DOE's mission in design and characterization of advanced materials.

Keywords: In-situ Surface UV-Raman Spectroscopy, Catalytic Surfaces, Catalyst Deactivation, Zeolite Based Materials

SMALL BUSINESS INNOVATION RESEARCH PROGRAM

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

PHASE I

High-Temperature Oscillator and Digital Clock - DOE Contact Raymond J. LaSala, (202) 586-4198; Linear Measurements, Inc. Contact Mr. Robert Hatch, (619) 535-2172

A Novel Potentiometric Pressure Sensor with a Temperature-Independent Signal for Geothermal Drilling - DOE Contact Paul Grabowski, (202) 586-0478; Materials and Systems Research, Inc. Contact Dr. Anil V. Virkar, (801) 973-1199

Capacitors for Extreme Temperature Applications - DOE Contact Gideon Varga, (202) 586-0082; Sigma Technologies International, Inc. Contact Dr. Angelo Yializis, (520) 575-8013

A High Temperature MEMS Inclination Sensor for Geothermal Drilling - DOE Contact Raymond J. LaSala, (202) 586-4198; Silicon Designs, Inc. Contact Mr. John C. Cole, (425) 391-8329

High Temperature Micromachined Sensor for Industrial Gas Streams - DOE Contact Eric Lightner, (202) 586-8130; Nanomaterials Research Corporation Contact Ms. Molly M. W. Kostelecky, (303) 702-1672

Thermoelectric Quantum Well Device - DOE Contact Jim Merritt, (202) 586-0903; Hi-z Technology, Inc. Contact Mr. Norbert Elsner, (619) 695-6660

N Type Quantum Well Films and Devices - DOE Contact Jim Merritt, (202) 586-0903; Hi-z Technology, Inc. Contact Mr. Norbert Elsner, (619) 695-6660

Economical Fabrication of Large Micro-Impingement Cooling Panels - DOE Contact Sam E. Berk, (301) 903-4171; Saddleback Aerospace Contact Ms. Elizabeth A. Campbell, (562) 598-3700

Helium Cooled Refractory Metal Divertor Panel - DOE Contact Sam E. Berk, (301) 903-4171; Thermacore, Inc. Contact Mr. Donald M. Ernst, (717) 569-6551

Fast Repetitive Arc Free Current Limiting Circuit Breaker - DOE Contact T. V. George, (301) 903-4957; Utron, Inc. Contact Dr. F. Douglas Witherspoon, (703) 369-5552

Nitride-based Cold Cathodes for Minature and Rugged Electron Sources - DOE Contact Jerry Peters, (301) 903-5228; Ionwerks Contact Dr. J. Albert Schultz, (713) 522-9880

RF Pulse Compression Using a Diamond Switch - DOE Contact Jerry Peters, (301) 903-5228; Alameda Applied Sciences Corporation Contact Dr. Mahadevan Krishnan, (510) 483-4156

Development of a High Current Density Nb_3Sn Conductor With Ga and Mg Dopants for High Field Application - DOE Contact Jerry Peters, (301) 903-5228; Supercon, Inc. Contact Mrs. Elaine Tarkiainen, (508) 842-0174

A High Current Very Low Cost Nb_3SnTi Doped Conductor Utilizing A Novel Internal Tin Process, with Separate Stabilizing Elements Scalable To Modern Niobium Titanium Production Economics - DOE Contact Jerry Peters, (301) 903-5228; Supergenics Contact Mr. Bruce A. Zeitlin, (941) 349-0930

Automated Diamond Turning Lathe for the Production of Copper Accelerator Cells - DOE Contact Jerry Peters, (301) 903-5228; DAC Vision, Inc. Contact Mr. James W. Drain, (805) 684-8307

High Power Switch - DOE Contact Jerry Peters, (301) 903-5228; Diversified Technologies, Inc. Contact Mr. Micheal A. Kempkes, (781) 275-9444

Adiabatic Forming of Copper Accelerator Cells for the NLC - DOE Contact Jerry Peters, (301) 903-5228; LMC, Inc. Contact Mr. Lennart J. Lindell, (815) 758-3514

Pulse Capacitors for Next Generation Linear Colliders - DOE Contact Jerry Peters, (301) 903-5228; Nanomaterials Research Corporation Contact Ms. Molly M. W. Kostelecky, (303) 702-1672

Carbon-Carbon Composite Closeout Frames for Space Qualified, Stable High Thermal Conductivity Detector Support Structures - DOE Contact Michael P. Procario, (301) 903-2890; Hytec, Inc. Contact Mr. William O. Miller, (505) 661-0080

Low Cost Support Structures, With New Advanced Composite Materials Tailored For Ultra-Stable Particle Tracking Detectors - DOE Contact Michael P. Procario, (301) 903-2890; Hytec, Inc. Contact Mr. William O. Miller, (505) 662-0080

New Fullerene-Based Resistor Technology for Use in Low Noise Instrumentation - DOE Contact Gene Henry, (301) 903-6093; Cremat Contact Mr. Fred Olschner, (617) 926-0661

SQUID Susceptometers for Read Out of Magnetic Microcalorimeters - DOE Contact Gene Henry, (301) 903-6093; Hypres, Inc. Contact Dr. Elie Track, (914) 592-1190

Large Volume Detectors from New CdZnTe Growth Process - DOE Contact Gene Henry, (301) 903-6093; Radiation Monitoring Devices, Inc. Contact Dr. Gerald Entine, (617) 926-1167

Fabrication of Seamless Niobium Superconducting Accelerating Cavities Using Directed Light Fabrication - DOE Contact Gene Henry, (301) 903-6093; Advanced Energy Systems, Inc. Contact Mr. Anthony Favale, (516) 575-9345

Electromagnetically Forming a Seamless Niobium Radio Frequency (RF) Superconducting Cavity - DOE Contact Gene Henry, (301) 903-6093; Advanced Energy Systems, Inc. Contact Mr. Anthony Favale, (516) 575-9345

Development of High Power RF Windows for Next-Generation Superconducting and Normal Conducting Accelerators - DOE Contact Gene Henry, (301) 903-6093; Advanced Energy Systems, Inc. Contact Mr. Anthony Favale, (516) 575-9345

A 200-kW Average Power Microwave Window for L-Band Applications - DOE Contact Gene Henry, (301) 903-6093; AMAC International, Inc. Contact Dr. Quan-Sheng Shu, (757) 269-5641

Mercury Cadmium Telluride Detectors for Near Infrared Applications - DOE Contact Rick Petty, (301) 903-5548; Avyd Devices, Inc. Contact Dr. Honnavalli R. Vydyanath, (714) 751-8553

Development of III-Nitride UV Detectors - DOE Contact Rick Petty, (301) 903-5548; Avyd Devices, Inc. Contact Dr. Honnavalli R. Vydyanath, (714) 751-8553

Low Temperature, High Altitude Humidity Sensor - DOE Contact Rick Petty, (301) 903-5548; Nanomaterials Research Corporation Contact Ms. Molly M. W. Kostelecky, (303) 702-1672

Low Cost Optical Moisture Sensor for Weather Balloons - DOE Contact Rick Petty, (301) 903-5548; Southwest Sciences, Inc. Contact Dr. Alan C. Stanton, (505) 984-1322

A Diode Laser Sensor for High Precision Measurement of Terrestrial CO_2 Sources and Sinks - DOE Contact Roger Dahlman, (301) 903-4951; Physical Sciences, Inc. Contact Dr. Byron David Green, (978) 689-0003

Low-Cost, High Resolution and High-Sensitivity PET Detector Modules - DOE Contact Prem Srivastava, (301) 903-4071; Tomotronics, Inc. Contact Ms. Pamela H. Worstell, (508) 653-4051

A Generic Approach to Improved Semi-Solid Forming of Metals - DOE Contact Yok Chen, (301) 903-3428; Chesapeake Composites Corporation Contact Dr. Alexander Brown, (302) 324-9110

High-Strain-Rate Superplastic Forging of Aluminum Alloys - DOE Contact Yok Chen, (301) 903-3428; Materials Modification, Inc. Contact Dr. T.S. Sudarshan, (703) 560-1371

Semi-Solid Metal Freeform Fabrication - DOE Contact Yok Chen, (301) 903-3428; Semi-solid Technologies, Inc. Contact Dr. Stuart B. Brown, (508) 652-8518

Supersmooth Neutron Optical Surfaces by Gas Cluster Ion Beam Processing - DOE Contact Helen Kerch, (301) 903-2346; Epion Corporation Contact Dr. Allen Kirkpatrick, (781) 275-3703

Three Dimensional Si Imaging Array For Cold Neutrons - DOE Contact Helen Kerch, (301) 903-2346; Intraspec, Inc. Contact Mr. John Walter, (423) 483-1859

Solid-State Neutron Detection Materials - DOE Contact Helen Kerch, (301) 903-2346; Radiation Monitoring Devices, Inc. Contact Dr. Gerald Entine, (617) 926-1167

Fluorescence Chemical Sensor for Chemical Warfare - DOE Contact Carl Friesen, (208) 526-1765; Altair Center, LLC Contact Dr. Sergei Krivoshlykov, (508) 845-5349

Chemosensor Array for Detecting the Proliferation of Weapons of Mass Destruction - DOE Contact Carl Friesen, (208) 526-1765; Intelligent Optical Systems, Inc. Contact Mr. Robert Lieberman, (310) 530-7130

PHASE II (FIRST YEAR)

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

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

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

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

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

A Photocatalytic TiO_2 Anode and Membrane Reactor for the Enhanced Destruction of Chloro-Organic Compounds in Water - DOE Contact Kamalendu Das, (304) 285-4065; Ceramem Corporation Contact Dr. Robert Goldsmith, (781) 899-4495

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

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

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

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

PHASE II (SECOND YEAR)

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

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

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

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

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

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

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

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

PHASE I

Intercalated Phosphonate-Clay Composites as Latent Heat Storage Materials for Masonry - DOE Contact Terrence Logee, (202) 586-1689; Cape Cod Research, Inc. Contact Ms. Katherine D. Finnegan, (508) 540-4400

Fiber Reinforced Polymer Composite Building Panels Capable of Energy Storage Through High Enthalpy Solid-State Phase Transition - DOE Contact Terrence Logee, (202) 586-1689; Dpd, Inc. Contact Ms. Farangis Jamzadeh, (517) 349-5653

SunGuard: A Roofing Tile for Natural Cooling - DOE Contact Terrence Logee, (202) 586-1689; Powerlight Corporation Contact Mr. Thomas L. Dinwoodie, (510) 540-0550

Evaluation of Integrated Wall Systems Incorporating Electrochromic Windows - DOE Contact Terrence Logee, (202) 586-1689; Sage Electrochromics, Inc. Contact Mr. Kenneth Ney, (507) 333-0078

Development of a High Resolution X-Ray Imaging-Spectrometer - DOE Contact Charles Finfgeld, (301) 903-3423; Radiation Science, Inc. Contact Dr. Allen S. Krieger, (617) 621-7076

Enabling Materials for Magnetic Fusion Energy - DOE Contact Sam E. Berk, (301) 903-4171; Ultramet Contact Mr. Craig N. Ward, (818) 899-0236

Low Cost Dispersion Strengthened Ferritic Steels - DOE Contact Sam Berk, (301) 903-4963; Powdermet, Inc. Contact Mr. Andrew J. Sherman, (818) 768-6420

Hg-Ba-Ca-Cu-O HTS Current Leads for High Energy Physics Applications at High Magnetic Field and Temperature - DOE Contact Jerry Peters, (301) 903-5228; Eurus Technologies, Inc. Contact Mr. John A. Romans, (850) 574-1800

High Performance Nb_3Sn (Ta) Wires by Tin Enrichment and Increased Filament Content - DOE Contact Jerry Peters, (301) 903-5228; Superconducting Systems, Inc. Contact Ms. Minou Mossavat, (781) 642-6702

Microwave-Absorbing Materials for Accelerators in Cryogenic Environments - DOE Contact Gene Henry, (301) 903-6093; Ceradyne, Inc. Contact Mr. Howard George, (714) 549-0421

An Advanced Avalanche-Photodiode Based Spectroscopic Radiation Imager - DOE Contact Kamalendu Das, (304) 285-4065; Radiation Monitoring Devices, Inc. Contact Dr. Gerald Entine, (617) 926-1167

Novel Solid State Electochemical Sensor - DOE Contact Paul Bayer, (301) 903-5324; H.V. Setty Enterprises, Inc. Contact Dr. H.V. Venkatasetty, (612) 894-2792

PHASE II (SECOND YEAR)

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

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

PHASE I

Ion-Conducting Oxide Ceramic Materials for Solid-Oxide Fuel Cells Using Novel Low Cost Combustion Chemical Vapor Deposition - DOE Contact Udaya Rao, (412) 386-4743; Microcoating Technologies, Inc. Contact Mr. Jerome J. Schmitt, (770) 457-8400

Cathode-Supported Thin-Film Solid Oxide Cells with Low Operating Temperatures - DOE Contact Richard A. Johnson, (304) 285-4564; Nextech Materials, Ltd. Contact Mr. William J. Dawson, (614) 842-6608

Thermally Stable Catalysts for Methane Combustion - DOE Contact Richard A. Johnson, (304) 285-4564; Tda Research, Inc. Contact Mr. Michael E. Karpuk, (303) 940-2301

Improved Carbon Molecular Sieve Membranes for Oxygen-Nitrogen Separation - DOE Contact Udaya Rao, (412) 386-4743; Advanced Fuel Research, Inc. Contact Dr. Michael A. Serio, (860) 528-9806

Improved Precursors for Oxygen-Selective Membranes in Practical Devices for Methane Conversion - DOE Contact Udaya Rao, (412) 386-4743; Ceramem Corporation Contact Dr. Robert L. Goldsmith, (781) 899-4495

Supported Flat Plate Thin Films for Oxygen Separation - DOE Contact Udaya Rao, (412) 386-4743; Eltron Research, Inc. Contact Ms. Eileen E. Sammells, (303) 440-8008

Mixed-Conducting Oxide Ceramic Membranes for Oxygen Separation Using Novel Low Cost Combustion Chemical Vapor Deposition - DOE Contact Udaya Rao, (412) 386-4743; Microcoating Technologies, Inc. Contact Mr. Jerome J. Schmitt, (770) 457-8400

A New Radiation Resistant Epoxy Resin System for Liquid Impregnation Fabrication of Composite Insulation - DOE Contact Warren Marton, (301) 903-4958; Eltron Research, Inc. Contact Ms. Eileen E. Sammells, (303) 440-8008

Advanced Heat Sink Materials for Fusion Energy Devices - DOE Contact Sam E. Berk, (301) 903-4171; Plasma Processes, Inc. Contact Mr. Timothy McKechnie, (256) 851-7653

Robust Ceramic Coatings for Vanadium Alloys to Use in Lithium Cooled Fusion Systems - DOE Contact Sam Berk, (301) 903-4171; Composite Technology Development, Inc. Contact Dr. Naseem A. Munshi, (303) 664-0394

Hybrid 3-D SiC/C High Thermal Conductivity Composites - DOE Contact T. V. George, (301) 903-4957; Mer Corporation Contact Mr. R. O. Loutfy, (520) 574-1980

A Novel Process for the Fabrication of Advanced High Temperature Superconductors - DOE Contact Jerry Peters, (301) 903-5228; American Superconductor Corporation Contact Mr. Tom Rosa, (508) 836-4200

Co-Processed Ceramic Insulation for High Field Accelerator Magnets - DOE Contact Jerry Peters, (301) 903-5228; Composite Technology Development, Inc. Contact Dr. Naseem A. Munshi, (303) 664-0394

Improvement of High Field Performance and Reliability of Nb_3Sn Conductor by PIT Method - DOE Contact Jerry Peters, (301) 903-5228; Supercon, Inc. Contact Mrs. Elaine Tarkiainen, (508) 842-0174

Ultra Low Loss RF Window Materials - DOE Contact Jerry Peters, (301) 903-5228; Tpl, Inc. Contact Dr. William F. Hartman, (505) 342-4414

Ultra-Hard Diamond-Like Nanocomposite Coatings for Wear Applications - DOE Contact Yok Chen, (301) 903-3428; Advanced Refractory Technologies, Inc. Contact Dr. Roger Storm, (716) 875-4091

Application of the Combinatorial Synthesis and LHPG Techniques to the Development of New Scintillator Materials - DOE Contact Gene Henry, (301) 903-6093; Lasergenics Corporation Contact Dr. Richard Schlecht, (408) 363-9791

Ultra-hard Nanolayered Coatings for Wear-resistant Applications - DOE Contact Yok Chen, (301) 903-3428; Applied Thin Films, Inc. Contact Dr. Sankar Sambasivan, (847) 491-4619

Functionally Graded, Nanocrystalline, Multiphase, Boron-and-Carbon-Based Superhard Coatings - DOE Contact Yok Chen, (301) 903-3428; Spire Corporation Contact Mr. Ronald S. Scharlack, (781) 275-7470

Large Area Filtered Arc Deposition of Carbon and Boron Based Hard Coatings - DOE Contact Yok Chen, (301) 903-3428; Ues, Inc. Contact Mr. Francis F. Williams, Jr., (937) 426-6900

Ultrahard Nanostructured Diamond Thin Films Using Inductively Coupled Plasma - DOE Contact Yok Chen, (301) 903-3428; UHV Technologies, Inc. Contact Dr. Nalin Kumar, (609) 608-0311

High Current Density in Bi2223 Tape and Low AC Loss Wire - DOE Contact Yok Chen, (301) 903-3428; American Superconductor Corporation Contact Dr. Tom Rosa, (508) 836-4200

Low Cost Bi-2223 Conductors for HTS Transformers - DOE Contact Yok Chen, (301) 903-3428; American Superconductor Corporation Contact Dr. Tom Rosa, (508) 836-4200

Meter Length YBCO Coated Conductor Development - DOE Contact Yok Chen, (301) 903-3428; American Superconductor Corporation Contact Dr. Tom Rosa, (508) 836-4200

Non-Vacuum, Reel-to-Reel Processing of High-Temperature Superconducting Coated Conductors - DOE Contact Yok Chen, (301) 903-3428; Microcoating Technologies, Inc. Contact Mr. Jerome J. Schmitt, (770) 457-8400

Novel Catalyst for CH_4-CO Conversion - DOE Contact Amy Manheim, (202) 586-1507; Ceramem Corporation Contact Dr. Robert L. Goldsmith, (781) 899-4495

Hydrophobic Ionic Liquid Biphase Catalysis - DOE Contact Brian Valentine, (202) 586-1739; Covalent Associates, Inc. Contact Dr. K.M. Abraham, (781) 938-1140

SiC-Based Hydrogen Selective Membranes for Catalytic Membrane Reactor Applications - DOE Contact Charlie Russomanno, (202)586-7543; Media And Process Technology, Inc. Contact Dr. Paul K. T. Liu, (412) 826-3721

Novel Non-Flammable Electrolytes for Lithium Batteries - DOE Contact Susan Rogers, (202) 586-8997; Cape Cod Research, Inc. Contact Ms. Katherine D. Finnegan, (508) 540-4400

Flame Retardant Electrolytes for Li-Ion Batteries - DOE Contact Susan Rogers, (202) 586-8997; EIC Laboratories Contact Dr. A. C. Makrides, (781) 769-9450

Nonflammable Lithium-Ion Battery Electrolytes - DOE Contact Susan Rogers, (202) 586-8997; Techdrive, Inc. Contact Dr. Robert Filler, (630) 910-3729

PHASE II (FIRST YEAR)

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

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

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

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

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

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

An Improved Reaction-Bonded Silicon Carbide Process for SiC/SiC Composites - DOE Contact Sam Berk, (301) 903-4171; TDA Research, Inc. Contact Mr. John D. Wright, (303) 940-2300

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

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

PHASE II (SECOND YEAR)

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

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

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

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

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 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

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

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

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 Alkenes with Syngas - DOE Contact Donald Krastman, (412) 892-4720; TDA Research, Inc. Contact Mr. Michael E. Karpuk, (303) 940-2301

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

High Speed Long Wavelength Infrared Detector Array/Preamplifier Development - DOE Contact Carl Friesen, (208) 526-1765; Fermionics Corporation Contact Dr. Peter C.C. Wang, (805) 582-0155

Development of Cadmium Germanium Arsenide Crystals - DOE Contact Carl Friesen, (208) 526-1765; Inrad, Inc. Contact Mr. James L. Greco, (201) 767-1910

An Easily Dispersed Reactive Coating for Surface Decontamination - DOE Contact Carl Friesen, (208) 526-1765; Lynntech, Inc. Contact Dr. Oliver J. Murphy, (409) 693-0017

Rapid Quench Nb_3Al for High Field Accelerator Applications - DOE Contact Jerry Peters, (301) 903-5228; Plastronic, Inc. Contact 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

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

SMALL BUSINESS TECHNOLOGY TRANSFER RESEARCH PROGRAM

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

PHASE I

Thin-Film Fiber Optic Sensors for Power Control and Fault Detection - DOE Contact Alec Bulawka, (202) 586-5633; Airak Engineering, Inc. Contact Mr. Paul Grems Duncan, (540) 864-6580

Novel Carbon Monoxide Sensor for PEM Fuel Cell Systems - DOE Contact Jim Merritt, (202) 586-0903; Nextech Materials, Ltd. Contact Mr. William J. Dawson, (614) 292-4903

Electrochemical Sensors for Volatile Nitrogen Compounds in Air - DOE Contact Donald Krastman, (412) 386-4720; J and N Enterprises, Inc. Contact Mr. J. Scott Kleppe

Organic Diodes Using ISAM Polymers - DOE Contact Samuel Barish, (301) 903-2917; Luna Innovations, Inc. Contact Ms. Garnett Linkous, (540) 953-4274

Ink-Jet Printing for Fabrication of Full-Color Polymer LED Displays - DOE Contact Samuel Barish, (301) 903-2917; Uniax Corporation Contact Mr. Boo J. L. Nilsson, (805) 562-9293

PHASE II (FIRST YEAR)

High Energy and Power Ultracapacitors Utilizing Novel Type III Polymers and Non-Aqueous Electrolytes - DOE Contact Susan Rogers, (202) 586-8997; Covalent Associates, Inc. Contact Dr. K.M. Abraham, (781) 938-1140

PHASE II (SECOND YEAR)

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

Advanced Ceramic Hot Gas Filters - DOE Contact Theodore McMahon, (304) 285-4865; LoTec, Inc. Contact Mr Santosh Y. Limaye, (801) 483-3100

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

PHASE II (FIRST YEAR)

Boron Carbide Coatings for Enhanced Performance of Radio-Frequency Antennas in Magnetic Fusion Devices - DOE Contact T. V. George, (301) 903-4957; Hy-tech Research Corporation Contact Dr. Robert Hazelton, (540) 639-4019

PHASE II (SECOND YEAR)

New High-Performance GaSb-Based Thermophotovoltaic (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

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.

An element of the fusion energy program is the development and validation of the materials for fusion experiments and, in the longer-term, for fusion energy systems. For future fusion energy systems, the OFES Advanced Materials Program develops and validates structural materials 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, "low activation" structural 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).

Development and validation of non-structural materials is carried out in OFES programs for plasma-facing components, diagnostic and control systems, breeding of tritium fuel, and for superconducting magnets.

These materials R&D programs are conducted with a high degree of international cooperation. Bilateral agreements with Japan and the Russian Federation enhance the ability of each party to mount fission reactor irradiation experiments. The Fusion Materials Agreement under the International Energy Agency (IEA) serves as a useful venue for the exchange of information and the coordination of programs.

266. STRUCTURAL MATERIALS DEVELOPMENT

$720,000
DOE Contact: S. Berk, (301) 903-4171
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

267. MODELING IRRADIATION EFFECTS IN SOLIDS

$50,000
DOE Contact: S. Berk, (301) 903-4171
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. Multiscale modeling applies these results to evaluate the effects on properties of materials, especially the interactions of the irradiation produced defects with the flow dislocations during deformation processes.

