DOE/SC-0040

ENERGY MATERIALS COORDINATING COMMITTEE (EMaCC)

Fiscal Year 2000

July 31, 2001

DEPARTMENT OF ENERGY · UNITED STATES OF AMERICA ·

Annual Technical Report

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

United States Government **Department of Energy**

memorandum

DATE: October 1, 2001

REPLY TO ATTN OF: Office of Science

SUBJECT: Energy Materials Coordinating Committee (EMaCC) Chairman's Report for Fiscal Year 2201

TO: James F. Decker, SC-1

Thru: Patricia M. Dehmer, SC-10 p.m.d 10/3/01
Iran L. Thomas, SC-13 ILT 10-3-01
William T. Oosterhuis, SC-132 WTO 10-2-01

As required by the Terms of Reference of the Energy Materials Coordinating Committee (EMaCC), I am submitting this memo to you as a report for the period of FY 2001. EMaCC provides a channel for discussions, information and coordination between the various materials-related programs within the Department of Energy. Through the forums of its meetings, topical seminars and its annual report, programmatic and budget information is shared and working relationships are established between the materials related programs in the Department.

EMaCC has six topical subcommittees, which conduct seminars surveying departmental materials program in their area of interest. These topical subcommittees are Electrochemical Technologies (Richard Kelley, SC-13), Metals (Sarah Dillich, EE-22), Radioactive Waste Containers (Matesh Varma, SC-13), Semiconductors (Jerry Smith, SC-13), Structural Ceramics (Charles Sorrell, EE-23), and Superconductivity (James Daley, EE-15).

The Energy Materials Coordinating Committee Annual Report (attached, DOE/SC-0040) provides an annual summary of non-classified materials-related research programs supported by various elements within the Department of Energy. The EMaCC Annual Report is a useful working tool for project managers who want to know what is happening in other divisions, and it provides a guide for persons in industry and academia to the materials program within the Department. The major task of EMaCC this year was to make the Annual Report a more user-friendly document by removing redundant program information and shortening the project summaries. In addition, useful contact person information for various programs within the Department is provided.

Five meetings of the coordinating committee were held during the past year. At these meeting representatives from the Office of Basic Energy Sciences, Office of Biological and Environmental Research, Office of Fusion Energy Sciences, Fossil Energy, Energy Efficiency and Renewable Energy, and Office of Nuclear Energy presented detailed information and priority on the materials program supported by their respective organizations. These presentations were very useful and will lead to better coordination of the materials program within the Department. Details on these presentations are given in the minutes from the EMaCC meetings.

I served as chairman of the Energy Materials Coordinating Committee during the past year, and David Hamilton (EE) served as the executive Secretary. For FY 2002, Uday Rao (FE) was elected by the voting representatives of EMaCC to serve as chairman, and Dale Koelling (SC) as Executive Secretary.

Matesh N. Varma
Chairman, EMaCC

Attachment

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Office of Basic Energy Science
Division of Materials Sciences
Germantown, MD 20874-1290

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INTRODUCTION

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

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

Electrochemical Technologies - Richard Kelly, 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-23 (202) 586-1514
Superconductivity - James Daley, EE-15 (202) 586-1165

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

Five meetings were scheduled for 2000-2001. The dates and minutes from the meetings are as follows:

Tuesday, October 3, 2000, 10:00 A.M.-11:30 A.M., Room E-141/GTN

Dr. Merril Smith from the Office of Power Technologies (OPT) presented an outline, objective and update of the Distributed Energy Resources (DER) program, with particular emphasis on the materials activities component of the program. Dr. Smith is the Program Manager for the DER program within the OPT. Budget for this program is approximately $50 million for FY 2001.

Dr. Charles Sorrell briefed on changes in the Materials Program supported by the Office of Industrial Technologies. He indicated that the subprogram "Continuous Fiber Ceramics Composites (CFCC)" will be completed by FY 2002. The Advanced Industrial Materials Program (AIM) will be transformed into a new program called "Industrial Materials of the Future (IMF)" and will consist of AIM and whatever is left from the CFCC program. It is the intention of the IMF program to open it to the laboratory as well as to the university community by FY 2004.

Tuesday, January 9, 2001, 10:00 A.M.-11:30 A.M., Room E-401/GTN

Dr. William Oosterhuis from the Office of Basic Energy Sciences (OBES) presented an overview of the programs within the Condensed Matter Physics and Materials Chemistry Team (Division of Materials Science and Engineering). Dr. Oosterhuis is the team leader and presented an outline of their organization and some examples of the research they are funding. Dr. Robert Gottschall from OBES presented an overview of the programs within the Metals, Ceramics and Engineering Team (Division of Materials Science and Engineering), of which he is