Keywords: Modeling, Irradiation Effects

268. FUSION SYSTEMS MATERIALS

$3,679,000
DOE Contact: S. Berk, (301) 903-4171
ORNL Contacts: S. J. Zinkle, (865) 576-7220 and A. F. Rowcliffe, (865) 574-5057

This program is directed at the development and qualification of structural materials and insulating ceramics for use in components of fusion power systems exposed to the intense neutron flux. Candidate low activation structural material systems include ferritic/martensitic steels, vanadium alloys and SiC/SiC composites. Investigations focus on the most critical questions or limiting properties in each of these systems: ferritic/martensitic steels—DBTT transition shifts and fracture toughness; vanadium alloys—welding processes, effects of irradiation on fracture toughness, and compatibility in proposed coolant systems; SiC/SiC composites—definition of the effects of irradiation on properties and structure and evaluation of advanced composite fibers and coatings. The insulating ceramic activity is developing an understanding of irradiation effects in alumina, spinel and other materials. The greatest concern is to establish the permanent and transient changes in electrical properties, requiring measurement while the specimen is under irradiation. Work on these material classes involves irradiation in fission reactors, including HFIR and other test reactors, as partial simulation of the fusion environment.

Keywords: Ceramics, Steels, Vanadium, Silicon Carbide, Composites, Irradiation Effects, Electrical Properties

269. **STRUCTURAL MATERIALS FOR FUSION SYSTEMS**
$1,270,000
DOE Contact: S. Berk, (301) 903-4171
PNNL Contacts: R. J. Kurtz, (509) 373-7515

The goal of this program is to develop an understanding of radiation effects that provides a basis for development of irradiation-insensitive materials. The objective is low activation materials for use as structures in divertor, first wall, and blanket components of fusion systems. Irradiation in fission reactors is used to simulate fusion conditions, with measurement of physical and mechanical properties used to track irradiation effects. A modeling activity complements the experimental measurements. The ultimate goal is optimized ferritic steels, vanadium alloys, and SiC/SiC composite materials for fusion power plant use.

Keywords: Steels, Vanadium, Silicon Carbide, Composites, Irradiation Effects, Modeling

270. **DEVELOPMENT OF RADIATION-HARDENED CERAMIC COMPOSITES FOR FUSION APPLICATIONS**
$94,000 (Two year funding provided to cover FY 1999 and 2000)
DOE Contact: S. Berk, (301) 903-4171
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

271. **MECHANISMS OF PLASTIC AND FRACTURE INSTABILITY FOR ALLOY DEVELOPMENT OF FUSION MATERIALS**
$285,000 (Two year funding provided to cover FY 1999 and 2000)
DOE Contact: S. Berk, (301) 903-4171
UCLA Contact: N. M. Ghoniem, (310) 825-4866

This research is focused on increasing the understanding of plastic instabilities and fracture processes in materials irradiated under projected fusion conditions. The effects of the many materials, irradiation, and mechanical loading parameters on the flow and fracture processes, especially embrittlement processes, will be evaluated and modeled to establish understanding of controlling mechanisms. Techniques in use include atomistic computer simulation, atomic cluster modeling, 3-D dislocation dynamics, and analysis using flow and fracture models. The goal is to develop the understanding needed to establish models and methods to extrapolate from the available data base to predict the behavior of structural components in future operating fusion power systems.

Keywords: Irradiation Effects, Fracture, Mechanical Properties, Modeling

272. **DAMAGE ANALYSIS AND FUNDAMENTAL STUDIES FOR FUSION REACTOR MATERIALS DEVELOPMENT**
$502,000 (Two year funding provided to cover FY 1999 and 2000)
DOE Contact: S. Berk, (301) 903-4171
UCSB Contacts: G. R. Odette, (805) 893-3525 and G. E. Lucas, (805) 893-4069

This research is directed at developing a fundamental understanding of both the basic damage process and microstructural evolution that take place in a material during neutron irradiation. This understanding is used with empirical data to develop physically-based models of irradiation effects. The focus is on the fracture properties of vanadium alloys and ferritic stainless steels, including helium effects, to: (a) develop an integrated approach to integrity assessment, (b) develop advanced methods of measuring fracture properties, and (c) analyze the degradation of the mechanical properties of steels. The program also contributes to the assessment of the feasibility of using these alloys in fusion systems.

Keywords: Vanadium, Steels, Irradiation Effects Fracture

273. **MATERIALS DEVELOPMENT FOR PLASMA FACING COMPONENTS**
$2,800,000
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, development of joining techniques for refractory metals (e.g., W, Mo, Nb, V) for plasma facing components, development of enhancement schemes for helium cooling or liquid lithium cooling of refractory alloys, determination of erosion rates of liquid lithium, tin-lithium alloy and Li_2BeF_4 under normal and disruption conditions, heat removal capability testing of liquid surfaces, and thermal fatigue testing of tungsten and other refractory materials. The joining techniques being investigated include diffusion bonding, hot-isostatic pressing, furnace brazing and inertial welding. Tritium retention and permeation measurements are being conducted on the Tritium Plasma Experiment. The refractory material work is centered on developing high temperature helium gas cooled or liquid metal cooled heat sinks for plasma facing components. The liquid surface work is focused on development of free surface flows and the heat removal capability of the designs. The erosion rates are measured on both plasma simulators and tokamaks. The thermal fatigue testing and heat removal capability measurements are carried out on electron beam test systems.

Keywords: Plasma-Facing Components, Lithium, Tungsten, Refractory Metals, Joining, Erosion, Thermal Fatigue, Flibe

274. **STRUCTURAL MATERIALS DEVELOPMENT FOR THE CONDUIT OF ITER CABLE-IN-CONDUIT-CONDUCTORS**
$100,000
DOE Contact: W. A. Marton, (301) 903-3068
MIT Contact: J. Minervini, (617) 253-5503

The conduit material selected for cable-in-conduit-conductors is the high strength superalloy Incoloy Alloy 908, developed via collaboration between INCO Alloys International (IAI) and MIT. During the year, work was started on development of an improved, modified Alloy 908 with increased resistance to Stress Accelerated Grain Boundary Oxidation (SAGBO). The principal goal is to reduce SAGBO sensitivity in order to reduce coil fabrication cost and risk. A review of the causes of SAGBO has been performed, and based on these results new designs for alloy modifications have been produced.

Keywords: Conduit, Incoloy, Magnet Materials

275. **DEVELOPMENT AND TESTING OF INSULATING COATINGS**
$310,000
DOE Contact: S. Berk, (301) 903-4171
ANL Contact: D. L. Smith (630) 252-4837

This program is directed at the development of coatings and coating technologies that can be used in elevated temperature flowing lithium blanket breeder/coolant circuits. The planned sequence of work is to identify promising candidate ceramics, develop the coating technology, and conduct the lithium exposure experiments to demonstrate stability and self-repair needed for fusion power system operation.

Keywords: Ceramics, Insulators, Coatings

276. **IDENTIFICATION AND EVALUATION OF INSULATING COATINGS**
$70,000
DOE Contact: S. Berk, (301) 903-4171
ORNL Contact: S. J. Zinkle, (865) 576-7220

This new program will initially focus on the stability of candidate ceramic insulators during long term, elevated temperature exposure to static lithium. The first experiments will use high purity, bulk ceramic samples, to provide a base line to be used in later tests of deposited coatings.

Keywords: Ceramics, Insulators

OFFICE OF ENVIRONMENTAL MANAGEMENT

	FY 1999
Office of Environmental Management - Grand Total	$8,708,996
Materials Properties, Behavior, Characterization or Testing	$8,708,996
The Influence of Radiation and Multivalent Cation Additions on Phase Separation and Crystallization of Glass	241,000
Chemical and Ceramic Methods Toward Safe Storage of Actinides Using Monazite	429,000
Atmospheric-Pressure Plasma Cleaning of Contaminated Surfaces	404,000
Chemical Decomposition of High-Level Nuclear Waste Storage/Disposal Glasses Under Irradiation	163,000
Analysis of Surface Leaching Processes in Vitrified High-Level Nuclear Wastes Using In-Situ Raman Imaging and Atomistic Modeling	186,333
Investigation of Microscopic Radiation Damage in Waste Forms Using ODNMR and AEM Techniques	232,667
In-Situ Spectro-Electrochemical Studies of Radionuclide Contaminated Surface Films on Metals and the Mechanism of Their Formation and Dissolution	335,000
Determination of Transmutation Effects in Crystalline Waste Forms	304,328
Radiation Effects on Materials in the Near-Field of Nuclear Waste Respository	136,000
An Alternative Host Matrix Based on Iron Phosphate Glasses for the Vitrification of Specialized Nuclear Waste Forms	208,278
Microstructural Properties of High Level Waste Concentrates and Gels with Raman and Infrared Spectroscopies	155,000
Fundamental Thermodynamics of Actinide-Bearing Mineral Waste Forms	383,333
Optimization of Thermochemical, Kinetic, and Electrochemical Factors Governing Partitioning of Radionuclides During Melt Decontamination of Radioactively Contaminated Stainless Steel	400,000
Mechanism of Pitting Corrosion Prevention by Nitrite in Carbon Steel Exposed to Dilute Salt Solutions	216,667
Stability of High-Level Waste Forms	254,000
Radiation Effects in Nuclear Waste Materials	960,000
New Silicotitanate Waste Forms: Development and Characterization	400,000
Distribution & Solubility of Radionuclides & Neutron Absorbers in Waste Forms for Disposition of Plutonium Ash & Scraps, Excess Plutonium, and miscellaneous Spent Nuclear Fuels	600,000
Modeling of Diffusion of Plutonium in Other Metals and of Gaseous Species in Plutonium-Based Systems	145,000
Radionuclides Immobilization in the Phases Formed by Corrosion of Spent Nuclear Fuel: The Long-Term Assessment	160,321
Direct Investigations of the Immobilized of Radionuclides in the Alteration Phases of Spent Nuclear Fuel	260,829
Decontamination of Radionuclides from Concrete During and After Thermal Treatment	271,907
Mechanisms of Radionuclide-Hydroxycarboxylic Acid Interactions for Decontamination of Metallic Surfaces	383,333
Physical, Chemical and Structural Evolutioon of Zeolite-Containing Waste Forms Produced from Metakaolinite and Calcined HLW	170,000
Mechanisms and Kinetics of Organic Aging in High-Level Nuclear Wastes	300,000
Modeling of Spinel Settling in Waste Glass Melter	291,667
Photooxidation of Organic Waste Using Semiconductor Nanoclusters	417,000
Ion-exchange Processes and Mechanisms in Glasses	300,333

OFFICE OF ENVIRONMENTAL MANAGEMENT

The Office of Environmental Management (EM) was established to effectively coordinate and manage the Department's activities to remediate the DOE Defense Complex and to properly manage waste generated by current operations. EM conducts materials research within two offices:

Office of Waste Management - The Office of Waste Management uses current technologies to minimize production of DOE-generated waste, alter current processes to reduce waste generation, and work with the Office of Science and Technology to develop innovative technologies for the treatment and disposal of present and future waste streams. The mission of the Office is to minimize, treat, store, and dispose of DOE waste to protect human health, safety, and the environment.

Office of Science and Technology - The Office of Science and Technology (OST) is responsible for managing and directing targeted basic research and focused, solution-oriented technology development programs to support the DOE Office of Environmental Management (EM). Programs involve research, development, demonstration, and deployment activities that are designed to produce innovative technologies and technology systems to meet national needs for regulatory compliance, lower life-cycle costs, and reduced risks to both people and the environment. Certain areas of the OST program focus on materials research in order to provide better, safer and less expensive approaches to identify, characterize and remediate DOE's waste problem.

Four Focus Areas have been formed to focus the EM-wide technology development activities on DOE's most pressing environmental management problems and are co-led by all EM offices:

Subsurface Contaminants. Hazardous and radioactive contaminants in soil and groundwater exist throughout the DOE complex, including radionuclides, heavy metals, and dense, nonaqueous phase liquids. Groundwater plumes have contaminated over 600 billion gallons of water and 50 million cubic meters of soil. In addition, the Subsurface Contaminants Focus Area is responsible for supplying technologies for the remediation of numerous landfills at DOE facilities. Technology developed within this speciality area provides effective methods to contain contaminant plumes and new or alternative technologies for remediating contaminated soils and groundwater.

Radioactive Tank Waste Remediation. Across the DOE Complex, hundreds of large storage tanks contain hundreds of thousands of cubic meters of high-level mixed waste. Primary areas of concern are deteriorating tank structures and consequent leakage of their contents. Research and technology development activities must focus on the development of safe, reliable, cost-effective methods of characterization, retrieval, treatment, and final disposal of the wastes.

Mixed Waste Characterization, Treatment, and Disposal. DOE faces major technical challenges in the management of low-level radioactive mixed waste. Several conflicting regulations together with a lack of definitive mixed waste *treatment standards hamper mixed waste treatment and disposal. Disposal capacity for mixed waste is also expensive* and severely limited. DOE now spends millions of dollars annually to store mixed waste because of the lack of accepted treatment technology and disposal capacity. In addition, currently available waste management practices require extensive, and hence costly waste characterization before disposal. Therefore, DOE must pursue technology that leads to better and less expensive characterization, retrieval, handling, treatment, and disposal of mixed waste.

Decontamination and Decommissioning. The aging of DOE's weapons facilities, along with the reduction in nuclear weapons production, has resulted in a need to transition, decommission, deactivate, and dispose of numerous facilities contaminated with radionuclides and hazardous materials. While building and scrap materials at the sites are a potential resource, with a significant economic value, current regulations lack clear release standards. This indirectly discourages the recovery, recycling, and/or reuse of these resources. The development of enhanced technologies for the decontamination of these materials, and effective communication of the low relative risks involved, will facilitate the recovery, recycle, and/or reuse of these resources. Improved materials removal, handling, and processing technologies will enhance worker safety and reduce cost.

The projects listed in this report are managed under the Environmental Management Research Program (EMSP). Basic research under the EMSP contributes to environmental management activities that decrease risk to the public and workers, provide opportunities for major cost reductions, reduce time required to achieve EM's mission goals, and, in general, address problems that are considered intractable without new knowledge. This program is designed to inspire breakthroughs in areas critical to the EM mission through basic research and is managed in partnership with ER. ER's well-established procedures are used for merit review of applications to the EMSP. Subsequent to the formal scientific merit review, applications that are judged scientifically meritorious are evaluated by DOE for relevance to the objectives of the EMSP. The current EMSP portfolio consists of 202 awards amounting to a total of $160 million in three-year funding. Twenty-eight of those awards were in scientific disciplines related to materials issues that have potential to solve Environmental Management challenges. The FY 1999 component of materials research is estimated to amount to $8,708,996. 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

277. THE INFLUENCE OF RADIATION AND MULTIVALENT CATION ADDITIONS ON PHASE SEPARATION AND CRYSTALLIZATION OF GLASS

$241,000
DOE Contact: Arnold Gritzke, (202) 586-3957
University of Arizona Contact:
Michael C. Weinberg, (520) 621-6909

Recent reviews which have dealt with critical issues regarding the suitability of glasses for nuclear waste disposal have identified liquid-liquid immiscibility and crystallization processes as having the potential to alter significantly storage behavior, especially chemical corrosion characteristics. These phase transformation processes can be abetted (or deterred) by radiation or the inclusion of small quantities of other components such as transition metals, rare earths, actinides, etc. Consequently, in order to minimize the chances for the occurrence of deleterious phase separation or crystallization, it is essential to examine the influence of these factors on phase transformation kinetics.

The major goal of this program is to study the influence of irradiation and multivalent cations and redox conditions upon the thermodynamics and kinetics of phase separation and crystallization in selected glass compositions. Any observed changes in transformation behavior will be related to structural modifications caused by radiation. Finally, guidelines will be developed to mitigate the deleterious effects of phase separation and crystallization by composition adjustments, based on the development of a database from ongoing and existing measurements and the development of appropriate models.

The characteristics of phase separation are being analyzed, experimentally, using SEM, EDS, HSEM, TEM, and SAXS. Crystallization is being studied using XRD, SEM, TEM, and optical microscopy. Structural changes are being examined using IR and Raman Spectroscopies and solid state NMR measurements.

Keywords: Radiation, Phase Separation, Crystallization, Glasses

278. CHEMICAL AND CERAMIC METHODS TOWARD SAFE STORAGE OF ACTINIDES USING MONAZITE

$429,000
DOE Contact: Arnold Gritzke, (202) 586-3957
Rockwell International Corporation Contact:
P.E.D. Morgan, (805) 373-4273
ORNL Contact: Lynn A. Boatner, (423) 574-5492

The program is investigating monazite ceramics for safe, secure, geologically tested, very long term, containment for actinides. The main outstanding fundamental research issues facing the use of monazite as a waste form necessitate the development of fundamental understanding of: sintering mechanisms involved in forming high density monazite ceramics; physical and chemical properties of grain boundaries in these ceramics; interactions with impurities and additives used to promote densification; physical properties of polycrystalline monazite ceramics; and the precipitation of monazite phases in an efficient, simple and economical manner. This program is addressing these issues to serve as a knowledge base for using monazite as a nuclear waste form.

Keywords: Monazite, Waste Form, Sintering, Densification

279. ATMOSPHERIC-PRESSURE PLASMA CLEANING OF CONTAMINATED SURFACES

$404,000
DOE Contact: Arnold Gritzke, (202) 586-3957
University of California at Los Angeles Contact:
Robert F. Hicks, (310) 206-6865
LANL Contact: Gary Selwyn, (505) 667-7824

Decommissioning of transuranic waste (TRU) into low-level radioactive waste (LLW) represents the largest cleanup cost associated with the nuclear weapons complex. This project is developing a low-cost technology for converting TRU into LLW based on the selective plasma etching of plutonium and other actinides from contaminated structures. Plasma etching has already been used to remove Pu films from materials. However, this process is operated under vacuum, making it both expensive and difficult to apply to many nuclear wastes. A major breakthrough in this field was the demonstration of the operation of a g-mode, resonant-cavity, atmospheric-pressure plasma jet (APPJ). This jet etches kapton at between 10 and 15 m/hour, and tantalum at between 1 and 2 m/hour. Etching occurs below 373 K, so that delicate materials will not be destroyed by this process. The plasma jet may be used to selectively remove plutonium and other actinide elements by converting them into volatile compounds that are trapped by adsorption and filtration. Since the jet operates outside a chamber, many nuclear wastes may be treated, including machinery, duct-work, concrete and other building materials. At LANL, the source physics is being studied using Stark-broadening, microwave interferometry, and laser-induced fluorescence (LIF). The metastables, neutrals and radical species produced with mixtures of NF3, CF4, C2F6, O2,He and Ar are being identified by LIF, optical emission spectroscopy (OES), laser Raman spectroscopy (LRS), coherent anti-Stokes Raman spectroscopy (CARS), and mass spectroscopy (MS). At UCLA, the elementary surface reactions of these species with tantalum and tungsten (surrogate metals for Pu) are being studied in ultrahigh vacuum using a supersonic molecular-beam coupled to the plasma jet. The surfaces are being characterized by X-ray photoemission (XPS), infrared spectroscopy (IR), low-energy electron diffraction (LEED), and scanning-tunneling microscopy (STM). In addition, plutonium etching experiments are being carried out at the Los Alamos Plutonium Facility.

Keywords: Plasma Etching, Plutonium

280. **CHEMICAL DECOMPOSITION OF HIGH-LEVEL NUCLEAR WASTE STORAGE/DISPOSAL GLASSES UNDER IRRADIATION**
$163,000
DOE Contact: Arnold Gritzke, (202) 586-3957
Naval Research Laboratory Contact:
David L. Griscom, (202) 404-7087

This project is addressing potential hazards of radiation-induced gas phase formation in borosilicate glasses intended for vitrification of high-level nuclear waste. The present research effort is designed to: (1) demonstrate unambiguously the nature(s) of any radiation-induced gas phases which may be dissolved in high-level-nuclear-waste-glass forms and lead to bubble formation; (2) provide fundamental knowledge necessary to assess the vulnerability of these forms to chemical explosion, particularly if dissolved oxygen is verified; and (3) develop an efficient method of surveying wide ranges of potential waste glass compositions to determine the dependence of radiolytic oxygen evolution on glass composition and hence determine compositions with superior resistance to decomposition.

Keywords: Borosilicate Glass, Gas Phases, High Level Waste

281. **ANALYSIS OF SURFACE LEACHING PROCESSES IN VITRIFIED HIGH-LEVEL NUCLEAR WASTES USING IN-SITU RAMAN IMAGING AND ATOMISTIC MODELING**
$186,333
DOE Contact: Arnold Gritzke, (202) 586-3957
University of Florida Contact: Joseph H. Simmons, (352) 392-6679

This research combines a novel investigative technique with novel modeling studies to analyze leaching processes in glasses. Its utility is that it will provide both a means of conducting fundamental studies of the corrosion behavior of high valence and multivalent ions in the waste glass as well as a proven in-situ method for monitoring the chemical corrosion behavior of radioactive waste glasses, remotely and in burial sites. The research has three major thrusts: (1) the development of in-situ Raman Imaging Spectroscopy for a detailed examination of leaching processes and associated structural changes and mineral precipitates on the surface of borosilicate glasses loaded with simulated high-level nuclear wastes, (2) the application of this method to the analysis of transition states and their energetics during surface leaching by novel modeling studies, and by comparison with existing methods of IR, Auger XPS and SIMS spectroscopy, SEM, TEM and STM/AFM microscopy and BET surface analysis; and (3) the extension of in-situ Raman Imaging Spectroscopy for conducting remote tests on radioactive loaded samples, and for the examination of variations over the surface of large ingots. The research comprises fundamental studies of (1) the relationship between leaching processes and Raman spectroscopy, using both tests on simple liquids and quantum mechanical modeling; and (2) the examination of transition states in hydration processes involving the higher valence and multivalent ions and their use in predicting, with high accuracy, their solubility in aqueous solutions using both experimental and quantum mechanical modeling methods. The combination of these two studies has the potential to offer a novel method which has both in-situ and remote capabilities for the analysis of leaching processes on high-level radioactive waste glasses. This method makes possible tests on radioactive materials with greatly reduced personnel exposure, and makes possible the examination of leaching processes in real-time in burial sites. Finally, this method can be applied to the continuous monitoring of the conditions of glass boules during actual disposal conditions.

Keywords: High Level Waste, Leaching, Glass

282. **INVESTIGATION OF MICROSCOPIC RADIATION DAMAGE IN WASTE FORMS USING ODNMR AND AEM TECHNIQUES**
$232,667
DOE Contact: Arnold Gritzke, (202) 586-3957
Argonne National Laboratory Contact: Guokui Liu, (630) 252-4630

This project investigates the microscopic effects of radiation damage in crystalline and glass high level waste forms (HLW). Information about the nature of electronic interaction and the chemical bonding properties of radionuclides in damaged phases is being developed. Connections between the consequences of alpha and beta-decay processes and radionuclide release and chemical decomposition in waste forms are being established. Detailed studies focus on the microscopic effects of alpha-decay of the transuranic isotopes 238,239Pu, 241,243Am, and 243,244Cm and the beta- and alpha-decay of 249Bk(249Cf) doped into crystalline materials 10 to 30 years ago and currently prepared borosilicate glasses. Electronic and chemical binding properties and local structural changes of parent radionuclide species and their decay daughters in the radiation damaged regions of the waste forms are being probed using nonlinear laser spectroscopic techniques, such as optically detected nuclear magnetic resonance (ODNMR), in concert with analytical electron microscopy (AEM) imaging and analysis and X-ray diffraction methods. Experimental information obtained using various techniques for the same materials is being compared and systematic measurements are being made after the samples undergo a series of annealing tests. Theoretical models based on electronic and nuclear interactions of the actinides and their surrounding ligands are being developed to interpret the experimental results and correlate the microscopic effects of radiation damage to the macroscopic mechanical and chemical properties of the HLW materials.

Keywords: High Level Waste, Radiation Damage

283. **IN-SITU SPECTRO-ELECTROCHEMICAL STUDIES OF RADIONUCLIDE CONTAMINATED SURFACE FILMS ON METALS AND THE MECHANISM OF THEIR FORMATION AND DISSOLUTION**
$335,000
DOE Contact: Arnold Gritzke, (202) 586-3957
Argonne National Laboratory Contact: Carlos A. Melendres, (630) 252-4346,
Northern Illinois University Contact: S. M. Mini, (815) 753-6484

The aim of this research is to gain a fundamental understanding of the structure, composition, and mechanism of formation of radionuclide-containing surface films on metals that are relevant to the problem of decontamination of piping systems and waste storage tanks at DOE nuclear facilities. This project seeks to expand our knowledge, while obtaining useful practical information, through the conduct of a systematic research activity that utilizes the unique facilities at Argonne National Laboratory, e.g., the Advanced Photon Source (APS) for X-ray absorption spectroscopy (XAS), as well as specialized laboratory facilities and instrumentation for carrying out experiments with radioactive materials. Formal collaboration with a university assures that a strong basic approach is taken in the analyses and methodologies used to achieve the desired goals.

The research consists of electrochemical studies of the corrosion and passivation behavior of iron, nickel, chromium, and stainless steel over a wide pH range and as a function of temperature from 25 to 95°C. The energetics and dynamics of film formation and dissolution and the effect of incorporation of heavy metal ions and radioactive elements are being investigated. Synchrotron X-ray absorption and vibrational (infrared and Raman) spectroscopic techniques are being used to define *in-situ* the structure and composition of the various oxide phases that are formed as a function of temperature.

Keywords: Surface Films, Metals, Piping, Waste Tanks

284. **DETERMINATION OF TRANSMUTATION EFFECTS IN CRYSTALLINE WASTE FORMS**
$304,328
DOE Contact: Arnold Gritzke, (202) 586-3957
Argonne National Laboratory Contact: Jeff Fortner, (630) 252-4479
PNNL Contact: Nancy J. Hess, (509) 375-2142

The objective of this study is to characterize the effects of transmutation in a candidate waste form for 137Cs by investigating samples of a cesium aluminosilicate mineral, pollucite, that have undergone "natural" decay of the Cs under ambient temperature while isolated from interfering chemical effects. There currently is no information on β-decay transmutation effects in waste forms in which transmutation has occurred over the natural decay time of the decaying isotope. This causes large uncertainty as to the effect of the transmutation on the physical and chemical properties of the waste form. As a result, uncertainties arise about the viability of the waste form as a long-term storage media for nuclear waste. Information on the effects of transmutation from β-decay will give support to the selection of alternate waste forms for separated 137Cs and give information on the long-term behavior of candidate waste forms.

The approach is to nondestructively examine small stainless steel capsules containing pure pollucite. The contents of these capsules will be examined with XANES, XAFS, and small angle anomalous X-rays. The synchrotron facilities at Stanford and ANL will be utilized. The scientific team is comprised of members from PNNL, ANL, and LANL.

Keywords: Transmutation, Crystalline Waste Forms, Synchrotron Radiation Facilities

285. **RADIATION EFFECTS ON MATERIALS IN THE NEAR-FIELD OF NUCLEAR WASTE REPOSITORY**
$136,000
DOE Contact: Arnold Gritzke, (202) 586-3957
University of Michigan Contacts: Lu-Min Wang, (313) 647-8530 and Rodney C. Ewing, (313) 647-8529

Successful, demonstrated containment of radionuclides in the near-field can greatly reduce the complexity of the performance assessment analysis of a geologic repository. The chemical durability of the waste form, the corrosion rate of the canister, and the physical and chemical integrity of the back-fill provide important barriers to the release of radionuclides. However, near-field containment of radionuclides depends critically on the behavior of these materials in a radiation field.

A systematic study is being performed of elastic and inelastic damage effects in materials in the near-field. These include: (1) waste forms (glass and crystalline ceramics); (2) alteration products of waste forms (clays and zeolites); (3) back-fill materials (clays and zeolites). The work draws on over twenty years of experience in studying radiation effects in minerals and complex ceramics and utilizes an unusual combination of studies of natural phases of great age with ion beam and electron irradiations of synthetic phases under carefully controlled conditions.

Keywords: Radiation Effects, Near-field, Geologic Repository

286. **AN ALTERNATIVE HOST MATRIX BASED ON IRON PHOSPHATE GLASSES FOR THE VITRIFICATION OF SPECIALIZED NUCLEAR WASTE FORMS**
$208,278
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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 pretreatment 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

287. **MICROSTRUCTURAL PROPERTIES OF HIGH LEVEL WASTE CONCENTRATES AND GELS WITH RAMAN AND INFRARED SPECTROSCOPIES**
$155,000
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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

288. **FUNDAMENTAL THERMODYNAMICS OF ACTINIDE-BEARING MINERAL WASTE FORMS**
$383,333
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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

289. **OPTIMIZATION OF THERMOCHEMICAL, KINETIC, AND ELECTROCHEMICAL FACTORS GOVERNING PARTITIONING OF RADIONUCLIDES DURING MELT DECONTAMINATION OF RADIOACTIVELY CONTAMINATED STAINLESS STEEL**
$400,000
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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

290. **MECHANISM OF PITTING CORROSION PREVENTION BY NITRITE IN CARBON STEEL EXPOSED TO DILUTE SALT SOLUTIONS**
$216,667
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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

291. **STABILITY OF HIGH-LEVEL WASTE FORMS**
$254,000
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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

292. **RADIATION EFFECTS IN NUCLEAR WASTE MATERIALS**
$960,000
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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

293. **NEW SILICOTITANATE WASTE FORMS: DEVELOPMENT AND CHARACTERIZATION**
$400,000
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This program outlines a new strategy for disposing of crystalline silicotitanate (CST) ion exchangers by *in situ* heat treatment to produce an alternate waste form. New waste forms and disposal strategies specific to CST secondary waste that are developed in this work will offer an alternative to current disposal plans which call for recombining the separated Cs, Sr-loaded CST into the high activity waste streams then dissolving it in borosilicate glass. This research is predicated by work at Pacific Northwest National Laboratory that shows that thermally treated CSTs have durabilities better than borosilicate glass. The goal of the program is to reduce the costs associated with CST waste disposal, to minimize the risk of contamination to the environment during CST processing, and to provide DOE with technical alternatives for CST disposal. Because there is uncertainty in repository availability and in waste acceptance criteria, it is likely that Cs and Sr loaded ion exchangers will require short term storage at Hanford or that new scenarios for long term storage or disposal of nuclides with relatively short half lives (such as 137Cs and 90Sr) will arise.

This research synthetically explores both low and high temperature stable and metastable phases involving the key component elements. This allows for characterization of all potential by-products from thermal treatment of CSTs. The technical objective of the work is to (1) fully characterize the phase relationships, structures and thermodynamic and kinetic stabilities of crystalline silocotitanate 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

294. **DISTRIBUTION & SOLUBILITY OF RADIONUCLIDES & NEUTRON ABSORBERS IN WASTE FORMS FOR DISPOSITION OF PLUTONIUM ASH & SCRAPS, EXCESS PLUTONIUM, AND MISCELLANEOUS SPENT NUCLEAR FUELS**
$600,000
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The objective of this multi-institutional, multi-national research effort is to understand the distributions, solubilities, and releases of radionuclides and neutron absorbers in waste forms. The results will provide the underpinning knowledge for developing, evaluating, selecting, and matching waste forms for the safe disposal of various wastes associated with Pu, miscellaneous spent nuclear fuels (SNF), and other transuranic (TRU) wastes and for developing deterministic model for the long-term performance assessment of radionuclide containment.

The scope of this project includes: (1) systematically investigate the solubility and partition behavior of selected waste forms as a function of composition, temperature, and processing conditions with the goal of enhancing our understanding of the physics and chemistry of radionuclides and neutron absorbers in simplified waste forms; (2) determine the local structure of radionuclides and neutron absorbers waste forms in various phases: (a) develop a microscale characterization to determine what phases are presented and how key elements are partitioned among those phases using optical, scanning, and transmission microscopies and XRD; (b) develop a molecular level characterization to understand local coordination using EXAFS and NMR; (c) perform an atomic level characterization to determine oxidation state using XANES; (3) selectively study waste form properties with the emphasis on the release behaviors of neutron absorbers and radionuclides.

Keywords: Radionuclides, Neutron Absorbers, Solubility, Waste Form

295. MODELING OF DIFFUSION OF PLUTONIUM IN OTHER METALS AND OF GASEOUS SPECIES IN PLUTONIUM-BASED SYSTEMS
$145,000
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The research is aimed at developing and utilizing computational-modeling-based methodology to treat two major problems. The first of these is to be able to predict the diffusion of plutonium from the surface into the interior of another metal such as uranium or stainless steel (fcc iron). The second is the more complicated situation of treating the diffusion of a gaseous species into plutonium-containing oxidized material, specifically the solid-state diffusion of O_2-driven by an oxygen gradient. The first class of problem, diffusion of plutonium into host metals, is pertinent to characterizing contamination and consequent clean-up procedures in situations where plutonium has been in contact with other metals for extended periods of time. The second situation is pertinent to complicated hydrogen generation mechanisms creating possibly catastrophic pressure in situations, such as storage barrels, where oxidized plutonium-containing material has been stored for long periods of time.

The investigation of thermally-activated diffusion makes use of transition state theory with dynamic corrections. In transition state theory the number of crossings of a specified counting surface that separates initial and final states is equated to the number of such crossings that occur in an equilibrium system. The use of ab-initio-based atomistic potentials allows efficient mapping of the pertinent energy barriers. Molecular dynamics can be used to treat realistically the nature of the hoppings as well as to correct for dynamical effects such as recrossings. Grain boundaries are simulated and incorporated into dynamic simulations to study the relative importance of grain boundary diffusion in allowing plutonium atoms to penetrate into the interior of the host metals.

The two main components of the modeling study are: (1) the treatment of diffusion and of the pertinent grain boundary modeling and (2) the development of physically accurate plutonium atomistic potentials. The physical quality of these potentials is the controlling quantity in determining the ability to be accurately predictive for the questions of interest.

Keywords: Diffusion, Plutonium, Modeling and Simulations

296. RADIONUCLIDE IMMOBILIZATION IN THE PHASES FORMED BY CORROSION OF SPENT NUCLEAR FUEL: THE LONG-TERM ASSESSMENT
$160,321
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The UO_2 in spent nuclear fuel is not stable under oxidizing conditions. Under oxidizing conditions, the U(IV) has a strong tendency to exist as U(VI) in the uranyl molecule, UO_2^{2+}. The uranyl ions react with a wide variety of inorganic and organic anions to form complexes which are often highly soluble. The result is rather rapid dissolution of UO_2 and the formation of a wide variety of uranyl oxide hydrates, uranyl silicates and uranyl phosphates. The reaction rates for this transformation are rapid, essentially instantaneous on geologic time scales. Over the long term, and depending on the extent to which these phases can incorporate fission products and actinides, these alteration phases become the near-field source term.

Fortunately, previous investigations (experimental studies and field studies) have established that natural uraninites and their alteration products can be used as natural analogues to study the corrosion of UO_2 in spent nuclear fuel. This research program is addressing the following issues:

1. What are the long-term corrosion products of natural UO_2+x, uraninite, under oxidizing conditions?

2. What is the paragenesis or the reaction path of the phases that form during alteration? How is the paragenetic sequence formation related to the structures and compositions of these uranyl phases?

3. What is the trace element content (as compared to the original UO_2+x), and does the trace element content substantiate models developed to predict fission product and actinide incorporation into these phases?

4. Are these the phases that are predicted from reaction path models (e.g., EQ3/6) which will be used in performance assessments?

5. How persistent over time are the metastable phase assemblages that form? Will these phases serve as barriers to radionuclide release?

6. Based on the structures of these phases (mostly sheet structures) can the thermodynamic stabilities of these phases be estimated, or at least bounded, in such a way as to provide for a convincing and substantive performance assessment?

Keywords: Uranium Oxides, Minerology, Corrosion, Phase Stability

297. **DIRECT INVESTIGATIONS OF THE IMMOBILIZATION OF RADIONUCLIDES IN THE ALTERATION PHASES OF SPENT NUCLEAR FUEL**
$260,829
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DOE is the custodian of several thousand tons of spent nuclear fuel that is intended for geological disposal. The direct disposal of spent nuclear fuel or of mixed oxide fuel (fabricated for the disposal of excess weapons plutonium) requires a careful analysis of the role of spent fuel as a waste form. During burn-up, as much as four percent of the uranium in the fuel will have fissioned to produce stable and radioactive fission products (e.g., Sr, Cs, Tc, I, Mo, Se). In addition, transuranic elements (e.g., Np, Pu, Am, Cm) will have formed from uranium by neutron capture. These radionuclides are cause for concern if they are released in to the biosphere.

In an oxidizing environment, such as in the proposed geological repository at Yucca Mountain, Nevada, rapid alteration rates are expected for spent nuclear fuel, based upon experimental studies of UO_2 and spent nuclear fuel. The alteration involves matrix dissolution of the UO_2 and will release the radionuclides contained within the spent fuel. Researchers in the Chemical Technologies Division of Argonne National Laboratory have ongoing experiments on the oxidative dissolution of both UO_2 and spent nuclear fuel. In both cases, the samples are exposed, by slow dripping in contact with air, to water similar in composition to that found at the Yucca Mountain site. The alteration rate of the UO_2 and spent fuel in the experiments is appreciable, and the alteration products are primarily U6+ phases. The generally low concentrations of the fission products and transuranic elements in spent fuel will probably preclude them from forming separate phases. Rather, current research at Argonne National Laboratories indicates that some of these radionuclides are being incorporated into the U^{6+} phases, significantly impacting upon the future mobility of the radionuclides.

Approximately 20 minerals that contain U^{6+} are of importance for spent fuel disposal. There is currently inadequate data pertaining to the migration of radionuclides in a repository setting. Only a limited database exists that relates to the effects of alteration phases on the retardation of radionuclides, but this information is necessary in providing a radionuclide release estimate as required for performance assessment modeling. This project will characterize the incorporation of radionuclides into the alteration products to enable a more realistic estimate of the rate of radionuclide migration from the near field environment. An accurate assessment of realistic radionuclide solubilities in the repository will allow for the development of an effective and cost-efficient engineered barrier system. The alteration products of spent nuclear fuel will be studied to identify in which phases, and to what extent, the radionuclides of environmental concern are being incorporated.

Keywords: Uranium Oxides, Minerology, Phase Stability, Corrosion, Radionuclides

298. **DECONTAMINATION OF RADIONUCLIDES FROM CONCRETE DURING AND AFTER THERMAL TREATMENT**
$271,907
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The total area of contaminated concrete within all DOE facilities is estimated at 7.9 x $10^8 ft^2$ or approximately 18,000 acres with the major contaminating radionuclides being U, ^{90}SR, ^{60}Co, and ^{137}Cs (Dickerson et. al. 1995). Techniques to decontaminate concrete through the application of heat (including microwaves, infrared radiation, lasers, plasma torch, etc.) have centered on the generally known deterioration of concrete strength with imposed thermal stress. These strategies have all attempted to spall or scabble contaminated solids from the concrete surface and to maximize the particular technology's capability to that end. However, in addition to the imprecisely defined knowledge of the physical effects of specific heat treatments on concrete (final temperature, heating rate, and type of concrete aggregate), concomitant behavior of DOE's major radioactive contaminants (^{137}Cs, U, ^{90}Sr, and ^{60}Co) during thermal treatment is very poorly known. This research will determine the thermal effects between 100 and 1400°C on concrete engineering properties (compressive strength, strain, porosity, bulk density, and cracking), chemical properties (dehydration, mineral phase change, and solubility), and contaminant behavior as a function of final temperature, heating rate, and aggregate type (none, limestone, or silica); thermal effects on contaminants and concrete are depicted conceptually in Figure 1. Major effects on radionuclide transport via direct volatilization (particularly for ^{137}Cs and ^{60}Co) during heating are anticipated to lead to *in situ* decontamination techniques. Changes in the extractability of radionuclides from heat affected concrete will be measured, using short-lived radioisotopes, to ascertain changes in decontamination potential following thermal treatment. Detailed finite-element modeling of heat flow in concrete and resulting mechanical stresses (from pore pressure and thermal expansion) of optimal thermal treatments will be completed so that effects on laboratory-sized specimens can be extrapolated to field-scale thermal treatments on concrete mechanical properties and contaminant behavior. Expected results will be a thorough and detailed understanding of the thermal effects on concrete engineering properties and concomitant radionuclide behavior including a detailed empirical data base. Specific decontamination technologies using thermal stressing of concrete will then be able to predict their effects rather than continue with DOE's apparent present approach of supporting novel thermal technologies without either a basic understanding of the limits of thermal effects on concrete or the fate and behavior of key radionuclides.

Keywords: Concrete, Radionuclides, Decontamination

299. MECHANISMS OF RADIONUCLIDE-HYDROXYCARBOXYLIC ACID INTERACTIONS FOR DECONTAMINATION OF METALLIC SURFACES

$383,333
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This project addresses key fundamental issues involved in the use of simple and safe methods for the removal of radioactive contaminants from slightly contaminated steel and other surfaces at the DOE sites so that the metals can be reused. The objectives are to (i) determine the nature of the association of radionuclides U, Pu, Co and Sr with stainless steel, and (ii) selectively remove the radionuclides using hydroxycarboxylic acids (citric acid and its analogs). The basic mechanisms involving coordination, complexation, dissolution and removal will be elucidated in a systematic manner.

This is a collaborative research project between Brookhaven National Laboratory (BNL) and the State University of New York at Stony Brook (SUNY-SB). This project is divided into three phases. In Phase I the basic mechanism of interaction of actinides with metal oxides on metallic surfaces will be investigated. Phase II will determine the interaction of hydroxycarboxylic acids citric, malic and tartaric acids with the actinide contaminated metallic surfaces. Phase III involves investigation of interaction of hydroxycarboxylic acid with actual contaminated samples from DOE sites and interpretation of results based on knowledge gained from Phases I and II. The nature of radionuclide association with representative metal oxides typically formed on metallic surfaces which have undergone oxidation characteristic of long term environmental exposure will be investigated. The rate and extent of incorporation of radionuclide into amorphous and crystalline forms of iron oxides (goethite, hematite, magnetite and lepidocrocite), and metallic coupons will be determined. Exposure of metallic coupons to radionuclides during and following accelerated aqueous corrosion will utilize standard electrochemical cells and equipment. Advanced spectroscopic techniques (XPS, XANES, EXAFS, EDX, SIMS, FTIR and LD-ITMS at PNNL) will be used to characterize the (1) nature of the radionuclide association with the metal oxides and contaminated surfaces, and (2) radionuclide-citrate complexes and mixed-metal (actinide-metal-citrate) complexes that have been removed from contaminated surfaces. In addition, the photochemical and biochemical degradation of the resulting actinide-organic complexes will be examined, with application to recovery of radionuclides in a concentrated form and reduction of secondary waste generation.

Keywords: Radionuclides, Decontamination, Actinides, Corrosion

300. PHYSICAL, CHEMICAL AND STRUCTURAL EVOLUTION OF ZEOLITE-CONTAINING WASTE FORMS PRODUCED FROM METAKAOLINITE AND CALCINED HLW

$170,000
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Natural and synthetic zeolites are extremely versatile materials. They can adsorb a variety of liquids and gases, and also take part in cation exchange reactions. Zeolites are easy to make, they can be synthesized from a wide variety of natural and man made materials. One such combination is metakaolinite and sodium hydroxide solution. The objective of this research is to adapt this well known reaction for use in site remediation and clean-up of caustic waste solutions now in storage in tanks at Hanford and the Savannah River sites.

It has been established that a mixture of calcined equivalent ICPP waste (sodium aluminate/hydroxide solution containing 3:1 Na:Al) and fly ash and/or metakaolinite can be cured at various temperatures to produce a monolith containing Zeolite A (80°C) or Na-P1 plus hydroxysodalite (130°C) dispersed in an alkali aluminosilicate hydrate matrix. The zeolitization process is a simple one and as such could be a viable alternative for fixation of low activity waste (LAW) salts and calcines. Dissolution tests have shown these materials to have superior retention for alkali, alkaline earth and heavy metal ions.

The technology for synthesizing zeolites is well documented for pure starting materials, but relatively little is known about the process if metakaolinite is mixed with a complex mixture of oxides containing nearly every element in the periodic table. The purpose of the proposed work is to develop a clearer understanding of the advantages and limitations of producing a zeolite-containing waste form from calcined radioactive waste, i.e. the effect of processing variables, reaction kinetics, crystal and phase chemistry, and microstructure on their performance. To accomplish this, two waste forms representative of solutions in storage at the Hanford and Savannah River sites will be simulated. Because nitrate is detrimental to the process, the LAW will be calcined at various temperatures (w/wo sugar) to maximize the reactivity of the resultant mix of oxide phases while minimizing the loss of volatiles. The oxides will be mixed with varying amounts and types of metakaolinite, small amounts of other chemicals (alkali hydroxides and/or carbonates, zeolite seeds, templating agents) and enough water to make a paste. The paste will then be cured (in-can) at a variety of temperatures (80°-100°C). Once reaction rates for the process are established, MAS NMR and TEM will be used to study the atomic-level structure of the solids. X-ray diffraction will be used to examine the degree of crystallinity of the waste forms. An environmental SEM will be used to track the development of microstructure in real time. An electron microprobe will be used to analyze the phases in the waste form. Attempts will be made to relate changes in phase chemistry and microstructure to distribution coefficients and dissolution data. Compressive and bending strength tests will be used to determine mechanical behavior and standard leach tests will be used to determine the potential consequences of cation exchange reactions. Since simulated waste is not an adequate predictor, a major portion of the proposed work will be carried out at the Savannah River Technology Center, using actual LAW samples obtained from the Savannah River site.

Keywords: Zeolites, Radioactive Waste

301. MECHANISMS AND KINETICS OF ORGANIC AGING IN HIGH-LEVEL NUCLEAR WASTES
$300,000
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Donald M. Camaioni, (509) 375-2739

Highly radioactive wastes stored at Hanford and Savannah River DOE sites have unresolved questions relating to safety of the stored waste, as well as needs for safe, effective, and efficient waste processing to minimize the volume of high-level waste (HLW) streams for disposal. HLW undergoes constant irradiation from decaying radionuclides resulting in an array of radiation and thermochemical effects that directly impact issues concerning storage, retrieval, and pretreatment of the wastes. Heat from nuclear decay and from chemical processing (e.g., evaporation campaigns and tank transfers) drive thermal reactions of waste constituents, especially organic complexants. Radiolytic and thermochemical processes have been shown to degrade ("age") organic solutes into smaller fragments of lower energy content, reducing hazards associated with deflagration of nitrate organic mixtures while contributing to hazards such as the generation of toxic, flammable and potentially explosive gases (i.e., volatile organics, NH_3, H_2, and N_2O).

The goal of this project is to develop a fundamental understanding of organic aging and to assemble a model which describes and predicts the thermal and radiolytic aging of organic compounds in high level wastes. Kinetics will be measured and products and mechanisms of organic reactions occurring under conditions of waste storage, retrieval, and processing will be elucidated. Much emphasis will be placed on studying thermal effects, since organic reaction mechanisms and effects of varying conditions are uncertain. Organic complexants are of greatest concern regarding both safety and pretreatment since they have been found to degrade to gases, combust in dry wastes, and interfere with radionuclide separations. Therefore, efforts will focus on studying the reactions of these organic chemicals and associated degradation products.

Keywords: Oxidation, Organics, Radionuclides, Aging

302. MODELING OF SPINEL SETTLING IN WASTE GLASS MELTER
$291,667
DOE Contact: Arnold Gritzke, (202) 586-3957
Pacific Northwest National Laboratory Contact: Pavel R. Hrma, (509) 376-5092
Czech Academy of Sciences Contact: Lubomir Nemec, 011-420-2-24-310-371
Glass Service Ltd. Contact: Petr Schill, 011-420-657-611-439

The topic of this multi-institutional bi-national research is the formation and settling of spinel, the most common crystalline phase that precipitates in molten high-level waste (HLW) glass. For the majority of HLW streams, spinel formation in the HLW melter limits the waste fraction in glass because accumulation of spinel interferes with melter operation and shortens its lifetime. Hence, understanding spinel formation and behavior is important for HLW vitrification technology and economy, which call for the highest waste loading that is compatible with the quality and processability of the waste form.

Spinel is a product of an interaction between Cr_2O_3, Fe_2O_3, NiO, FeO, and other oxides, which are components of virtually all HLW streams at Hanford and Savannah River. Understanding and modeling the kinetics of spinel formation and the dynamics of spinel behavior in a waste glass melter will result in a reliable prediction and control of the rate of spinel settling and accumulation. The spinel settling rate will be predicted by mathematical modeling for which reliable experimental values of coefficients and material parameters will be obtained by laboratory studies. This approach combines the materials science, hydrodynamics, and mathematical modeling of spinel behavior in HLW glass melters.

Keywords: Spinel Formation, Equilibria, High-Level Waste Glass

303. PHOTOOXIDATION OF ORGANIC WASTE USING SEMICONDUCTOR NANOCLUSTERS
$417,000
DOE Contact: Arnold Gritzke, (202) 586-3957
SNL Contact: J. P. Wilcoxon, (505) 844-3939

Solar detoxification is a process wherein sunlight is captured by a semiconductor particle in suspension to create electrons and holes that then diffuse to the particulate surface to effect the oxidation and reduction of toxic pollutants. Using solar energy to oxidize organic chemicals to carbon dioxide and dilute mineral acids is very energy efficient compared to other methods such as incineration. 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: Solar Detoxification, Semiconductor Nanoclusters, Electron-Hole Recombination

304. ION-EXCHANGE PROCESSES AND MECHANISMS IN GLASSES
$300,333
DOE Contact: Arnold Gritzke, (202) 586-3957
PNNL 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 will be 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 will provide a signature characteristic of specific ion-exchange reactions. X-ray absorption spectroscopy will be 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: Nuclear Waste, Glass, Ion-exchange Reactions, X-ray Absorption Spectroscopy

OFFICE OF NUCLEAR ENERGY, SCIENCE AND TECHNOLOGY

Office of Nuclear Energy, Science and Technology - Grand Total	$73,917,000
Office of Space and Defense Power Systems	$3,617,000
Space and National Security Programs	$3,617,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$3,537,000
Development of an Improved Process for the Manufacture of Dop-26 Iridium Alloy Blanks and Clad Vent Sets, Product Characterization and Exploratory Alloy Improvement Studies	1,940,000
Carbon-bonded Carbon Fiber Insulation Production Maintenance Manufacturing Process Development and Product Characterization	320,000
A New High Temperature Solar Cell/selective Emitter for Thermophotovoltaic (TPV) Systems	272,000
Carbon-carbon Composites with Improved Mechanical and Thermal Characteristics for Radioisotope Power Systems	300,000
Enhancement of High Temperature Performance of Nd-fe-b Permanent Magnets for Sterling Engine/linear Alternator Power Generation	225,000
Amtec Electrode and Beta" Alumina Solid Electrolyte Development	300,000
Amtec Cell Assembly Process Development for Haynes-25 Niobium-1% Zirconium Cells	180,000
Materials Properties, Behavior, Characterization or Testing	$80,000
Emissivity Measurement and Sodium Compatibility Tests on Amtec Cell Materials	80,000
Office of Naval Reactors	70,300,000[1]

[1]This excludes $49.2 million for the cost of irradiation testing in the Advanced Test Reactor (ATR).

OFFICE OF NUCLEAR ENERGY, SCIENCE AND TECHNOLOGY

OFFICE OF SPACE AND DEFENSE POWER SYSTEMS

SPACE AND NATIONAL SECURITY PROGRAMS

Space and National Security Programs include the development and production of radioisotope power systems for both space and terrestrial applications and the technical direction, planning, demonstration and delivery of space nuclear reactor power and propulsion systems. During FY 1999, essentially all materials programs were aimed at: (1) transfer of clad vent set production operation from the Y-12 plant to Oak Ridge National Laboratory, (2) maintenance of iridium alloy and carbon bonded carbon fiber (CBCF) insulation radioisotope heat source material and components manufacturing capability, (3) continued improvement in heat source materials and their production processes and product characterization and (4) materials support for future terrestrial system applications and advanced high efficiency space power systems, particularly the alkali thermal to electric conversion (AMTEC) radioisotope power systems.

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

305. DEVELOPMENT OF AN IMPROVED PROCESS FOR THE MANUFACTURE OF DOP-26 IRIDIUM ALLOY BLANKS AND CLAD VENT SETS, PRODUCT CHARACTERIZATION AND EXPLORATORY ALLOY IMPROVEMENT STUDIES
$1,940,000
DOE Contact: W. Barnett, (301) 903-3097
ORNL Contacts: E. P. George, (865) 574-5085 and E. K. Ohriner, (865) 574-8519

An iridium alloy, DOP-26 (i.e., Ir-0.3 wt.% W with Th and Al dopant additions), serves as the fuel clad or capsule material for isotope heat sources employed in recent and contemporary space power systems for NASA deep space missions. This program is aimed at the optimization of the new improved process route previously selected for the production of DOP-26 iridium alloy sheet, namely a consumable vacuum arc cast/extrusion/"warm" rolling route. The effectiveness of this production process was further demonstrated in the production of DOP-26 alloy blanks, foil and clad vent sets for the Cassini Mission. Production yields have continued to exceed our goals.

During FY 1997, production of DOP-26 iridium alloy blanks, foil and clad vent set hardware for the Cassini mission was completed. Transfer of the clad vent set manufacturing operation from the Y-12 plant to the Oak Ridge National Laboratory was continued. Iridium alloy manufacturing capabilities are being maintained in a production maintenance mode.

Iridium process improvement activities were continued. Scale-up and evaluation of a new DOP-40 low thorium alloy (Ir-0.3 wt. % tungsten with dopant additions of 40 ppm cerium and 15 ppm thorium) was continued. A study of laser welding for fuel clad closure was continued.

Keywords: Consumable Arc Melt, Extrusion, Noble Metal, Rolling, Forming

306. CARBON-BONDED CARBON FIBER INSULATION PRODUCTION MAINTENANCE MANUFACTURING PROCESS DEVELOPMENT AND PRODUCT CHARACTERIZATION
$320,000
DOE Contact: W. Barnett, (301) 903-3097
ORNL Contact: G. Romanowski, (865) 574-4838

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 1999 program encompassed (1) continued maintenance of capability for both tube and plate billet production, (2) qualify a new X-ray inspection process and upgrade chemical analyses capability.

Keywords: Insulators/Thermal, High Temperature Service, Fibers

307. **A NEW HIGH TEMPERATURE SOLAR CELL/SELECTIVE EMITTER FOR THERMOPHOTOVOLTAIC (TPV) SYSTEMS**
$272,000
DOE Contact: W. Barnett, (301) 403-3097
Auburn University, Space Power Institute Contact: H. W. Brendhurst, (334) 844-5894

Selective rare earth emitters are being developed and matched with solar cells for TPV operation of 200°PC or higher.

Keywords: Selective Emitters, Solar Cells, Thermophotovoltaics

308. **CARBON-CARBON COMPOSITES WITH IMPROVED MECHANICAL AND THERMAL CHARACTERISTICS FOR RADIOISOTOPE POWER SYSTEMS**
$300,000
DOE Contact: W. Barnett, (301) 903-3097
Auburn University Contact: R. Zee, (334)844-3320
ORNL Contact: G. Romanowski, (865) 574-4838

Carbon-carbon composites having variations in cylindrical reinforcement architecture are being evaluated for replacement of the fine weave pierced fabric orthogonal structure currently being employed in the General Purpose Heat Source Graphite Impact Shell. Impact behaviors are being investigated.

Keywords: Carbon-Carbon, Impact Shell

309. **ENHANCEMENT OF HIGH TEMPERATURE PERFORMANCE OF Nd-Fe-B PERMANENT MAGNETS FOR STERLING ENGINE/LINEAR ALTERNATOR POWER GENERATION**
$225,000
DOE Contact: W. Barnett, (301) 903-3097
Iowa State University Contacts: F. McAllum, (515) 294-4726 and M. Russel, (515) 294-9225

Structure modifications via developed of functionally graded materials were persuaded to significantly enhance the Curie temperature with minimal degradation of the energy product.

Keywords: Permanent Magnets, Rare Earth Magnets

310. **AMTEC ELECTRODE AND BETA" ALUMINA SOLID ELECTROLYTE DEVELOPMENT**
$300,000
DOE Contact: W. Barnett, (301) 903-3097
Texas A&M University Contact: M. Schuler, (409) 845-8767

The development of improved performance electrode materials, principally iridium and mixed conductor electrode materials, was initiated for potentially improved performance AMTEC cells.

Keywords: Electrode Materials, AMTEC

311. **AMTEC CELL ASSEMBLY PROCESS DEVELOPMENT FOR HAYNES-25 NIOBIUM-1% ZIRCONIUM CELLS**
$180,000
DOE Contact: W. Barnett, (301) 903-3097
ORNL Contact: J. King, (923) 574-4807

Electron beam weld procedures and fixture were developed and applied to the manufacture of developmental AMTEC cell test hardware.

Keywords: Electron Beam Welding, AMTEC

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

312. **EMISSIVITY MEASUREMENT AND SODIUM COMPATIBILITY TESTS ON AMTEC CELL MATERIALS**
$80,000
DOE Contact: W. Barnett, (301) 903-3097

Emissivity measurements on AMTEC cell materials were continued. Measurements were conducted before and after sodium exposure tests.

Keywords: Emissivity, Sodium Compatibility, AMTEC

OFFICE OF NAVAL REACTORS

The materials program supports the development and operation of improved and longer life reactors and pressurized water reactor plants for naval nuclear propulsion.

The objective of the materials program is to develop and apply, in operating service, materials capable of use under the high power density and long life conditions required of naval ship propulsion systems. This work includes irradiation testing of reactor fuel, poison, and cladding materials in the Advanced Test Reactor at the Idaho National Engineering Laboratory. This testing and associated examination and design analysis demonstrates the performance characteristics of existing materials as well as defining the operating limits for new materials.

Corrosion, mechanical property, and wear testing is also conducted on reactor plant structural materials under both primary reactor and secondary steam plant conditions to confirm the acceptability of these materials for the ship life. This testing is conducted primarily at two Government laboratories—Bettis Atomic Power Laboratory in Pittsburgh and Knolls Atomic Power Laboratory in Schenectady, New York.

One result of the work on reactor plant structural material is the issuance of specifications defining the processing and final product requirements for materials used in naval propulsion plants. These specifications also cover the areas of welding and nondestructive testing.

Funding for this materials program is incorporated in naval projects jointly funded by the Department of Defense and the Department of Energy. This funding amounts to approximately $119.5 million in FY1999. Approximately $49.2 million represents the cost for irradiation testing in the Advanced Test Reactor. The Naval Reactors contact is David I. Curtis, (703) 603-5565.

OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT

	FY 1998
Office of Civilian Radioactive Waste Management - Grand Total	$29,121,295
Materials Properties, Behavior, Characterization or Testing	$29,121,295
Waste Packages	$29,121,295

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 OR TESTING

313. WASTE PACKAGES

$29,121,295
DOE Contact: Paige Russell, (702) 794-1315
M&O Contacts: Hugh Benton, (702) 295-4389 and V. (Pasu) Pasupathi, (702) 295-4507

The development of the nation's high-level waste repository has been delegated to DOE's Yucca Mountain Site Charactization Project Office. Framatome Cogema Fuels (formerly B&W Fuel Company), as part of the Civilian Radioactive Waste Management System Management & Operating (M&O) Contractor, is responsible for designing the waste package and related portions of the engineered barrier system. The advanced conceptual design was completed in 1996 and Viability Assessment design was completed in 1998. Progress on the waste package and the supporting materials studies has been documented in various reports.

The waste package design effort includes the development of waste packages to accommodate uncanistered commercial spent nuclear fuel (SNF), canistered SNF, canistered defense high-level waste, Navy fuel, and other DOE-owned spent nuclear fuel. The analytical process that is underway to support these designs included thermal, structural, and neutronic analyses. Also included are materials selection and engineering development. During FY99, barrier materials for the Site recommendation design were finalized with the selection of Alloy 22 as the outer corrosion resistant barrier over a stainless steel structural shell on the inside and titanium as the drip shield material.

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. These materials include alloy UNS# N06022, titanium grade 7, 316L stainless steel and alloy 22. The testing includes general aqueous and atmospheric testing, localized attack such as pitting and service corrosion, micro-biologically-influenced corrosion, galvanic corrosion, and stress corrosion cracking. The corrosion test facility started the long-term (at least five-year) test program in FY97. Evaluation of two year UNS# N06022 specimens were initiated and documented in project reports. Waste form materials are also being evaluated for alteration and leaching under repository-relevant conditions. In 1999, the short-term test program was continued to support waste package material degradation model development effort. The short-term test program focuses on stress corrosion cracking, hydrogen embrittlement, crevice corrosion, galvanic effects among the candidate materials and determination of the appropriate test environment that will represent saturated aqueous condition on the waste package surface.

Keywords: Yucca Mountain Repository, Waste Package, Engineered Barrier System

OFFICE OF DEFENSE PROGRAMS

	FY 1999
Office of Defense Programs - Grand Total	$45,869,600
The Weapons Research, Development and Test Program	$45,869,600
Sandia National Laboratories	$22,264,600
Materials Preparation, Synthesis, Deposition, Growth or Forming	$10,102,000
Scientifically Tailored Materials	3,140,000
Materials Processing	3,040,000
Atomic-Scale Studies of Surface Defect Chemistry	615,000
Exploiting Lens Technology Through Novel Materials	615,000
Enabling Science & Technology for Cold Spray Direct Fabrication Properties	195,000
Atomic-Level Studies of Surfactant-Directed Materials Growth	460,000
Freeforming of Ceramics and Composites from Colloidal Slurries	475,000
Laser-Assisted Arc Welding for Aluminum Alloys	210,000
Functional Materials for Microsystems: Smart Self-Assembled Photochromic Films	375,000
Self-Healing Molecular Assemblies for Control of Friction and Adhesion In MEMS	502,000
Self-Assembled Templates for Fabricating Novel Nano-Arrays and Controlling Materials Growth	475,000
Materials Properties, Behavior, Characterization or Testing	$9,310,000
Aging and Reliability	2,440,000
From Atom-Picoseconds to Centimeter-Years in Simulation and Experiment	600,000
Hardening and Tribological Improvement of Mems Ni Alloys by Ion Implantation	300,000
Corrosion Behavior of Plasma-Passivated Copper	400,000
In-Situ Stress Relaxation During Annealing of Amorphous Carbon Films	300,000
Physics of Photosensitivity in Novel Thin Films	250,000
The Shock Properties of PZT 95/5	200,000
The Properties and Physics of Relaxor Ferroelectrics	150,000
Photonic Band Gap Structures as a Gateway to Nano-Photonics	375,000
The Initiation and Propagation of Nano-Scale Cracks at an Adhesive/Solid Interface	400,000
Fundamental Aspects of Micromachine Reliability	370,000
Intelligent Polymers for Nanodevice Performance Control	400,000
Quantum Dot Arrays	450,000
Molecular Characterization of Energetic Material Initiation	60,000
Innovative Experimental and Computational Diagnostics for Monitoring Corrosion in Weapons Environments	300,000
Linking Atomistic Computations with Phase Field Modeling	352,000
A Combinatorial Microlab Investigation of Critical Copper-Corrosion Mechanisms	600,000
Microscale Shock Wave Physics Using Photonic Driver Techniques	400,000
Wetting and Spreading Dynamics of Solder and Braze Alloys	600,000
Improved Materials Aging Diagnostics and Mechanisms through 2D Hyperspectral Imaging Methods and Algorithms	363,000

OFFICE OF DEFENSE PROGRAMS

	FY 1999
The Weapons Research, Development and Test Program (continued)	
Sandia National Laboratories (continued)	
Device or Component Fabrication, Behavior or Testing	$1,632,600
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	600,000
Non-Volatile Protonic Memory	300,000
Instrumentation and Facilities	$1,220,000
Advanced Analytical Techniques	1,220,000
Los Alamos National Laboratory	$17,000,000
Enhanced Surveillance Campaign	17,000,000
Lawrence Livermore National Laboratory	$6,605,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$3,440,000
Engineered Nanostructure Laminate	2,000,000
Energetic Materials Strategic Chemistry	350,000
Cheetah Thermochemical Code	190,000
Explosives Development	900,000
Materials Properties, Behavior, Characterization or Testing	$665,000
Interfaces, Adhesion, and Bonding	265,000
Laser Damage: Modeling and Characterization	400,000
Instrumentation and Facilities	$2,500,000
Scanning Tunneling Microscopy (STM), Atomic Force Microscopy (AFM), near Field Scanning Optical Microscopy (NSOM)	250,000
Atomic Level Explosive Calculations	325,000
Metastable Solid-phase High Energy Density Materials	535,000
AFM Investigations of Crystal Growth	290,000
Polyimide Coating Technology for ICF Targets	500,000
Beryllium Ablator Coatings for NIF Targets	600,000

OFFICE OF DEFENSE PROGRAMS

THE WEAPONS RESEARCH, DEVELOPMENT AND TEST PROGRAM

SANDIA NATIONAL LABORATORIES

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

314. SCIENTIFICALLY TAILORED MATERIALS
$3,140,000
DOE Contact: Bharat Agrawal, (301) 903-2057
SNL Contact: Jill Hruby, (925) 294-2596

The Scientifically Tailored Materials effort addresses the need for materials with specific properties or performance characteristics to be used in the enduring stockpile. Projects emphasize achieving scientific understanding of how the materials properties depend on composition, microstructure, and preparation conditions. Research focuses on materials that can serve as direct replacements for those in current use whose availability is curtailed by sunset technologies or ES&H regulations, on new materials to simplify production or surveillance, on new technological solutions to current component functions, or on enhanced reliability or surety. Current areas of emphasis are:

New Encapsulant Concepts to create easily removable encapsulants, enhance their adhesion and dielectric breakdown strength, develop the required visco-elastic response of alumina-loaded epoxy, and incorporate chemical getters.

Optical, Electronic, and Sensor Materials to determine what limits the dynamics of PZT switching, create a new optical medium for information storage, and explore microporous materials for high energy density storage.

Advanced Engineering Materials to determine the degradation of gas transfer system materials due to hydrogen.

Keywords: New Materials, Materials by Design, Encapsulants, Optical, Electronic, Sensor Materials

315. MATERIALS PROCESSING
$3,040,000
DOE Contact: Bharat Agrawal, (301) 903-2057
SNL Contact: Julia M. Phillips, (505) 844-1071

The Materials Processing effort seeks to develop a fundamental understanding of new and existing processes that are anticipated to be critical for defense programs needs. The effort emphasizes developing the understanding that will enable us to fabricate parts faster, with fewer defects, and at lower cost. The results of this sub-program are used to develop advanced manufacturing techniques for component production. Projects are supported in three theme areas.

Joining to understand the composition effects of alloy weldability, model laser weld penetration, and discover *the surface reactions needed for metal/ceramic* bonding.

Direct and Micro-Fabrication to find the most direct way to fabricate structures from computer-aided design models using micropens to create electrical circuits for packaging; develop plasma spray for radiation shield coatings; electrodeposited (LIGA) structures; and determine the mechanical properties of nanoscale structures and measure and control the molecular level friction and wear.

Model-based Processing to optimize the compaction, densification, and sintering of ceramic powders and develop coutergravity withdrawal casting.

Keywords: Processing, Fabrication

316. ATOMIC-SCALE STUDIES OF SURFACE DEFECT CHEMISTRY
$615,000
DOE Contact: Gerald Green, (202) 586-8377
SNL Contact: Nancy B. Jackson, (505) 272-7619

We propose to use a combination of experimental and theoretical techniques to explore atomic scale defect chemistry on technologically important surfaces, with the goal of determining the salient factors that control defect chemistry. The formation, mobility, reactivity, and dissolution of atomic scale surface defects play an important role in materials areas such as catalysis, corrosion, thin film growth, semiconductor processing, sensors, and magnetic devices. Important defects include single adatoms, surface steps and kinks, dislocations, and vacancies. It is generally believed that a small number of localized surface defects may be particularly reactive and thereby dominate the surface chemistry of many materials. While past studies of this important problem have been limited by an absence of appropriate experimental probes for imaging atomic scale defects, the recent advent of specialized scanning probe microscopies largely overcomes this problem and now allows more detailed studies of defect chemistry than previously possible. The unique Atom Tracking scanning tunneling microscope (STM) recently developed at Sandia is a particularly powerful new technique that allows measurement of atomic-scale kinetic processes on a time scale that is more than three orders of magnitude faster than previous techniques. Similarly, a lack of sufficient computing power has severely limited previous theoretical studies of defect properties. The recent development of massively parallel computational techniques at Sandia, which now allows calculations on systems containing hundreds of atoms per unit cell, will enable studies of surface defects with a level of detail and sophistication far greater than previously possible. By studying well defined, well ordered surfaces, we can greatly simplify the study of defect chemistry and obtain detailed fundamental information on defect formation and reactivity. Coupling experimental results with theoretical studies will allow the development of models that explain, predict, and ultimately help to control surface defect reactivity.

Keywords: Atomic Scale, Chemistry, Defects

317. EXPLOITING LENS TECHNOLOGY THROUGH NOVEL MATERIALS
$615,000
DOE Contact: Gerald Green, (202) 586-8377
SNL Contact: Brian Damkroger, (505) 845-3592

LENS (Laser Engineered Net Shaping) is a direct fabrication process in which metal powders are deposited into a laser melted pool, with succeeding layers being deposited to build up complex engineering shapes. In this age of model based designs and requirements the ability to directly transform design information into a manufactured product is extremely desirable. LENS is a rapid, low cost, low footprint direct fabrication process that lends itself to this concept for advanced manufacturing. However, previous work has developed LENS as an advanced manufacturing tool, rather than exploiting its unique attributes. These attributes include: real time microstructural control, tailored material properties at different locations in the same part, the production of graded CTE parts. This project will develop a science based approach to utilize LENS to "process for properties" in a controlled fashion, or for the production of components that cannot be made using other methods. Three materials: a tool steel with an optimized structure/property mix, a graded structure based on stainless steel compositions, and a ceramic-to-metal transition are novel material systems through which LENS will be investigated and exploited.

This goal will be achieved by first developing a thorough understanding of the process in terms of how it impacts solidification and microstructure development. Factors like solidification rate, thermal profiles, cooling rate, powder input, and residual stresses must be understood, as well as their effects on material responses such as dendrite tip velocity and undercooling, microsegregation, precipitation and transformation kinetics. Using pyrometry and thermocouple techniques in conjunction with accurate data regarding powder flow, gas flow, laser power and feed rate, the conditions present in the molten pool will be used to develop models of solidification and microstructural evolution. Additionally, the unique attributes and capabilities of the LENS process will be studied and understood. From this knowledge base, will be designed and produced a suite of experimental materials and structures that optimally exploit the LENS process and demonstrate its unique potential. An understanding of the residual stresses in LENS parts, and what mitigation techniques may be available will be developed.

Keywords: Metals, Processing, Laser, Solidification

318. ENABLING SCIENCE & TECHNOLOGY FOR COLD SPRAY DIRECT FABRICATION PROPERTIES
$195,000
DOE Contact: Gerald Green, (202) 586-8377
SNL Contact: Mark Smith, (505) 845-3256

Direct Fabrication is envisioned as a rapid, agile, economical process technology that additively builds up a net or near-net shaped component made of one or more materials directly from a computer model; such technology would be of enormous benefit to SNL's core National Security Mission and U.S. industry. Cold Spray Processing (CSP) is a recently discovered, poorly understood, Russian technology that can rapidly deposit (mm/sec) metals, polymers, and composites at temperatures <200°C by accelerating powder particles up to 600-1000 m/s in a supersonic compressed air or gas jet. The Russians have used CSP for high-rate coating deposition, but no one has attempted direct fabrication via CSP. One can envision a radical new fabrication technology in which a highly focused CSP particle "beam" is combined with a multi-axis robotic motion system in order to spray-fabricate a single- or multi-material component directly from a computer model. CSP build rates should be substantially higher than present layer-wise direct fabrication techniques and, since CSP particles are never fully melted, superior surface finishes, microstructures, and properties might be achieved (e.g., finer grain size, no brittle phases, minimal oxidation, less residual stress). With CSP, one might also deposit functionally graded or layered materials at low temperatures, thus eliminating joining operations, simplifying design/fabrication, reducing part counts, and decreasing stress cracking. (For example, aluminum has been CSP-deposited directly onto smooth, unprepared glass with excellent adhesion.) CSP may also be an environmentally friendly alternative to problem technologies, such as copper electroplating and soldering or painting of aircraft and weapons.

This project explores the use of cold spray processing for direct fabrication of simple proof-of-concept shapes.

Keywords: Cold Spray Processing, Direct Fabrication

319. **ATOMIC-LEVEL STUDIES OF SURFACTANT-DIRECTED MATERIALS GROWTH**
$460,000
DOE Contact: Gerald Green, (202) 586-8377
SNL Contact: Terry Michalske, (505) 844-5829

This project is investigating converting surface impurities from a nuisance to a systematically applicable nano-fabrication tool. Combining Sandia's special facilities, including the "atom-tracker" Scanning Tunneling Microscope (AT-STM), Low Energy Electron Microscopy (LEEM), and Massively Parallel Computation (MPC), the objective is to learn how common adsorbed atoms ("surfactants") can be used to manipulate and direct thin-film growth, and to develop a "surfactant toolkit" that enables production of either atomically flat or 3-dimensionally nano-structured surfaces. The approach is to start with model systems, studying surfactant-modified diffusion on and near metal and semiconductor surfaces, and integrating real-time experimental and advanced computational modeling capabilities. The AT-STM is being used to study H-assisted Si adatom diffusion on Si(001), and the LEEM to investigate both H-assisted step fluctuations on the same surface and O-assisted island growth on Pt(111). Ge segregation versus adsorbate overlayer coverage is being investigated in Si-Ge alloys via novel surface stress measurements. Theoretical efforts are closely coupled to experiments—MPC is indispensable in developing reliable, atomic-scale, mechanistic models.

Keywords: AT-STM, LEEM, MPC

320. **FREEFORMING OF CERAMICS AND COMPOSITES FROM COLLOIDAL SLURRIES**
$475,000
DOE Contact: Gerald Green, (202) 586-8377
SNL Contact: Duane Dimos, (505) 844-6385

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

321. **LASER-ASSISTED ARC WELDING FOR ALUMINUM ALLOYS**
$210,000
DOE Contact: Gerald Green, (202) 586-8377
SNL Contact: Brian Damkroger, (505) 845-3592

At this time, there exists a strong need in the defense programs, automotive, aerospace and transportation industries for a rapid, robust, high quality process for welding aluminum alloys, especially for relatively thin gauge product. While laser beam welding is widely applied in these industries it has not proved valuable for aluminum because of problems with reflectivity and weld joint variability. Gas metal arc welding (GMAW) is widely used for thick section aluminum welding because the process can compensate for part fit-up and metallurgical deficiencies. Under this project a new welding process is being developed by combining together a fiber optic-delivered pulsed Nd:YAG laser with a miniaturized GMAW system. The new laser-assisted arc welding (LAAW) process couples the process advantages of these two unique heat sources and will also enable process capabilities never before envisioned in arc welding. These two heat sources are being combined in a compact (likely patentable) device that can be manipulated on the end of a robotic arm. The focused pulsed Nd:YAG laser beam assures deep weld penetration and ablative removal of the tenacious aluminum oxide. The arc is focused and located by the metal vapor and gas ions generated by the high intensity laser beam. Increased arc stability is anticipated since the gas metal arc is known to be stabilized by thermal ionization of the shielding gas. The project is a System of Laboratories (SOL) collaboration among ORNL, INEEL and SNL. These three laboratories have distinguished themselves for their contributions to the science and technology of materials joining. The team established through this SOL interaction should allow the U.S. to successfully compete with international entities, such as Germany's Fraunhofer Institute, in developing (and hence owning) advanced joining technologies for commercially critical markets.

Keywords: Laser-Assisted Arc Welding

322. FUNCTIONAL MATERIALS FOR MICROSYSTEMS: SMART SELF-ASSEMBLED PHOTOCHROMIC FILMS
$375,000
DOE Contact: Gerald Green, (202) 586-8377
SNL Contact: Terry A. Michalske, (505) 844-5829

The objective of this project is to scientifically-tailor smart interfacial films and 3-D composite nanostructures to exhibit photochromic responses to specific, highly-localized chemical and/or mechanical stimuli, and to integrate them into optical microsystems. The project will involve the design of functionalized chromophoric self-assembled materials that possess intense and environmentally-sensitive optical properties (absorbance, fluorescence) enabling their use as detectors of specific stimuli and transducers when interfaced with optical probes. Particularly strong candidates for initial studies are the conjugated polydiacetylenes. The organic functional material will be immobilized in an ordered, mesostructured inorganic host matrix which will serve as a perm-selective barrier to chemical and biological agents and provide structural support for improved material durability. Construction of these hybrid organic/inorganic layers will be facilitated by advanced self-assembly techniques. Multi-task scanning probe techniques (atomic force microscopy, near-field scanning optical microscopy) offering simultaneous optical and interfacial force capabilities will drive the chromophoric materials with localized and specific interactions for detailed characterization of physical mechanisms and parameters. The composite films will be directly interfaced with microscales devices as optical elements (e.g. intracavity mirrors, diffraction gratings), taking advantage of the very high sensitivity of device performance to real-time dielectric changes in the films.

Keywords: Microsystems, Self-Assembly, Photochromic Materials

323. SELF-HEALING MOLECULAR ASSEMBLIES FOR CONTROL OF FRICTION AND ADHESION IN MEMS
$502,000
DOE Contact: Gerald Green, (202) 586-8377
SNL Contact: Terry A. Michalske, (505) 844-5829

Major barriers to implementing MEMS technologies are the ability to chemically passivate and lubricate the surface of micromechanical structures to prevent adhesion and reduce friction and wear, and to prevent electrostatic charging of devices in radiation environments. We propose a new class of molecular coatings that offer Si surface passivation, elimination of surface oxide layers, self-healing lubrication properties, and a built-in mechanism to release shear energy through reversible chemical cleavage. Two approaches will be investigated, first separately, then in combination. We will investigate molecular assemblies that form liquid crystalline lamellar structures with robust mechanical properties, and a novel method of chemically modifying the polycrystalline Si surface directly, without an intermediary oxide layer, in a process that occurs simultaneously with the etching step used to remove the sacrificial oxide. Used separately, the first method may improve high shear stress micromachine performance, while the second may be suitable for applications where adhesion control is critical. Most exciting is combining both methods, where the self-healing lubricant is used to form a protective layer over the chemically treated surface prepared by the second method. Mechanical stress studies on these materials at the nanometer scale will be performed using both new and existing scanning probe techniques. We will also employ molecular dynamics simulation techniques to calculate the lubricants response to shear and compressive forces, determine the molecular mechanisms involved, and propose lubricant structures by understanding the molecular structure-function relationship.

Keywords: Microsystems, Friction and Adhesion Control

324. **SELF-ASSEMBLED TEMPLATES FOR FABRICATING NOVEL NANO-ARRAYS AND CONTROLLING MATERIALS GROWTH**
$475,000
DOE Contact: Gerald Green, (202) 586-8377
SNL Contact: Robert Q. Hwang, (925) 294-1570

Novel and exciting phenomena which have the potential to revolutionize science, materials, next-generation production methods are manifested as structural dimensions approach the nanometer level. However, advances in lithography are insufficient to achieve this feature scale. As a result, molecular self-assembly has attracted a great deal of interest, since this provides a possible spontaneous mechanism by which nanometer sized arrays can be formed without mechanical intervention. Although these low tech processes are *highly dependent on system/material specifics, new* techniques and the science which underlies them can be developed in a manner that allows extension of the natural order of self-assembling systems. The approach is based on previous work in which we fabricated templates of unprecedented size and regularity. These templates will then be applied to form nano-arrays based on a wide range of materials with tunable properties and nano-scale selective area over-growth patterns for improving the materials quality of thin films.

Keywords: Self-Assembly, Nano-Materials, Materials Growth

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

325. **AGING AND RELIABILITY**
$2,440,000
DOE Contact: Bharat Agrawal, (301) 903-2057
SNL Contact: Richard J. Salzbrenner, (505) 844-9408

The Materials Aging and Reliability effort addresses the chemical and physical mechanisms which cause materials properties to change with time. Important mechanisms that must be understood involve both the intrinsic thermodynamic drivers associated with the materials and extrinsic drivers associated with the environments in which the materials are used. The scientific results developed here become the basis for quantitative predictions of component reliability as a function of time in the stockpile. The main themes are:

Surfaces and Interfaces to determine the effect of impurities on the reliability of metal thin films, develop micro- and nano-probes for localized corrosion of aluminum alloys, and discover the fundamental mechanism of polymer bonding to nickel alloys.

Bulk Degradation to measure the thermo-mechanical degradation of solder joints and develop a methodology for measuring polymer degradation near room temperature.

Keywords: Aging, Reliability

326. **FROM ATOM-PICOSECONDS TO CENTIMETER-YEARS IN SIMULATION AND EXPERIMENT**
$600,000
DOE Contact: Gerald Green, (202) 586-8377
SNL Contact: John Hamilton, (925) 294-2457

Stockpile stewardship is perhaps Sandia's most important mission in the coming millennium. The understanding of aging phenomena is a critical aspect of stockpile stewardship. Accelerated aging tests and examinations of stockpile components play an important role, but both have their limitations. Accelerated aging tests at elevated temperatures skew the relative probabilities of various reactions. Examination of stockpile components provides a limited database and tends to leave us in a reactive rather than proactive position, i.e., we may learn about a problem only when it is almost too late to do anything about it. Consequently, it is a vital part of stockpile stewardship to develop simulation techniques that are accurate and valid over much greater time and length scales than those presently available. Most importantly, the simulation techniques should be tested by experiment at various length and time scales so that they can be validated and improved.

The state of the art in computer simulation allows precise studies of the atomic electronic structure, detailed calculations of atomic trajectories, modeling of long time scales OR modeling of large length scales. These capabilities tend to be mutually exclusive at present due to limits in communication between disciplines, limits in algorithm development, and limits in computer power. This project will use a coordinated multidisciplinary research effort to incorporate the accuracy presently available in atomistic molecular dynamics and electronic structure calculations into simulations at much longer time and length scales.

Four novel complementary computational techniques will be developed and/or employed: hyper molecular dynamics, chain of states method, transition state theory, and stochastic lattice dynamics. The simulations will be coupled with experiments on three specific *materials problems critical to Sandia missions: (1) The* relationship between hardening, strain, and length scale in microcomponents. The response of submicron solid structures to torsion and planar simple shear will be measured.; (2) Permeation through microporous media (polymers and zeolites).; (3) Semiconductor deposition. The atom tracker will be used to examine the motion of silicon atoms which occurs during growth of silicon films.

Keywords: Aging, Simulation, Atomic Scale, Molecular Dynamics

327. **HARDENING AND TRIBOLOGICAL IMPROVEMENT OF MEMS NI ALLOYS BY ION IMPLANTATION**
$300,000
DOE Contact: Bharat Agrawal, (301) 903-2057
SNL Contact: Charles Barbour, (505) 844-5517

The performance and lifetime of micro-electromechanical systems (MEMS) constructed from electroformed nickel alloys would be greatly enhanced by surface hardening and reductions in unlubricated friction and wear. Processing to achieve these benefits must minimize dimensional changes and heating, and must avoid the introduction of surfaces layers susceptible to debris-forming exfoliation or aging degradation. Ion implantation satisfies these constraints, and the technique has been shown to allow controlled modification of near-surface composition and microstructure leading to strengthening and reduced friction and wear. We are therefore exploring the use of ion implantation to harden the surfaces and reduce the friction and wear of Ni-based alloys used in MEMS. A scientific objective is to understand and quantify the relationship of mechanical properties to implantation-modified microstructure. Dual ion implantation of titanium and carbon has been demonstrated to produce an amorphous layer with superior mechanical properties in annealed bulk Ni and in the electroformed Ni and $Ni_{75}Fe_{25}$ of MEMS. The intrinsic yield strength of the amorphous Fe-Ti-C layer was determined from nanoindentation and finite-element modeling to be 5 GPa. This exceeds by a factor of two the strength of maximally hardened martensitic bearing steel, and it is also about twice the strength of conventional, metalloid-stabilized amorphous Ni-Fe alloys. Such exceptional resistance to plastic flow is ascribed to the absence of dislocation glide combined with strong atomic-pairing reactions between Ti and C. The near-surface strengthening resulting from implantation is found to suppress the destructive adhesion-and-fracture wear characteristic of untreated Ni surfaces in sliding contact. Scientifically, the present investigation is the first to quantify and mechanistically account for the intrinsic mechanical properties of an implantation-amorphized alloy.

Keywords: Micromachines, Hardening, Friction and Wear

328. **CORROSION BEHAVIOR OF PLASMA-PASSIVATED COPPER**
$400,000
DOE Contact: Bharat Agrawal, (301) 903-2057
SNL Contact: Charles Barbour, (505) 844-5517

Predictive understanding of corrosion is needed to ensure reliability in both electronics and microelectronics components. To date, modeling has been hindered by limited knowledge of primary corrosion mechanisms and the large number of coupled chemical reactions, which depend on complex interactions of materials with the environment. This multidimensional problem requires new approaches for quantitative identification of critical phenomena occurring in corrosion phase space. We are examining combinatorial techniques as a first step toward developing these new experimental approaches and determining mechanisms critical to copper sulfidation. In initial experiments, parallel experimentation was used in which the thickness of Cu oxide and the level of irradiation-induced defects were varied to efficiently identify mechanisms for Cu sulfidation. A Cu film was deposited on an SiO_2 covered Si wafer and then masked and oxidized in an electron cyclotron resonance (ECR) plasma to form different thicknesses of CuO_x on Cu. The sample was then implanted with 200 keV Cu^+ ions with different fluences to create different levels of point defects in the oxide and Cu. The sample matrix as well as a control sample, which had been exposed to air to form a native oxide, were then exposed to an H_2S environment. The variation in oxide thickness had little effect on the formation of and quantity of Cu_2S, while the level of irradiation affected the Cu_2S formation greatly. The plasma-oxidized Cu yields a surface which is more resistant to sulfidation than an air-oxidized Cu, thus providing a means to treat Cu for minimizing corrosion in sulfidizing environments. The results of this experiment show that the type of Cu-oxide (CuO vs. Cu_2O) and defect levels in the oxide are more important for controlling the sulfidation reaction than is the oxide thickness.

Keywords: Corrosion, Aging, Reliability

329. **IN-SITU STRESS RELAXATION DURING ANNEALING OF AMORPHOUS CARBON FILMS**
$300,000
DOE Contact: Bharat Agrawal, (301) 903-2057
SNL Contact: Charles Barbour, (505) 844-5517

Amorphous carbon thin films grown by pulsed laser deposition can have properties approaching those of diamond. In particular, we have measured thin films of this material that are 90 percent as hard and stiff as crystalline diamond, classing them as the second hardest material known to man. In addition, these films are electrically resistive, have low friction coefficient, and have extremely low wear rates, thus earning the name of amorphous diamond. One major limitation of these films is that very large compressive stresses (10 GPa) are generated during growth. This ultimately limits many applications of amorphous diamond (in particular tribological applications) since thicker films are often required. However, it has been demonstrated that simple thermal annealing treatments can *completely* relax the residual stress in these films. Surprisingly, the films retain their diamond-like nature with only minor changes in the bonding structure due to the annealing procedure. A detailed understanding of the stress relaxation in amorphous diamond is emerging from this work. Importantly, this understanding is predictive and is being used to guide applications development for this new material. In particular, stress relief enables the production of arbitrarily thick films and very thin large-area free-standing membranes. These thick films and membranes have applications in tribological coatings, X-ray and/or electron transparent windows and sensors; and as a material for microelectromechanical (MEMS) devices.

Keywords: Coatings, Stability, MEMS

330. **PHYSICS OF PHOTOSENSITIVITY IN NOVEL THIN FILMS**
$250,000
DOE Contact: Bharat Agrawal, (301) 903-2057
SNL Contact: Gerry Hays, (505) 844-4135

Photosensitive (PS) materials permanently change their refractive index upon exposure to intense light, enabling a wide range of integrated optical device structures to be rapidly patterned via a single, direct-write optical process step. This project is attempting to merge the development of highly photosensitive films with existing efforts to introduce optical subsystems into the enduring stockpile to produce relevant photonic devices with unique functionality. The ability to produce highly photosensitive germanosilicate thin films using a novel sputtering approach has been developed and has enabled the largest reported Δn ($-5x10^{-3}$) in as-synthesized materials. In addition, control of processing parameters has allowed engineering, at an atomic level, the defect interactions responsible for the PS response of our films. As a result, the unique ability now exists to control not only the magnitude of the optical response of our films, but also the sign of the induced refractive index change. Optical data transmission and signal manipulation offer significant advantages over more conventional, electronic approaches. Commercial telecommunications and remote sensing technologies rely on the ultrafast data transfer rates, insensitivity to signal interference, and robust physical design that characterize photonic systems based on both optical fibers and waveguides. These characteristics can also provide enhanced nuclear weapons safety in DOE/DP applications as efforts continue at Sandia to integrate optical systems into the enduring stockpile.

Keywords: Optical Materials, Photosensitivity

331. **THE SHOCK PROPERTIES OF PZT 95/5**
$200,000
DOE Contact: Bharat Agrawal, (301) 903-2057
SNL Contact: George Samara, (505) 844-6653

Although pulsed power devices utilizing shock-induced depoling of the ferroelectric ceramic PZT 95/5 have been in use for many years, an important responsibility currently being addressed is the design and certification of several new devices. A strong desire to progress beyond the historical "build and test" approach has resulted in a substantial effort to achieve accurate numerical simulations of device operation. A major challenge at the start of this effort, however, was the fact that very few studies of the complex dynamic behavior of poled PZT 95/5 had been conducted during the past twenty years. Consequently, an extensive experimental program was started to provide insight and well-characterized data for the development of improved models for PZT 95/5. Initially, this study addressed the mechanical behavior of unpoled PZT 95/5 over the range of axial stresses of interest (5 to 50 kbar). Planar impact techniques were used with both PVDF film gauges and laser interferometry (VISAR) to characterize wave evolution under conditions that examined the FE to AFE phase transition and dynamic pore collapse. Current emphasis is placed on shock-induced depoling of samples that are either normally or axially poled (poled perpendicular or parallel to the intended shock motion, respectively). Twenty experiments examined the depoling process and corresponding wave evolution over the full range of impact stresses. The database now available represents a substantial challenge to the ongoing development of improved models for PZT 95/5. However, successful simulation of these planar experiments, together with a number of multi-dimensional experiments planned for the coming year, will signify the achievement of an essential goal in the effort to accurately simulate the operation of pulsed power devices.

Keywords: Ferroelectrics, Shock Physics, Power Supplies

332. **THE PROPERTIES AND PHYSICS OF RELAXOR FERROELECTRICS**
$150,000
DOE Contact: Bharat Agrawal, (301) 903-2057
SNL Contact: George Samara, (505) 844-6653

Complex mixed oxides based on Pb $(Zr_{1-x}Ti_x)O_3$, or PZT, find several applications in nuclear weapons components. One such material based on Pb $(Zr_{.70}Ti_{.30})O_3$, is PBZT-Bi which is used in explosively-driven pulsed power sources. The substitution of Ba^{2+} for Pb^{2+} ions and the addition of a small amount of Bi impart unto this material slim loop ferroelectric (SFE) character and properties qualitatively different from those of PZTs and other normal ferroelectrics. PBZT and related mixed perovskites with random site disorder represent a class of materials referred to as relaxors or relaxor ferroelectrics. Their properties have not been studied in any detail and the physics is not understood. The combined effects of temperature, hydrostatic pressure, frequency, and dc biasing fields on the electrical properties are being investigated along with the complementary differential scanning calorimetry, X-ray diffraction and TEM measurements. The results of the work make it clear that the properties and physics of these materials are very different from those of normal ferroelectrics. Thus, models developed to describe the response of ferroelectrics such as the PZTs will be inappropriate for Relaxors. The present work will provide the basis for an appropriate model.

Keywords: Ferroelectrics, Performance Modeling, PBZT-Bi

333. **PHOTONIC BAND GAP STRUCTURES AS A GATEWAY TO NANO-PHOTONICS**
$375,000
DOE Contact: Gerald Green, (202) 586-8377
SNL Contact: Mial Warren, (505) 844-7208

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

Keywords: Photonics, Bandgap, Epitaxy

334. **THE INITIATION AND PROPAGATION OF NANO- SCALE CRACKS AT AN ADHESIVE/SOLID INTERFACE**
$400,000
DOE Contact: Gerald Green, (202) 586-8377
SNL Contact: Michael Kent, (505) 845-8178

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

335. **FUNDAMENTAL ASPECTS OF MICROMACHINE RELIABILITY**
$370,000
DOE Contact: Gerald Green, (202) 586-8377
SNL Contact: Terry Michalske, (505) 844-5829

A fundamental basis for designing micromechanical devices with high yield, reliable performance and long life is lacking. Mechanical design tools for macro-scale machines relate reliability to inertial forces. However, the performance of micron-scale structures of high aspect ratio is dominated by surface forces. The technical goal of this project is to use experimental reliability results obtained directly from micromachined test structures to develop and verify mechanics models containing interaction terms appropriate to the micron scale (e.g., capillarity, van der Waals forces, electro statics). Issues to be addressed include auto-adhesion (stiction), friction and wear. Microbridge structures with varying geometry and surface properties (e.g., roughness, chemical coatings) are being designed and built. Deformations are being monitored by interferometry in an environmental chamber. Finite element models incorporating new surface elements are being developed, verified and refined by comparing against experimental results. An additional objective is to investigate friction and wear using smart micro machined structures that enable self-diagnosis by electrical monitoring of capacitance and Q factor changes. Optical detection technique is being explored. Dynamical response models incorporating internal friction terms as well as damping are being verified and refined using experimental results. Friction due to energy loss at rubbing surfaces can then be extracted.

This project is developing a new tool set based on an experimental and theoretical foundations. The tool set can be used to calculate and characterize reliability of micromachines for integrated microsystem applications.

Keywords: Micromachine, Reliability

336. **INTELLIGENT POLYMERS FOR NANODEVICE PERFORMANCE CONTROL**
$400,000
DOE Contact: Gerald Green, (202) 586-8377
SNL Contact: Roger Clough, (505) 844-3492

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

337. **QUANTUM DOT ARRAYS**
$450,000
DOE Contact: Gerald Green, (202) 586-8377
SNL Contact: George Samara, (505) 844-6653

This project integrates two areas of Sandia research to fabricate new molecularly engineered, cluster-based, nanocomposite materials. First, Sandia has patented the inverse micellar synthesis of highly monodisperse metal and semiconductor nanoclusters, or "quantum dots." These 10-100 Å nanoclusters have many interesting properties, including large catalytic activity, room temperature luminescence, size dependent bandgaps, etc., and are sufficiently monodisperse that size-dependent cluster properties can be easily resolved. However, these clusters are currently stable only in the reaction bath. Second, Sandia has developed an expertise in synthesizing bulk periodic mesoporous materials by templating silica around liquid crystalline surfactant assemblies. These surfactant-templated porous materials (STPMs) are similar to zeolites, but the unit cell size is 40Å versus the 4-8Å typical for zeolites. These are the first periodic materials whose uniform pore size is commensurate with the typical dimensions of quantum dots. These new materials should be an ideal matrix for quantum dots; moreover, the quantum dots should form a highly periodic array, which may give rise to a host of new coherent phenomena. The goal of this project is to synthesize a new class of materials, "Quantum Dot Arrays" (QDAs), that consists of metal or semiconductor clusters periodically arrayed in an isolating silica matrix. Such cluster-based materials will have unique optical, catalytic, and dielectric properties: gold clusters in silica would give a high dielectric material for super capacitors; low work function clusters could make a good field emitter; luminescent silicon clusters could make optical arrays; supported nanocluster catalysts could be made as thin films.

Keywords: Quantum Dot, Nanocluster

338. **MOLECULAR CHARACTERIZATION OF ENERGETIC MATERIAL INITIATION**
$60,000
DOE Contact: Gerald Green, (202) 586-8377
SNL Contact: Lloyd L. Bonzon, (505) 895-8989

Sandia has responsibility for a diverse mix of energetic materials (EMs) and components. Determining the microscale chemical and physical responses of EMs to abnormal thermal environments is fundamental to understanding the safety of these EMs. The high explosive HMX (1,3,5,7-tetranitro-1,3,5,7-tetraazacyclooctane) is an energetic material used in many applications and Sandia-responsible components. The high temperature polymorph (designated d-HMX) is of special concern due to our recent discovery that it appears to control reaction progress for thermal initiation. The solid-solid phase transition of HMX is dependent on pressure and temperature, with high pressures favoring the less sensitive b-HMX and high temperatures favoring the sensitive d-HMX. We believe we have established a clear link between the HMX b-d phase transition and increased reactivity, sensitivity to initiation and subsequent burning. However, sampling techniques used in our preliminary tests are not amenable to most component configurations. We propose to develop an in situ probe to monitor the phase transition using Raman spectroscopy and second harmonic generation detection, both of which distinguish the two phases. Probe development and incorporation of second harmonic generation detection into the probe will be the main focus of the project. Following development of the experimental probe, the phase behavior of HMX and HMX-containing plastic bonded explosives (PBXs) will be studied at elevated temperatures and pressures relevant to component and system cookoff environments. Understanding the rate and extent of the solid-solid phase transition as functions of confinement, pressure, temperature, particle size and density at time of cookoff is vital to improving our safety analyses of the material. We will apply this experimental development to monitor the kinetics of the phase transition and how the phase transition affects subsequent decomposition and cookoff. These results will be used to further Sandia's Hazard Analysis Program (funded by the Office of Munitions).

Keywords: Energetic Materials, Raman Spectroscopy

339. **INNOVATIVE EXPERIMENTAL AND COMPUTATIONAL DIAGNOSTICS FOR MONITORING CORROSION IN WEAPONS ENVIRONMENTS**
$300,000
DOE Contact: Gerald Green, (202) 586-8377
SNL Contact: Julia M. Phillips, (505) 284-3093

This project is advancing capabilities to detect and quantify aluminum alloy degradation in atmospheric environments by leveraging expertise in nano-fabrication technology to produce electrode microstructures and micro-electrochemical test platforms amenable to testing in thin adsorbed water layers. Planar arrays of individually addressable microelectrodes are used to perform both passive and perturbing electrochemical testing under conditions in which conventional electrochemical techniques are not applicable. Precisely engineered sample microstructures make it possible to systematically vary material characteristics and derive causal relationships with atmospheric degradation. Secondary phases in Al alloys can polarize surrounding material due to galvanic interactions, and many proposed degradation mechanisms include galvanic driving force as a critical component. In order to understand how secondary phases affect corrosion, it is necessary to describe the potential and current distributions on a sample surface. A meso-scale electrical model is being developed to incorporate arbitrary second phase distributions and variable adsorbed electrolyte morphology in order to predict combinations of environment and microstructure that enhance the propensity for galvanic degradation. Particle-particle interactions as well as particle-matrix interactions are taken into account. To predict material performance in atmosphere it is also necessary to describe the absorbed environment. Surface acoustic wave (SAW) technology provides a means of detecting a fraction of a monolayer change in adsorbed species. By nano-fabricating electrodes on a SAW platform, we can determine how microstructure and geometry impact water adsorption. SAW devices can also be used to sense changes in the acoustic properties of material oxides due to damage accumulation, and may operate as early warning sensors for atmospheric degradation. Efforts will also be made to spatially resolve SAW signals to determine where as well as when damage initiates. The focusing of speciment design, electrochemical measurements, modeling and environmental characterization to the mesoscale level is critical to lifetime predictions in stockpile environments.

Keywords: Corrosion

340. **LINKING ATOMISTIC COMPUTATIONS WITH PHASE FIELD MODELING**
$352,000
DOE Contact: Gerald Green, (202) 586-8377
SNL Contact: Stephen M. Foiles, (505) 844-9781

The phase field model has proven to be a very powerful tool for modeling microstructural evolution during complex materials processing techniques. Although the method can be used to study grain growth and particle coarsening, the phase field model is particularly effective in predicting dendrite formation and solute redistribution during solidification and is therefore very useful in the numerical modeling of joining operations–welding, soldering and brazing. To date most of the work utilizing the phase field concept has focused on the development of the numerical technique and the study of generic microstructures; microstructure modeling applied to specific alloy systems has been rare. The lack of direct comparison between model predictions and actual microstructures in real alloys stems from the fact that many materials parameters-mobilities, free energies, surface energies, gradient energy coefficients, etc.—required as input in the phase field model and often these parameters are difficult to obtain experimentally. The purpose of this project is to employ atamistic calculations to obtain numerical values of all parameters necessary to model microstructural evolution. We plan to concentrate our initial efforts on the Cu-Ni system which represents a model brazing alloy.

Keywords: Computational Materials Science, Modeling of Materials Properties

341. **A COMBINATORIAL MICROLAB INVESTIGATION OF CRITICAL COPPER-CORROSION MECHANISMS**
$600,000
DOE Contact: Gerald Green, (202) 586-8377
SNL Contact: Charles Barbour, (505) 844-5517

An important aspect in developing a capability to predict stockpile reliability is a physics-based understanding of atmospheric corrosion. Corrosion modeling is hindered by limited knowledge of primary mechanisms and large numbers of coupled chemical reactions, which depend on complex interactions of materials with environment and functionality. This multidimensional problem requires fundamentally new experimental approaches which can provide timely quantitative information on critical phenomena occurring in corrosion phase space. We are combining parallel miniature experimentation with ultrasensitive microanalytical techniques to efficiently explore this phase space and identify mechanisms and kinetics for copper sulfidation in the Microdomain Laboratory. This approach differs from convention by focusing on microscopic length scales, the relevant scale for corrosion. Combinatorial experiments (arrays of microlabs) will quantify the direct and synergistic effects of morphological and metallurgical variables (alloying, defect density in the Cu oxide and bulk, diffusivities, porosity), environmental variables (sulfur content in air, light exposure, water droplet size and distribution versus humidity), and functionality (e.g., electric-current conduction). Novel diagnostics include conductivity microsensors to locally quantify pH_2O and pH_2S, in-situ electrical conductivity and light scattering to monitor real-time evolution of corrosion reactions, local ion-selective potentiometric monitoring of reaction products, and ultimately microcalorimetry sensors. This LDRD enables a new and rapid approach to determine physical models for complex chemical processes of key importance to ASCI and other DOE technology needs.

Keywords: Corrosion, Combinatorial Techniques

342. **MICROSCALE SHOCK WAVE PHYSICS USING PHOTONIC DRIVER TECHNIQUES**
$400,000
DOE Contact: Gerald Green, (202) 586-8377
SNL Contact: George A. Samara, (505) 844-6653

The goal of this program is to establish a new capability for conducting shock wave physics experiments at low per-experiment costs through a significant reduction in experimental length and time scales. Based on the earlier development of laser-based optical detonator technology at Sandia, this new capability will utilize the rapid absorption of optical energy from large, Q-switched, solid-state lasers to accelerate small planar films (a launch process known as photonic driving). The films subsequently impact another material, generating shock waves in both materials having amplitudes and durations that depend on the impact velocity and film thickness, respectively. Sub-nanosecond interferometric diagnostics were developed previously to examine the motion and impact of these films. To address a useful range of materials and stress states, photonic driving levels must be scaled up considerably from optical detonator levels. An order of magnitude increase permits the study of the dynamic mechanical behavior of materials having thicknesses up to 10s of microns. Some important materials, such as polycrystalline silicon (the basic structural material in surface micromachines), can be studied at this stage. An additional order of magnitude increase is the goal of the second program year. To enable practical studies of the shock wave response of a broad range of materials, however, photonic driving levels at least three orders of magnitude above detonator levels are necessary, and this is the final objective of this program. At these levels the dynamic behavior of materials up to a fraction of a millimeter thick can be studied, including a number of materials of current interest (such as materials in shock-activated components). However, significant increases in laser energies pose sever challenges to be overcome with respect to laser-induced damage in optics, beam shaping, thermally driven phase transitions in the laser-accelerated materials, and instabilities in these materials during acceleration.

Keywords: Shock Wave Physics, Microscale Materials Characterization

343. WETTING AND SPREADING DYNAMICS OF SOLDER AND BRAZE ALLOYS

$600,000
DOE Contact: Gerald Green, (202) 586-8377
SNL Contact: Terry A. Michalske, (505) 844-5829

The purpose of this program is to develop a scientific understanding of the microscopic processes that control wetting and spreading dynamics in materials systems related to soldering and brazing. The program exploits new advances in experimental surface science techniques and atomistic modeling methods to study wetting and spreading phenomena on length scales that range from Angstroms to microns. The unique imaging capabilities of the low energy electron microscope (LEEM) and the scanning tunneling microscope (STM) are being used to test the validity of atomic potentials being developed to simulate wetting and spreading dynamics. The LEEM is also being used to measure the spreading behavior of small molten droplets on well-characterized metal surfaces. The extent to which the flow properties at these small length scales obey classical wetting and spreading models will being determined by continuum mechanics calculations. More detailed information on the flow behavior will be obtained from molecular dynamics simulations. Building on these results, the investigations will be extended to braze alloys and how active components promote spreading on inert substrates.

Keywords: Materials Joining

344. IMPROVED MATERIALS AGING DIAGNOSTICS AND MECHANISMS THROUGH 2D HYPERSPECTRAL IMAGING METHODS AND ALGORITHMS

$363,000
DOE Contact: Gerald Green, (202) 586-8377
SNL Contact: Julia M. Phillips, (505) 284-3093

Twenty years ago, new quantitative multivariate spectral analysis methods caused a quantum leap in the capabilities of quantitative spectroscopy over previous univariate methods. The opportunity now exists to make a more significant revolution in the capabilities of quantitative spectral analyses. By combining the massive amounts of data generated using new commercial 2-dimensional (2D) infrared (IR) imaging spectrometers with the Sandia invention of powerful new hyperspectral information extraction algorithms, the ability will soon exist to perform quantitative spectroscopy without the need for calibration standards. This will enable rapid 2D spectral images of aging polymeric and energetic materials to directly extract pure-component spectra of all spectrally active chemical species in samples, which will include the spectra of degradation products. This information combined with hyperspectral analysis algorithms will facilitate accurate compositional maps of materials with low-micrometer spatial resolution. This new work will be able to directly impact materials degradation diagnostics by distinguishing multiple aging mechanisms and activation energies and by greatly improving infrared sensitivity and chemical selectivity. The chemical specificity and spatial mapping of 2D IR spectroscopy will allow quantification of degradation products to help understand degradation mechanisms, kinetics, and diffusion. In the first year of this project, the scheduled milestones have been met and exceeded. New proprietary algorithms for improved spectral image analysis have been programmed on both single-processor and parallel-processor computers, tested on various data sets, and their impact demonstrated when applied to the non-image spectral data from aged materials of importance in the stockpile stewardship program.

Keywords: Hyperspectral Image Analysis, FT-IR Spectroscopy, Chemometrics

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

345. **WIDE-BANDGAP COMPOUND SEMICONDUCTORS TO ENABLE NOVEL SEMICONDUCTOR DEVICES PROJECT**
$290,000
DOE Contact: Gerald Green, (202) 586-8377
SNL Contact: Jerry Simmons, (505) 844-8402

This project is an interdisciplinary investigation into the growth and physical properties of wide-bandgap compound semiconductors for the purpose of enabling both optoelectronic and microelectronic device development. The AlGaInN material system is widely considered to be essential to the development of a wide array of UV and blue optical devices as well as high-temperature microelectronics. A critical limiting factor in the demonstration of advanced III-N based devices is the lack of an in-depth understanding of the physics and chemistry that govern the unique properties of these materials. This work focuses on two important areas in the development of these materials. A portion of the effort concentrates on understanding the growth of III-N materials by gas-source molecular beam epitaxy (GSMBE), specifically the effects of substrate preparation, substrate temperature, V/III ratio, and growth rate on the nucleation and growth of AlGaInN on 6H-SiC (0001) surfaces using *in situ* reflection high-energy electron diffraction (RHEED), reflection mass spectroscopy (REMS), and scanning tunneling microscopy (STM). In combination with efforts to study crystal growth processes in these materials, the physical properties of the AlGaInN material system are being investigated. Analytical investigations include calculations to determine band structure and development of a model for optical gain and lasing which will include an exact treatment of Coulomb effects. Steady state and time-resolved luminescence is used to evaluate the nature of defect states in these materials as well as to study the excitonic properties which are expected to be enhanced for wide-bandgap semiconductors. Magnetoluminescence experiments determine energy dispersion and effective masses and these results are directly compared with band structure calculations. Another aspect of the work is an evaluation of how various processing techniques which are relevant for device fabrication, such as post-growth annealing, reactive ion etching and implantation, affect the optical and electronic properties of the III-N materials.

Keywords: MBE, HEED, REMS, STM

346. **SCANNING PROBE-BASED PROCESSES FOR NANOMETER-SCALE DEVICE FABRICATION**
$442,600
DOE Contact: Gerald Green, (202) 586-8377
SNL Contact: Terry Michalske, (505) 844-5829

Nanometer-scale electronic device technology requires a novel physics base that includes fabrication processes, characterization techniques and materials properties allowing reliable performance of devices at this very small length scale. This program integrates and expands Sandia's expertise in scanning-probe based fabrication and characterization of nanostructures with capabilities in microelectronic fabrication to produce fully accessible nanostructures for electronic evaluation. The objective is an order of magnitude decrease in feature size compared to conventional fabrication technology. Approaches to nanostructure fabrication using scanning probe-based (STM, AFM) processes in combination with extensive device fabrication are being explored. For prototype device structures critical nanoscale components are being integrated with conventional test structures to allow full electrical accessibility. Two approaches to nanostructure fabrication are being explored: investigation of molecular layer resists based on simple adsorbed atoms and molecules which can be patterned by electron-induced desorption or reaction, and development of a more general AFM-based nanolithographic capability, based on anodic oxidation under an AFM tip. In parallel with these fabrication approaches, low temperature electrical measurements are being performed, and selected nanoelectronic devices are being fabricated and characterized.

Keywords: Nanoscale, Device Fabrication

347. **SURFACE MICROMACHINED FLEXURAL PLATE WAVE DEVICE INTEGRATED ON SILICON**
$600,000
DOE Contact: Gerald Green, (202) 586-8377
SNL Contact: Kent Schubert, (505) 844-5935

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

348. **NON-VOLATILE PROTONIC MEMORY**
$300,000
DOE Contact: Gerald Green, (202) 586-8377
SNL Contact: Gilbert V. Herrera, (505) 284-6701

A new principle for non-volatile memory devices has recently been discovered at Sandia, in which the space charge in the oxide layer of silicon/silicon dioxide/silicon structures can be rapidly changed by applied electric fields. Because of their simplicity, process-compatibility, and apparent radiation hardness, these structures may have great potential in low-power non-volatile memory applications. We are investigating two issues that stand between this technology and its incorporation into microelectronics fabrication, 1) formation of the memory state and 2) memory-retention stability. At present the memory state in the oxide is created by immersion in either forming gas (5% hydrogen in nitrogen), or rarified hydrogen, at ~600°C, but this process is neither optimized nor physically well understood. Furthermore, a central assumption that mobile protons are primarily responsible for the memory remains controversial. Our studies have included H-plasma treatment and we will attempt to implant protons directly into the oxide using an H-ion beam. Surface-sensitive techniques will be applied to the elucidation of the hydrogen anneal process and to determining its spatial uniformity, and whenever appropriate deuterium loading will be exploited to advantage. A variety of voltage-response measurements are currently underway to characterize not only memory retention, but the transport kinetics of these devices in general. Transport modeling is also in progress, as an aid in understanding the complex behavior that is being observed. The complementary goal of this investigation is to understand the chemistry of proton-induced memory activation via quantum molecular modeling.

Keywords: Non-Volatile Memories

INSTRUMENTATION AND FACILITIES

349. **ADVANCED ANALYTICAL TECHNIQUES**
$1,220,000
DOE Contact: Bharat Agrawal, (301) 903-2057
SNL Contact: Richard J. Salzbrenner, (505) 844-9408

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

LOS ALAMOS NATIONAL LABORATORY

350. **ENHANCED SURVEILLANCE CAMPAIGN**
$17,000,000
DOE Contacts: E. Cochran (301) 903-7330 and S. Zaidi (301) 903-3446
LANL Contacts: J. Martz (505) 667-2323 and G. Buntain (505) 667-4748

Nuclear weapons will be retained in the stockpile for lifetimes beyond the design intent and our experience. The Department of Energy [DOE] needs a technically sound basis for determining when stockpile systems must be refurbished or reconditioned before reliability or safety are impacted. If new refurbishment capability is needed, the DOE needs to know:

- When these capabilities must be operational and what the required capacity should be;
- If the capacity for existing facilities is adequate and when potential refurbishment for the various stockpile systems must be scheduled;
- A basis from which to characterize the functional reliability of aged components, as part of the annual assessment process.

The Enhanced Surveillance Campaign will protect the health of the stockpile by providing advance warning (through prediction and detection) of manufacturing and aging defects to allow refurbishment before performance or safety are impaired. We will strive to understand the science behind material and component aging to establish a predictive capability to support annual certification, refurbishment scope and timing, and nuclear weapon complex planning. The Campaign will provide diagnostics for screening of weapons systems to identify units that must be refurbished as well as for early detection of material or component aging trends or defects. We apply the knowledge we have gained to make improvements to the core Surveillance Program.

Keywords: Nuclear Weapons, Pits, Plutonium, CSA, Canned Subassembly, Case, High Explosive, Non-Nuclear Materials, Non-Nuclear Components, Systems, Reliability, Energetic Materials, Stockpile, Enhanced Surveillance, Campaign 8, Accelerated Aging

LAWRENCE LIVERMORE NATIONAL LABORATORY

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

351. ENGINEERED NANOSTRUCTURE LAMINATES
$2,000,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LLNL Contact: Troy W. Barbee, Jr., (925) 423-7796

Multilayers are man-made materials in which composition and structure are varied in a controlled manner in one dimension during synthesis. Individual layers are formed using atom by atom processes (physical vapor deposition) and may have thicknesses of from one monolayer (0.2nm) to hundreds of monolayers (>100nm). At this time more than 75 of the 92 naturally occurring elements have been incorporated in multilayers in elemental form or as components of alloys or compounds. In this work deposits containing up to 225,000 layers of each of two materials to form up to 500μ thick samples have been synthesized for mechanical property studies of multilayer structures.

These unique man-made materials have demonstrated extremely high mechanical performance as a result of the inherent ability to control both composition and structure at the near atomic level. Also, mechanically active flaws that often limit mechanical performance are controllable so that the full potential of the structural control available with multilayer materials is accessible. Systematic studies of a few multilayer structures have resulted in free-standing foils with strengths approaching those of whiskers, approximately 70 percent of theory. Also, new mechanisms for mechanically strengthening materials are accessible with nanostructure laminates.

Applications now under development include: coatings for aircraft gas turbine engines; EUV, soft X-ray and X-ray optics spectroscopy and imaging; high performance capacitors for energy storage; capacitor structures for industrial applications; high performance tribological coatings; strength materials; integrated circuit interconnects; machine tool coatings; projection X-ray lithography optics.

Keywords: Thin Films, Multilayer Technology

352. ENERGETIC MATERIALS STRATEGIC CHEMISTRY
$350,000
DOE Contact: Bharat Agrawal, (301) 903-6688
LLNL Contact: R. L. Simpson, (925) 423-0379

Vicarious nucleophilic substitution chemistry is being used to synthesize energetic materials. New explosive molecules are being synthesized. Alternate routes to existing molecules, such as TATB, have been developed.

Keywords: Examination, Explosive, Energetic, TATB

353. CHEETAH THERMOCHEMICAL CODE
$190,000
DOE Contact: Bharat Agrawal, (301) 903-6688
LLNL Contact: R. L. Simpson, (925) 423-0379

A thermochemical code for the prediction of detonation performance is being developed. In addition to detonation performance, thermochemical calculations of impetus and specific impulse for propellant applications may also be made.

Keywords: Examination, Explosive, Energetic, TATB

354. EXPLOSIVES DEVELOPMENT
$900,000
DOE Contact: Bharat Agrawal, (301) 903-6688
LLNL Contact: R. L. Simpson, (925) 423-0379

New explosives are being developed for hard target penetrators. The goals include insensitivity to shock loading and significantly higher energy density than that of currently available materials.

Keywords: Explosive

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

355. **INTERFACES, ADHESION, AND BONDING**
$265,000
DOE Contact: Iran L. Thomas, (301) 903-6688
LLNL Contact: Wayne E. King, (925) 423-6547

The experimental effort is producing results that are directly comparable with theoretical calculations. Planar metal/metal interfaces and metal/ceramic interfaces (in anticipation of improvements in the theory) of well defined misorientations are being investigated. In order to span the entire range of length scales, macroscopic bicrystals a few millimeters thick, with interfacial areas on the order of a square centimeter, are required. In order to obtain such bicrystals, diffusion bonding is used. An ultra-high-vacuum diffusion bonding machine has been developed in parallel with this research project.

Keywords: Interfaces, Bonding, Electronic Structure

356. **LASER DAMAGE: MODELING AND CHARACTERIZATION**
$400,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LLNL Contact: T. Diaz de la Rubia, (925) 422-6714

The objective of this project is to understand the mechanisms for laser-induced damage in optical materials used in high-peak-power laser systems such as the National Ignition Facility (NIF). The material system of primary interest is polished fused silica surfaces. The primary characterization tools used in the studies include luminescence spectroscopy and microscopy, total internal reflection microscopy (TIRM), near-field scanning optical microscopy (NSOM), and photothermal microscopy (PTM). Efforts are focused on the understanding of damage growth due to successive pulses and the mitigation of the growth through removal of the damaged material. The damage growth rate determines the functional lifetime of the optic in the laser system. The dependence of the damage growth rate on laser wavelength, pulse length, and pulse repetition rate is being determined. Also of interest is the influence of optic environment (air vs. vacuum) on the damage processes.

Keywords: Silica, Luminescence, Laser Damage

INSTRUMENTATION AND FACILITIES

357. **SCANNING TUNNELING MICROSCOPY (STM), ATOMIC FORCE MICROSCOPY (AFM), NEAR FIELD SCANNING OPTICAL MICROSCOPY (NSOM)**
$250,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LLNL Contact: W. Siekhaus, (925) 422-6884

A large stage scanning probe microscope that can perform scanning tunneling as well as contact and non-contact atomic force microscopy on the surface of objects as large as 6" in diameter, a small stage modified so that it can perform non-contact AFM and STM as well as nano-indentation, and an ultra-high vacuum instrument that can perform non-contact AFM and STM measurements and STM. An additional large-stage and a small stage scanning probe microbe have been added and modified to perform near field scanning probe microscopy.

Properties of Nano-scale Particles, Nanometer-scale clusters of various materials, deposited by laser ablation and by evaporation in a noble gas atmosphere onto various substrates are analyzed by AFM and STM to determine their size distribution and by optical spectroscopy and electron spectroscopy to determine their size-dependent optical properties and electronic Structure.

Optical properties of materials on the nanometer scale are being investigated by NSOM. NSOM analysis is restricted to the near field of the scanning probe, and hence is ideally suited to probe the evanescent field on the surface of optical material. NSOM is used to determine local field enhancement by surface irregularities and thus to establish the relationship between surface features and laser damage threshold.

Combined Scanning Probe Microscopy/Nano-Indentation is used to identify the local mechanical properties of composite materials such as fiber reinforced plastics, bone-, tooth- and arterial-tissue from healthy and diseased arteries, and also to identify aging-induced changes in local properties of materials in stockpile.

Keywords: NDE, Chemical Reaction, Stockpile Stewardship, Etching, Cluster, Nano-Indentation, Near Field Scanning Probe Microscopy, Optical Properties, Mechanical Properties, Biomaterials, Tooth, Artery, Bone

358. **ATOMIC LEVEL EXPLOSIVE CALCULATIONS**
$325,000
DOE Contact: Maurice Katz, (202) 586-5799
LLNL Contacts: Larry Fried, (925) 422-7796

A package of atomic-level calculations has been assembled that will allow design of new explosive molecules. The package includes calculations of solid density, heat of formation, chemical stability and sensitivity. This package is being tried on various new postulated compositions in concert with feedback from three organic and inorganic synthesis chemists. The intent is to couple Molecular Design with actual synthesis routes at the start so that the final selected design will be something with a good chance of being made in the lab. Several new target molecules were found with the system in FY98.

Keywords: Energetic Materials, High Explosives, Molecular Design, Detonation

359. **METASTABLE SOLID-PHASE HIGH ENERGY DENSITY MATERIALS**
$535,000
DOE Contact: Maurice Katz, (202) 586-5799
LLNL Contacts: H. Lorenzana, (925) 422-8982 and M. Finger, (925) 422-6370

Conventional energetic materials such as propellants, explosives and fuel cells store energy within internal bonds of molecules. This work is exploring the predicted existence of novel materials that are calculated to store two to four times the energy content per volume of existing explosives, a dramatic improvement in performance. Though the atomic components are similar to standard energetic materials, these new materials differ from conventional molecular systems in that they form infinite, three-dimensional networks of covalent bonds, otherwise known as extended solids. Every bond in these new systems is energetic; the result is a correspondingly larger storage of energy per volume. Specifically, pure nitrogen is calculated to be recoverable at ambient conditions as an energetic solid with three times the energy content of HMX, a very high performance explosive. Since these materials are predicted to exist at high pressures and high temperatures, experimental capabilities have been developed for synthesizing and characterizing such compounds at megabar pressures.

Keywords: Energetic Materials, High Energy Density Materials

360. **AFM INVESTIGATIONS OF CRYSTAL GROWTH**
$290,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LLNL Contact: J. J. DeYoreo, (925) 423-4240

The nanometer-scale morphology of crystalline surfaces exerts a strong control on materials properties and performance. While many researchers have studied vapor deposited metal and semiconductor surfaces grown far from equilibrium, few studies have given attention to the morphology of crystal surfaces grown from melts or solutions near equilibrium despite the fact that most bulk crystals are grown in this regime. Understanding the mechanisms of growth and the origin of defects in such crystals can impact materials performance in a number of fields including optics, electronics, molecular biology, and structural biology. This project is using atomic force microscopy (AFM) to investigate the growth of single crystal surfaces from solution in order to determine the mechanism of growth, the kinetics of step advancement, the effect of impurities, and the origin of defects.

This method has been applied to inorganic, organic and macromolecular crystals each of which serve as important model systems. These include KH_2PO_4, $CaCO_3$ doped with amino acids, molecular tapes of diketopipeizine derivatives, the protein canavalin and the satellite tobacco mosaic virus. The results of these investigations are providing an understanding of the fundamental physical controls during solvent mediated crystallization.

Keywords: Morphology, Crystal Surfaces, Atomic Force Microscopy

361. **POLYIMIDE COATING TECHNOLOGY FOR ICF TARGETS**
$500,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LLNL Contacts: R. Cook, (925) 422-3117 and Steve Letts, (925) 422-0937

This program has as its objective the development of a vapor based, high strength polyimide coating technology that will allow production of a smooth, 150 to 200μm polyimide ablator coating on a 2mm diameter capsule target for the National Ignition Facility (NIF).

Such targets should be strong enough to hold the full DT fuel load (about 300 atm) at room temperature, allowing us important flexibility in fielding these capsules for ignition experiments.

Keywords: Polymers, Laser Fusion Targets, Polyimide, Ablator

362. **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 and R. Wallace, (925) 423-7864

This program has as its objective the development of materials and processes that will allow sputter-deposition of up to 200μm of a uniform, smooth, high-Z doped Be-based ablator on a spherical hollow mandrel. Capsules made with this type of ablator have been shown by calculation to offer some important advantages as ignition targets for the National Ignition Facility (NIF). Emphasis in the past year has been on improving coating homogeneity and smoothness. Both new materials (glassy boron-beryllium alloys) and process modifications are being studied.

Keywords: Beryllium, Laser Fusion Targets, Ablator, Sputter Deposition

OFFICE OF FOSSIL ENERGY

	FY 1999
Office of Fossil Energy - Grand Total	$10,004,000
Office of Advanced Research	$10,004,000
Fossil Energy AR&TD Materials Program	$6,004,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$1,821,000
Development of Iron Aluminides	105,000
Ultrahigh-Temperature Cr-X Alloys	104,000
Mo-Si Alloy Development	150,000
Development of Modified Austenitic Alloys	151,000
Development of Recuperator Materials	85,000
Influence of Processing on Microstructure and Properties of Aluminides	168,000
Investigation of Electrospark-Deposited Coatings for Protection of Materials in Sulfidizing Atmospheres	12,000
Fabrication of Fiber-Reinforced Composites by Chemical Vapor Infiltration and Deposition	274,000
Compliant Oxide Coating Development	90,000
Development of Oxidation/Corrosion-Resistant Composite Materials and Interfaces	130,000
Modeling of Fibrous Preforms for CVD Infiltration	89,000
Development of a Commercial Process for the Production of Silicon Carbide Fibrils	161,000
Corrosion Protection of SiC-Based Ceramics with CVD Mullite Coatings	44,000
Ceramic Coating and Native Oxide Scales Evaluation	70,000
Development of Novel Activated Carbon Composites	238,000
Carbon Fiber Composite Molecular Sieves Technology Transfer	50,000
Materials Properties, Behavior, Characterization or Testing	$1,202,000
Oxide Dispersion Strengthened (ODS) Alloys	231,000
Investigation of the Weldability of Polycrystalline Iron Aluminides	64,000
Friction Welding of ODS Alloys	12,000
Evaluation of the Intrinsic and Extrinsic Fracture Behavior of Iron Aluminides	34,000
Investigation of Iron Aluminide Weld Overlays	39,000
In-Plant Corrosion Probe Tests of Advanced Austenitic Alloys	19,000
Corrosion and Mechanical Properties of Alloys in FBC and Mixed-Gas Environments	174,000
Optimization of Corrosion-Resistant Iron Aluminide Coatings and Claddings	160,000
Reduction of Defect Content in ODS Alloys	71,000
Corrosion Protection of Ultrahigh Temperature Intermetallic Alloys	200,000
Support Services for Ceramic Fiber-Ceramic Matrix Composites	24,000
Development of Nondestructive Evaluation Methods and Effects of Flaws on the Fracture Behavior of Structural Ceramics	174,000

OFFICE OF FOSSIL ENERGY (continued)

	FY 1999
Office of Advanced Research (continued)	
Fossil Energy AR&TD Materials Program (continued)	
Device or Component Fabrication, Behavior or Testing	$2,881,000
Materials and Components in Fossil Energy Applications Newsletter	60,000[1]
Development of Ceramic Membranes for Hydrogen Separation	344,000
Investigation of the Mechanical Properties and Performance of Ceramic Composite Components	47,000
Solid State Electrolyte Systems for Fuel Cells and Gas Separation	723,000
Improved Fuel Cell Materials and Economical Fabrication	39,000
Bismuth Oxide Solid Electrolyte Oxygen Separation Membranes	260,000
Metallic Filters for Hot-Gas Cleaning	50,000
Refractory Materials Issues in Gasifiers	96,000
Pd-Ag Membranes for Hydrogen Separation	96,000
High-Temperature Materials Testing in Coal Combustion Environments	550,000
Molecular Sieves for Hydrogen Separation	144,000
Oxide-Dispersion-Strengthened Fe_3Al Based Alloy Tubes: Application-Specific Development for the Power Generation Industry	44,000
Fatigue and Fracture Behavior of Cr-X Alloys	24,000
Management of the Fossil Energy AR&TD Materials Program	400,000
Gordon Research Conference Support	4,000
Advanced Metallurgical Processes Program	$4,000,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$2,200,000
Advanced Casting Technologies	1,160,000
Advanced Foil Lamination Technology	340,000
Advanced Titanium Processing	700,000
Materials Properties, Behavior, Characterization or Testing	$1,800,000
Advanced Refractory Research	600,000
Service Life Prediction	1,200,000

[1]Matching funding provided by EPRI.

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 the Advanced Research and Technology Development (AR&TD) Materials Program. The goal of the Fossil Energy AR&TD Materials Program is to provide a materials technology base to assure the success of coal fuels and advanced power generation systems being pursued by DOE-FE. The purpose of the Program is to develop the materials of construction, including processing and fabrication methods, and functional materials necessary for those systems. The scope of the Program addresses materials requirements for all fossil energy systems, including materials for coal fuels technologies and for advanced power generation technologies such as coal gasification, heat engines, combustion systems, and fuel cells. The Program is aligned with the development of those technologies that are potential elements of the DOE-FE Vision 21 concept, which aims to address and solve environmental issues and thus remove them as a constraint to coal's continued status as a strategic resource.

The principal development efforts of the Program are directed at ceramic composites for high-temperature (~1200°C) heat exchanger applications; new corrosion- and erosion-resistant alloys with unique mechanical properties for advanced fossil energy systems; functional materials, particularly metal and ceramic hot-gas filters and gas separation materials based on ceramic membranes (porous and ion transport) and activated carbon materials; and corrosion research to understand the behavior of materials in coal-processing environments. Included as part of the responsibilities of Oak Ridge National Laboratory (ORNL) on the Fossil Energy AR&TD Materials Program is, with DOE-ORO, the technical management and implementation of all activities on the DOE Fossil Energy Advanced Research and Technology Development (AR&TD) Materials Program. DOE-FE administration of the Program is through the Federal Energy Technology Center (FETC) and the Advanced Research Product Team.

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

363. **DEVELOPMENT OF IRON ALUMINIDES**
$105,000
DOE Contacts: F. M. Glaser, (301) 903-2784, V. U. S. Rao, (412) 892-4743, M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: M. L. Santella, (423) 574-4805

The objective of this task is to develop low-cost and low-density intermetallic alloys based on Fe_3Al with an optimum combination of strength, ductility, weldability, and corrosion resistance for use as components in advanced fossil energy conversion systems. Emphasis is on the development of iron aluminides for heat recovery applications in coal gasification systems.

Keywords: Alloys, Aluminides, Intermetallic Compounds

364. **ULTRAHIGH-TEMPERATURE Cr-X ALLOYS**
$104,000
DOE Contacts: F. M. Glaser, (301) 903-2784, V. U. S. Rao, (412) 892-4743, M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: C. T. Liu, (423) 574-4459

The objective of this task is to develop high-strength, oxidation- and corrosion-resistant intermetallic alloys for use as hot components in advanced fossil energy conversion and combustion systems to help meet the 65 percent efficiency goal of the Vision 21 Concept. The successful development of these alloys is expected to improve thermal efficiency through increased operating temperatures and decreased cooling requirements. The development effort will be devoted to *in-situ* composite alloys based on $Cr\text{-}Cr_2Nb$ and similar $Cr\text{-}Cr_2X$ (X = refractory elements) systems.

Keywords: Alloys, Chromium-Niobium, Corrosion, Intermetallic Compounds

365. **Mo-Si ALLOY DEVELOPMENT**
$150,000
DOE Contacts: F. M. Glaser, (301) 903-2784, V. U. S. Rao, (412) 892-4743, M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: J. H. Schneibel, (423) 574-4644

The objective of this task is to develop new-generation corrosion-resistant Mo-Si alloys for use as hot components in advanced fossil energy conversion and combustion systems. The successful development of Mo-Si alloys is expected to improve the thermal efficiency and performance of fossil energy conversion systems through increased operating temperatures, and to increase the service life of hot components exposed to corrosive environments at temperatures as high as 1600°C. This effort thus contributes directly to Vision 21, one goal of which is to significantly reduce greenhouse emissions. The effort focuses presently on Mo-Si-B alloys containing high volume fractions of molybdenum silicides and borosilicides.

Keywords: Alloys, Molybdenum, Silicon

366. **DEVELOPMENT OF MODIFIED AUSTENITIC ALLOYS**
$151,000
DOE Contacts: F. M. Glaser, (301) 903-2784, V. U. S. Rao, (412) 892-4743, 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

367. **DEVELOPMENT OF RECUPERATOR MATERIALS**
$85,000
DOE Contacts: F. M. Glaser, (301) 903-2784, V. U. S. Rao, (412) 892-4743, M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: R. W. Swindeman, (423) 574-5108

The purpose of this task is provide stainless steel technology that will assist Solar Turbines to design and construct an advanced recuperator for a simple cycle gas turbine.

Keywords: Alloys, Austenitics, Technology Transfer

368. **INFLUENCE OF PROCESSING ON MICROSTRUCTURE AND PROPERTIES OF ALUMINIDES**
$168,000
DOE Contacts: F. M. Glaser, (301) 903-2784, V. U. S. Rao, (412) 892-4743, M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: I. G. Wright, (423) 574-4451
Idaho National Engineering and Environmental Laboratory Contact: R. N. Wright, (208) 526-6127

This program will determine the influence of processing on improved properties of alloys based on the intermetallic compound Fe_3Al. Thermomechanical processing of these alloys will be pursued to improve their ambient and elevated temperature properties. The response of the microstructure to elevated temperature deformation and subsequent annealing will be characterized in terms of the establishment of equilibrium phases, equilibrium degree of long-range order, and secondary recrystallization. Oxide dispersion strengthened (ODS) alloys fabricated by reaction synthesis will be developed for improved high-temperature strength. Tensile properties of the ODS materials will be determined at room and elevated temperature and related to the microstructure. Creep properties of these alloys will be studied in detail and compared to current theories for creep strengthening by oxide dispersions. The processing/properties relationships determined using reaction-synthesized materials will be applied to more conventional high energy ball milled ODS alloys being developed at Oak Ridge National Laboratory (ORNL). Compositions of the dispersion strengthened Fe_3Al alloys will be determined in collaboration with the program at ORNL.

Keywords: Aluminides, Processing, Microstructure

369. **INVESTIGATION OF ELECTROSPARK-DEPOSITED COATINGS FOR PROTECTION OF MATERIALS IN SULFIDIZING ATMOSPHERES**
$12,000
DOE Contacts: F. M. Glaser, (301) 903-2784, V. U. S. Rao, (412) 892-4743, M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: I. G. Wright, (423) 574-4451
Pacific Northwest National Laboratory Contact: R. N. Johnson, (509) 375-6906

The purpose of this task is to examine the use of the electrospark deposition coating process for the application of corrosion-, erosion-, and wear-resistant coatings to candidate heat exchanger (including superheater and reheater) alloys. Materials to be deposited may include MCrAl, MCrAlY, highly wear-resistant carbides, and other hardsurfacing materials.

Keywords: Coatings, Materials, Deposition

370. **FABRICATION OF FIBER-REINFORCED COMPOSITES BY CHEMICAL VAPOR INFILTRATION AND DEPOSITION**
$274,000
DOE Contacts: F. M. Glaser, (301) 903-2784, V. U. S. Rao, (412) 892-4743, M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: T. M. Besmann, (423) 574-6852

The purpose of this task is to develop a process for the fabrication of fiber-reinforced ceramic composites having high fracture toughness and high strength. This process utilizes a steep temperature gradient and a pressure gradient to infiltrate low-density fibrous structures with gases, which deposit solid phases to form the matrix of the composite. Further development of this process is needed to fabricate larger components of more complex geometry and to optimize infiltration for shortest processing time, greatest density, and maximum strength. In addition, isothermal chemical vapor infiltration will be used to develop oxide-based composite systems for structural and thermochemical (solid oxide fuel cell) applications.

Keywords: Composites, Fiber-Reinforced, Ceramics

371. **COMPLIANT OXIDE COATING DEVELOPMENT**
$90,000
DOE Contacts: F. M. Glaser, (301) 903-2784, V. U. S. Rao, (412) 892-4743, M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: D. P. Stinton, (423) 574-4556

SiC-based materials in the form of sintered SiC, siliconized SiC, or SiC-matrix composites are being developed for use as heat exchangers in industrial waste incinerators and advanced fossil- or biomass-fueled power systems. Unfortunately, these SiC-based heat exchangers and filters are susceptible to corrosion by alkali metal salts at elevated temperatures. Protective oxide coatings typically crack and spall when applied to SiC substrates because of the large thermal expansion mismatch. The purpose of this task is to develop low-expansion, low-modulus corrosion-resistant coatings for Si-based ceramics and evaluate candidate materials in facilities at the DOE Federal Energy Technology Center.

Keywords: Ceramics, Oxides, Coatings

372. **DEVELOPMENT OF OXIDATION/ CORROSION-RESISTANT COMPOSITE MATERIALS AND INTERFACES**
$130,000
DOE Contacts: F. M. Glaser, (301) 903-2784, V. U. S. Rao, (412) 892-4743, M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: R. A. Lowden, (423) 576-2769

The performance and life of ceramic fiber-reinforced ceramic composites are diminished when they are exposed to fossil energy environments because of the corrosion of the composite constituents, especially the fiber and interface coating. Corrosives such as oxygen or steam can penetrate cracks formed in the ceramic matrix and react with the interface coating and fiber. Corrosion of the interface coating and attack of the fiber cause the mechanical properties to deteriorate and the composite to eventually fail. The purpose of this task is to develop fiber-matrix interface coatings that optimize the mechanical behavior of the ceramic composites at room temperature and at elevated temperatures, and protect the fibers from processing and corrosive environments typical of applications of interest to Fossil Energy programs.

Keywords: Composites, Ceramics, Fiber-Reinforced, Interfaces

373. **MODELING OF FIBROUS PREFORMS FOR CVD INFILTRATION**
$89,000
DOE Contacts: F. M. Glaser, (301) 903-2784, V. U. S. Rao, (412) 892-4743, M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: D. P. Stinton, (423) 574-4556
University of Louisville Contact: T. L. Starr, (502) 852-1073

There are two critical requirements for successful, ambient pressure CVD of solid oxide electrolyte films: maintain uniformity in thickness and composition over a reasonably large substrate, and avoid gas-phase nucleation that degrades film quality. The proposed research addresses both requirements and is based on the unique characteristics of stagnation point flow.

Stagnation point flow describes the characteristics of a fluid stream impinging upon a planar substrate. With this geometry, modeling of mass and energy transport between the stream and the substrate surface can be reduced to a one-dimensional, boundary layer problem. Further, with proper selection of flow conditions, the effective boundary layer thickness is essentially uniform over an appreciable portion of the substrate. Also, by utilizing a cold-wall design—cool stream impinging on a heated substrate—the "residence time at temperature" for the stream is small, minimizing gas phase reactions.

The proposed research shall investigate the application of stagnation point flow to the deposition of yttrium-stabilized zirconia (YSZ) solid electrolyte films. This program shall involve an experimental effort at ORNL and a modeling effort at the University of Louisville.

Keywords: Ceramics, Composites, Modeling

374. **DEVELOPMENT OF A COMMERCIAL PROCESS FOR THE PRODUCTION OF SILICON CARBIDE FIBRILS**
$161,000
DOE Contacts: F. M. Glaser, (301) 903-2784, V. U. S. Rao, (412) 892-4743, M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: D. P. Stinton, (423) 574-4556
ReMaxCo Technologies, Inc. Contact: R. D. Nixdorf, (423) 483-5060

The DOE Fossil Energy Program has an interest in silicon carbide fibrils as a material for high-temperature heat exchanger and recuperation components in advanced coal combustion plants. The purpose of this project is to develop a commercial process for the production of silicon carbide fibrils. The slow growth of the fibrils and excessive waste of raw materials have been the major impediments. This work is an effort to bring new technology solutions to the future volume production of silicon carbide fibrils.

Keywords: Ceramics, Composites, Fibrils, Modeling

375. **CORROSION PROTECTION OF SiC-BASED CERAMICS WITH CVD MULLITE COATINGS**
$44,000
DOE Contacts: F. M. Glaser, (301) 903-2784, V. U. S. Rao, (412) 892-4743, 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

376. **CERAMIC COATING AND NATIVE OXIDE SCALES EVALUATION**
$70,000
DOE Contacts: F. M. Glaser, (301) 903-2784, V. U. S. Rao, (412) 892-4743, M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: P. F. Tortorelli, (423) 574-5119

The purpose of this work is to generate the information needed for the development of improved (slow growing, adherent, sound) protective oxide coatings and scales. The specific objectives are to: (1) systematically investigate the relationships among substrate composition and surface oxide structure, adherence, soundness, and micromechanical properties, (2) use such information to predict scale and coating failures, (3) identify and evaluate compositions and synthesis routes for producing materials with damage-tolerant scales and coatings and (4) apply the approaches developed for surface oxide characterization to other ceramic coatings.

Keywords: Coatings, Corrosion

377. **DEVELOPMENT OF NOVEL ACTIVATED CARBON COMPOSITES**
$238,000
DOE Contacts: F. M. Glaser, (301) 903-2784, V. U. S. Rao, (412) 892-4743, M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: T. D. Burchell, (423) 576-8595

Hydrogen recovery technologies are required to allow the upgrading of heavy hydrocarbons to transport fuels, thus reducing the amount of carbon rejected during the conversion of fossil resources into hydrocarbon products. The purpose of this work is to develop carbon molecular sieves (CMS) starting with porous Carbon Fiber Composites (CFC) manufactured from petroleum pitch-derived carbon fibers. The Carbon Fiber Composite Molecular Sieves (CFCMS) will be utilized in Pressure Swing Adsorption (PSA) units for the efficient recovery of hydrogen from refinery purge gases, and for other gas separation operations associated with petroleum refining. Moreover, natural gas frequently contains large fractions of diluents and contaminants such as CO_2 and H_2S. CFCMS materials will be developed to effect the separation of diluents and contaminants from natural gas. Additionally, H_2O must be removed from natural gas to minimize pipeline corrosion. Novel separation techniques, that exploit the unique combination of properties of CFCMS, will be developed to effect the above-mentioned separations. The separation of air (O_2/N_2) is gaining importance because of the need for a compact separation system for vehicles powered by fuel cells. The combination of a suitably modified version of CFCMS and our electrical swing adsorption technology offers considerable potential for this application. Hence, research is being directed toward the tailoring of CFCMS for the separation of O_2/N_2.

Keywords: Carbon Fibers, Sieves, Composites

378. **CARBON FIBER COMPOSITE MOLECULAR SIEVES TECHNOLOGY TRANSFER**
$50,000
DOE Contacts: F. M. Glaser, (301) 903-2784,
V. U. S. Rao, (412) 892-4743, M. H. Rawlins,
(423) 576-4507
Oak Ridge National Laboratory Contact:
T. D. Burchell, (423) 576-8595

Hydrogen and methane gas recovery technologies are required to: (1) allow the upgrading of heavy hydrocarbons to transport fuels, thus reducing the amount of carbon rejected during crude oil refining and (2) improve the yield and process economics of natural gas wells. The purpose of this work is to develop carbon fiber composite molecular sieves (CFCMS) from porous carbon fiber composites manufactured from solvent extracted coal tar pitch derived carbon fibers.

Keywords: Carbon Products

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

379. **OXIDE DISPERSION STRENGTHENED (ODS) ALLOYS**
$231,000
DOE Contacts: F. M. Glaser, (301) 903-2784,
V. U. S. Rao, (412) 892-4743, M. H. Rawlins,
(423) 576-4507
Oak Ridge National Laboratory Contact:
I. G. Wright, (423) 574-4451

The purpose of this task is to address the materials-related barriers to expediting the use of oxide dispersion-strengthened (ODS) alloys in components which are required in DOE's Office of Fossil Energy Vision 21 processes to operate at temperatures higher than are possible with conventionally-strengthened alloys. Specific goals are to develop a detailed understanding of ODS alloy behavior in all phases of their use, including fabrication, service performance, life prediction, mode of failure, repair, and refurbishment. The scope of the effort includes the development of ODS iron-aluminum alloys that combine strength levels of the same order as commercially-available ODS-FeCrAl alloys, but with the superior resistance to high-temperature sulfidation and carburization attack demonstrated by the best iron aluminides. The data generated will form a resource for designers wishing to incorporate ODS alloys into components which may require modification of alloy processing to maximize strength or environmental resistance of particular forms of the alloys.

Keywords: Aluminides

380. **INVESTIGATION OF THE WELDABILITY OF POLYCRYSTALLINE IRON ALUMINIDES**
$64,000
DOE Contacts: F. M. Glaser, (301) 903-2784,
V. U. S. Rao, (412) 892-4743, 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

381. **FRICTION WELDING OF ODS ALLOYS**
$12,000
DOE Contacts: F. M. Glaser, (301) 903-2784,
V. U. S. Rao, (412) 892-4743, M. H. Rawlins,
(423) 576-4507
Oak Ridge National Laboratory Contact:
I. G. Wright, (423) 574-4451
The Welding Institute Contact:
P. L. Threadgill, 011-44-1223-891162

The purpose of this project is to establish that friction welding is a feasible method for joining iron aluminide tubes to other iron aluminide tubes, and to austenitic alloys. A companion objective is to establish optimized procedures for making welds, based on ambient temperature properties.

Keywords: Joining, Welding

382. EVALUATION OF THE INTRINSIC AND EXTRINSIC FRACTURE BEHAVIOR OF IRON ALUMINIDES
$34,000
DOE Contacts: F. M. Glaser, (301) 903-2784, V. U. S. Rao, (412) 892-4743, 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

383. INVESTIGATION OF IRON ALUMINIDE WELD OVERLAYS
$39,000
DOE Contacts: F. M. Glaser, (301) 903-2784, V. U. S. Rao, (412) 892-4743, 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

384. IN-PLANT CORROSION PROBE TESTS OF ADVANCED AUSTENITIC ALLOYS
$19,000
DOE Contacts: F. M. Glaser, (301) 903-2784, V. U. S. Rao, (412) 892-4743, 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

385. CORROSION AND MECHANICAL PROPERTIES OF ALLOYS IN FBC AND MIXED-GAS ENVIRONMENTS
$174,000
DOE Contacts: F. M. Glaser, (301) 903-2784, V. U. S. Rao, (412) 892-4743, M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: I. G. Wright, (423) 574-4451
Argonne National Laboratory Contact: K. Natesan, (708) 252-5103

The purposes of this task are to (1) evaluate mechanisms of oxidation, sulfidation, and breakaway corrosion in mixed gas atmospheres typical of both combustion and gasification systems, (2) develop an understanding of corrosion processes that occur in ceramic materials and surface modified alloys, (3) characterize the physical, chemical, and mechanical properties of surface scales that are resistant to sulfidation attack, (4) evaluate the role of deposits containing sulfur and/or chlorine and ash constituents in the corrosion behavior of metallic alloys, selected coatings, and monolithic/composite ceramics, and (5) evaluate the residual mechanical properties of materials after exposure in corrosive environments and quantify the effects of corrosion on the properties to enable life prediction of components.

Keywords: Corrosion, Gasification, Creep Rupture, Fluidized-Bed Combustion

386. **OPTIMIZATION OF CORROSION-RESISTANT IRON ALUMINIDE COATINGS AND CLADDINGS**
$160,000
DOE Contacts: F. M. Glaser, (301) 903-2784,
V. U. S. Rao, (412) 892-4743, M. H. Rawlins,
(423) 576-4507
Oak Ridge National Laboratory Contact:
P. F. Tortorelli, (423) 574-5119

The purpose of this task is to evaluate the high-temperature corrosion behavior of iron-aluminum alloys as part of the effort to develop highly corrosion-resistant iron-aluminide alloys and coatings for fossil energy applications consistent with the Office of Fossil Energy's Vision 21. One primary objective is to investigate the resistance of the alloys to mixed-oxidant (oxygen-sulfur-chlorine-carbon) environments that arise in the combustion or gasification of coal, including the determination of the influence of sulfur and other reactive gaseous species on corrosion kinetics and oxide scale microstructures and of long-term durability (including lifetime). A second objective is to maximize the high-temperature corrosion resistance of iron aluminides by examining the influence of alloying additions and oxide dispersoids on protective alumina scale formation and integrity.

Keywords: Corrosion, Aluminides, Mixed-Gas, Scales

387. ***REDUCTION OF DEFECT CONTENT IN ODS ALLOYS***
$71,000
DOE Contacts: F. M. Glaser, (301) 903-2784,
V. U. S. Rao, (412) 892-4743, M. H. Rawlins,
(423) 576-4507
Oak Ridge National Laboratory Contact:
I. G. Wright, (423) 574-4451
The University of Liverpool Contact:
A. R. Jones, 151-794-8026

The purpose of this work is to assess the sources of defects in oxide-dispersion-strengthened (ODS) alloys. Experiments to confirm key features of defects in ODS alloys shall be devised and performed, and recommendations shall be made for the reduction of defects in these alloys.

Keywords: Aluminides, Defects

388. **CORROSION PROTECTION OF ULTRAHIGH TEMPERATURE INTERMETALLIC ALLOYS**
$200,000
DOE Contacts: F. M. Glaser, (301) 903-2784,
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(423) 576-4507
Oak Ridge National Laboratory Contact:
P. F. Tortorelli, (423) 574-5119

The objective of this task is to develop high-strength, oxidation- and corrosion-resistant intermetallic alloys for use as hot components in advanced fossil energy conversion and combustion systems to help meet the 65 percent efficiency goal of the Vision 21 Concept. The successful development of these alloys is expected to improve thermal efficiency through increased operating temperatures and decreased cooling requirements. The development effort will be devoted to in-situ composite alloys based on $Cr\text{-}Cr_2Nb$ and similar $Cr\text{-}Cr_2X$ (X=refractory elements) systems.

Keywords: Corrosion, Chromium-Niobium, Mixed-Gas, Scales

389. **SUPPORT SERVICES FOR CERAMIC FIBER-CERAMIC MATRIX COMPOSITES**
$24,000
DOE Contacts: F. M. Glaser, (301) 903-2784,
V. U. S. Rao, (412) 892-4743, M. H. Rawlins,
(423) 576-4507
Oak Ridge National Laboratory Contact:
D. P. Stinton, (423) 574-4556
University of North Dakota Energy and
Environmental Research Center (UNDEERC)
Contact: J. P. Hurley, (701) 777-5159

This task will review and, if appropriate, propose modifications to plans, materials, and tests planned by researchers on the AR&TD Materials Program in work to test materials for coal-fueled energy systems. The changes shall be suggested in order to make the corrosion experiments more reflective of the actual conditions that will be encountered by the materials in the energy systems. UNDEERC shall accomplish this task by reviewing the major advanced energy system projects being funded by the DOE, and by working with the company's technical monitor and staff to prepare a summary of the expected corrosion problems. Both gasification and combustion systems will be included. Ceramic materials in two subsystems will be the focus of this work: (1) hot gas cleanup systems and (2) high-temperature heat exchangers. UNDEERC shall review and suggest improvements to materials testing procedures that are used to determine material behavior when used in hot-gas cleanup or heat exchanger applications. A limited amount of computer modeling and laboratory experimentation shall be a part of this effort.

Keywords: Composites, Ceramics, Fibers

390. **DEVELOPMENT OF NONDESTRUC TIVE EVALUATION METHODS AND EFFECTS OF FLAWS ON THE FRACTURE BEHAVIOR OF STRUCTURAL CERAMICS**
$174,000
DOE Contacts: F. M. Glaser, (301) 903-2784, V. U. S. Rao, (412) 892-4743, M. H. Rawlins, (423) 576-4507
Oak Ridge National Laboratory Contact: D. P. Stinton, (423) 574-4556
Argonne National Laboratory Contacts: W. A. Ellingson, (708) 252-5068 and J. P. Singh, (708) 252-5123

The purpose of this project is to study and develop acoustic and radiographic techniques and possible novel techniques such as nuclear magnetic resonance, to characterize structural ceramics with regard to presence of porosity, cracking, inclusions, amount of free silicon, and mechanical properties, and to establish the type and character of flaws that can be found by nondestructive evaluation (NDE) techniques. Both fired and unfired specimens are being studied to establish correlations between NDE results and failure of specimens.

Keywords: Nondestructive Evaluation, Ceramics, Flaws, Fracture

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

391. ***MATERIALS AND COMPONENTS IN FOSSIL ENERGY APPLICATIONS* NEWSLETTER**
$60,000[1]
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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

392. **DEVELOPMENT OF CERAMIC MEMBRANES FOR HYDROGEN SEPARATION**
$344,000
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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

393. **INVESTIGATION OF THE MECHANICAL PROPERTIES AND PERFORMANCE OF CERAMIC COMPOSITE COMPONENTS**
$47,000
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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

[1]Matching funding provided by EPRI.

394. SOLID STATE ELECTROLYTE SYSTEMS FOR FUEL CELLS AND GAS SEPARATION

$723,000

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This project seeks to develop functional ceramic materials for applications in fossil energy conversion and gas separation. This project is composed of the following activities: (1) Stability of Solid Oxide Fuel Cell (SOFC) Materials - Aging of fuel cell materials and interfaces under high dc current loads is the principal focus of this task. Aging processes are accelerated through the use of dc currents higher than typical of an operating solid oxide fuel cell. Alternative electrolyte and electrode materials are being developed that would enable operation at reduced temperature and/or at higher efficiencies. (2) Gas Separation Using Mixed-Conducting Ceramic Membranes - Mixed ion and electron-conducting metal oxide ceramics are being developed that can be used to passively separate oxygen of high purity from air. Other uses include application as the cathode in an SOFC operating at reduced temperatures, as the membrane in a reactor to produce synthesis gas, and in the partial oxidation of hydrocarbons to produce more valuable products. This task seeks to develop promising ceramic membrane compositions and forms, to characterize the electrical, physical, and chemical properties of these ceramics, and to demonstrate applications on a laboratory scale. (3) Bismuth Oxide-Based Gas Separation Membranes - In collaboration with Oak Ridge National Laboratory (ORNL), this task will develop bismuth oxide-based solid electrolytes for use in driven oxygen separation membranes. Such compositions offer exceptionally high ionic conductivities, at least a factor of ten higher than zirconia at moderate temperatures. Research at ORNL will focus on the synthesis of alkaline earth-doped bismuth oxide electrolytes, structural characterization, and the development of processing techniques. Research at PNNL will focus on the evaluation of electrical and mechanical properties, on processing methodology, and on compatible electrode development.

Keywords: Fuel Cells, SOFC, Membranes Testing

395. IMPROVED FUEL CELL MATERIALS AND ECONOMICAL FABRICATION

$39,000

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East Tennessee Technology Park Contact: D. E. Fain, (423) 574-9932

The purpose of this project is to develop and demonstrate the capability of porous materials technology existing at the East Tennessee Technology Park as a low-cost fabrication process for the production of air electrodes for the Westinghouse Electric Company's tubular solid oxide fuel cell.

Keywords: Fuel Cells, SOFC

396. BISMUTH OXIDE SOLID ELECTROLYTE OXYGEN SEPARATION MEMBRANES

$260,000

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The purpose of this task is to develop bismuth oxide-based ionic conducting solid electrolytes for use as oxygen separation membranes. To produce efficient materials which will be competitive with existing materials and processes will require experimental studies in the following areas: optimization of the crystal chemistry of the solid solutions of bismuth oxide to maximize the oxygen ion transport at moderate operating temperatures, development of processing techniques which will enhance the orientation texture of the ceramic for increased ionic transport; and characterization and evaluation of the performance of selected compositions for comparison with competing materials and technologies.

Keywords: Membranes

397. METALLIC FILTERS FOR HOT-GAS CLEANING
$50,000
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The objective of this study is to design and develop metallic filters having uniform, closely controlled porosity using a unique spherical powder processing and sintering technique. The corrosion resistance of the filter materials will be evaluated under simulated PFBC/IGCC gaseous environments in order to determine the optimum alloy composition and filter structure. The corrosion tests will also provide a means to estimate the service lives of experimental filter materials when subjected to either normal or abnormal PFBC/IGCC plant operating conditions. Metallic filters are expected to offer the benefits of non-brittle mechanical behavior and improved resistance to thermal fatigue compared to ceramic filter elements, thus improving filter reliability. Moreover, the binder-assisted powder processing and sintering techniques to be developed in this study will permit additional filter design capability (e.g., highly controlled filter porosity/permeability with greatly enhanced processing simplification), thus enabling more efficient and effective filtration.

Keywords: Filters

398. REFRACTORY MATERIALS ISSUES IN GASIFIERS
$96,000
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The purpose of this research is to characterize and understand slag component interactions with the refractories used in coal gasifiers. It is anticipated that once these interactions are understood, it will be possible to find a means of controlling, i.e., limiting, the slag-refractory interactions and extending the refractory lifetime.

Keywords: Refractories

399. Pd-Ag MEMBRANES FOR HYDROGEN SEPARATION
$96,000
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The Palladium Membrane Reactor was developed for processing tritiated water and tritiated hydrocarbons found in fusion energy, weapons, and environmental applications. In addition to these applications, the PMR has the potential to revolutionize fossil fuel processing. However, in order to use the PMR in fuel applications, further performance data and development are needed. A state-of-the-art PMR will be used to evaluate performance and determine the best operating conditions for production of pure hydrogen from coal gas. The PMR has only been tested at atmospheric pressure, whereas coal-gas processing will need to be done at higher pressures. Performance at elevated pressures will be determined. Coal gas contains impurities such as sulfur that are potentially poisonous to PMRs. This effect will be determined. Also, in order to make the technology practical for industrial use, a higher flux Pd membrane is needed. Such a membrane has been developed at Los Alamos. An advanced PMR will be constructed with the high-flux membrane and tested with simulated coal gas. Successful demonstration of the advanced PMR could lead to a radical decrease in the cost of fossil fuel processing.

Keywords: Membranes

400. HIGH-TEMPERATURE MATERIALS TESTING IN COAL COMBUSTION ENVIRONMENTS
$550,000
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Structural and functional materials used in solid- and liquid-fueled energy systems are subject to gas- and condensed-phase corrosion, and erosion by entrained particles. The material temperature and composition of the corrodents determine the corrosion rates, while gas flow conditions and particle aerodynamic diameters determine erosion rates for a given material. Corrodent composition depends on the composition of the fuel, the temperature of the material, and the size range of the particles being deposited. It is difficult to simulate under controlled laboratory conditions all of the possible corrosion and erosion mechanisms to which a material may be exposed in an energy system. Therefore, the University of North Dakota Energy & Environmental Research Center and the U.S. Department of Energy, National Energy Technology Laboratory are working with Oak Ridge National Laboratory to provide materials scientists with no-cost opportunities to expose materials in pilot-scale systems to conditions of corrosion and erosion similar to those in occurring in commercial power systems.

NETL is operating the Combustion and Environmental Research Facility (CERF). In recent years, the 0.5 MMBtu/hr CERF has served as a host for exposure of over 60 ceramic and alloy samples at ambient pressure as well as at 200 psig (for tubes). Samples have been inserted in five locations covering 1700-2600F, with exposures exceeding 1000 hours. In the present program, the higher priority metals are to be tested at 1500-1600 F in one CERF location and near 1800-2000F at other locations to compare results with those from the EERC tests.

Keywords: Testing

401. **MOLECULAR SIEVES FOR HYDROGEN SEPARATION**
$144,000
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The purpose of this program is to develop and test three novel inorganic-organic materials for hydrogen separation and purification. The program will combine experimental and theoretical efforts to develop and test the following three materials as the working thin film in asymmetric Interfacial composite membranes (on alumina supports): In-situ generated bridged polysilsesquioxanes, organic templated silicates and catalytic membranes. (1) bridged polysilsesquioxanes belong to a class of hybrid organic-inorganic materials with thermal stability to 500°C and resistance to acids, strong bases and organic solvents. The organic bridging group can be varied to give an enormous range of materials with differing physical and chemical properties, including hydrogen permeation, (2) Organic templated silicates are designed to exhibit greater thermal and chemical stability while still forming the molecular sieving layer in asymmetric membranes. These materials are prepared from silane precursors whose organic group chemically reacts during the membrane formation to generate the membrane. (3) We will team these synthetic strategies with catalyst syntheses such as micelle-mediated preparation of metal nanoclusters to generate a revolutionary catalyst separation system combining highly dispersed metal nanoclusters in hybrid membranes with precisely modulated permselectivity. These catalytic membranes will provide a technology to perform reactions such as hydrogen reforming and the water shift reaction on-line. Pure hydrogen is removed from the reaction zone with a subsequent advantage to the reaction equilibrium.

Keywords: Membranes

402. **OXIDE-DISPERSION-STRENGTHENED Fe_3Al-BASED ALLOY TUBES: APPLICATION-SPECIFIC DEVELOPMENT FOR THE POWER GENERATION INDUSTRY**
$44,000
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University of California at San Diego Contact: Bimal K. Kad, (619) 534-7059

The objective of this work is to explore experimental and computational means by which inherent material and processing-induced anisotropies of ODS Fe_3Al-base alloys can be exploited to meet in-service mechanical and creep-life requirements of the power generation industry. The research shall examine microscopic and microstructural issues with a view to addressing optimum material design for macroscopic components under well prescribed in-service loading criteria. The economic incentive is the low cost of Fe_3Al-based alloys and its superior sulfidation resistance, in comparison to the competing Fe-Cr-A1 base alloys and the Ni-base superalloys currently in service.

The development of suitable ODS Fe_3A1 materials and processes shall endeavor to achieve high mechanical strength at temperature, as well as prolonged creep-life in service. Post-deformation recrystallization or zone annealing processes shall be examined as necessary to increase the grain size and to modify the grain shape for the anticipated use.

Keywords: Alloys

403. **FATIGUE AND FRACTURE BEHAVIOR OF Cr-X ALLOYS**
$24,000
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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 are conducted for the purpose of evaluating crack initiation and fatigue life of Cr_2Nb-based alloys as well as other intermetallic alloys.

Keywords: Alloys

404. **MANAGEMENT OF THE FOSSILENERGY AR&TD MATERIALS PROGRAM**
$400,000
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The goal of the Fossil Energy AR&TD Materials Program is to provide a material technology base to assure the success of coal fuels and advanced power generation systems being pursued by DOE-FE. The purpose of the program is to develop the materials of construction, including processing and fabrication methods, and functional materials necessary for those systems. The scope of the program addresses materials requirements for all fossil energy systems, including materials for coal fuels technologies and for advanced power generation technologies such as coal gasification, heat engines, combustion systems, and fuel cells. The program is aligned with the development of those technologies that are potential elements of the DOE-FE Vision 21 concept, which aims to address and solve environmental issues and thus remove them as a constraint to coal's continued status as a strategic resource.

The principal development efforts of the program are directed at ceramic composites for high-temperature (~1200°C) heat exchanger applications; new corrosion- and erosion-resistant alloys with unique mechanical properties for advanced fossil energy systems; functional materials, particularly metal and ceramic hot-gas filters and gas separation materials based on ceramic membranes (porous and ion transport) and activated carbon materials; and corrosion research to understand the behavior of materials in coal-processing environments. Included as part of the responsibilities of Oak Ridge National Laboratory (ORNL) on the Fossil Energy AR&TD Materials Program is, with DOE-ORO, the technical management and implementation of all activities on the DOE Fossil Energy Advanced Research and Technology Development (AR&TD) Materials Program. DOE-FE administration of the program is through the Federal Energy Technology Center (FETC) and the Advanced Research Product Team.

Keywords: Management, Materials Program

405. **GORDON RESEARCH CONFERENCE SUPPORT**
$4,000
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The task provides funds for partial support of the annual Gordon Research Conference.

Keywords: Technology Transfer

ADVANCED METALLURGICAL PROCESSES PROGRAM

The materials program at the Albany Research Center (ARC), formerly with the Bureau of Mines, incorporates Advanced Metallurgical Processes that provide essential life-cycle information for evaluation and development of materials. The research at ARC directly contributes to FE objectives by providing information on the performance characteristics of materials being specified for the current generation of power systems, on the development of cost-effective materials for inclusion in the next generation of fossil fired power systems, and for solving environmental emission problems related to fossil fired energy systems. The program at ARC stresses full participation with industry through partnerships and emphasizes cost sharing to the fullest extent possible.

The materials research in the Program focuses on extending component service lifetimes through the improvement and protection of current materials, by the design of new materials, and by defining the service operating conditions for new materials in order to ensure their safe and effective use. This process involves developing a better understanding of specific failure modes for materials in severe operating environments, addressing factors which limit their current use in these environments, and by designing new materials and materials processing procedures to overcome anticipated usage challenges in severe operating environments, such as those typically found in fossil energy generating plants and in structures and supporting facilities associated with oil and gas production. Emphasis is placed on high-temperature erosion testing and modeling in environments anticipated for Vision 21 plants, on the development of sulfidation/oxidation resistant materials which can also resist thermal cycling for pressurized circulating fluidized bed reactors, the production of low-cost titanium for use as drill strings or coiled tubing in drilling applications, and repair and development of refractory materials for coal gasifiers.

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

406. ADVANCED CASTING TECHNOLOGIES

$1,160,000
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To develop modified austenitic stainless steels with performance characteristics necessary for process streams in advanced heat recovery and hot gas cleanup systems employed with advanced power generation systems (IGCC, PFBC and IGFC). The most difficult near term R&D challenges are development of hot gas particulate and sulfur cleanup systems employed with these advanced power generation systems. Primary focus is on the development of TiC-reinforced *cast* austenitic stainless steels with Al and Si additions for oxidation and sulfidation resistance.

Keywords: Alloys, Casting, Cast Austenitic Stainless Steel, Titanium Carbide

407. ADVANCED FOIL LAMINATION TECHNOLOGY

$340,000
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ARC researchers have developed a materials fabrication approach that utilizes dissimilar foils to produce a variety of materials (e.g., layered composites, monolithic metallic and intermetallic alloys). This technique has also been used to join dissimilar metals. The goal of this research is to use conventional deformation processing techniques (such as extrusion or rolling) to bond foils to substrates and to each other.

Keywords: Alumindes, Coatings, Foil-Lamination Process

408. ADVANCED TITANIUM PROCESSING

$700,000
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Nearly 50 percent of the cost of titanium can be attributed to fabrication. Currently, all wrought products are produced from cylindrical ingot which must be broken down in multiple steps of forging and rolling. The process, although more lengthy, is analogous to the same process that was once used to make wrought steel products prior to the advent of continuous casting. A similar continuous and lower cost process to prepare commercially pure titanium and titanium alloys in a variety of shapes including slab, plate, and billet would reduce costs, increase the usage of titanium, and lead to environmental benefits and energy savings. A successful conclusion of this project will result in a continuous melting and ingot making process that directly utilizes titanium sponge or scrap. Development of a melting process to produce a billet or slab surface finish that is suitable for rolling without the necessity of forging or other preparation will significantly increase yields and productivity.

Keywords: Titanium, Continuous Casting

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

409. ADVANCED REFRACTORY RESEARCH

$600,000
DOE Contact: Richard P. Walters, (541) 967-5873
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The emphasis of this high temperature material research has been driven by both short range industrial needs and long range issues in gasifiers. Program emphasis is on the following: (1) identifying material failure mechanisms, (2) identifying/ developing materials that will extend the lifetime of primary refractory liners in slagging gasifier systems, (3) developing ways to shorten system downtime caused by refractory maintenance and, (4) developing improved thermocouples/temperature monitoring techniques.

Keywords: Refractories

410. **SERVICE LIFE PREDICTION**
$1,200,000
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Abrasion and erosion are significant materials-related problems in the operation of fossil energy plants. Abrasion is a problem in the production of pulverized coal for use in the burners, and erosion is a problem in the daily operation of the plant. Improvements in abrasion and erosion resistance will result in higher efficiency, less maintenance, and less catastrophic failures in fossil energy plants. An understanding of how materials behave as a result of particle impact will be developed through understanding the contact mechanics of the impact process and by investigating and characterizing the damage inflicted on various materials by impact of particles.

Large temperature gradients and heat fluxes occur in turbines, heat exchangers, and walls of fossil energy power plants. The effects of temperature gradient and heat flux on oxidation, sulfidation, and hot corrosion rates and mechanisms are not well understood. This study also examines non- isothermal oxidation and hot corrosion.

Keywords: Abrasion, Erosion, Oxidation, Corrosion, Wear

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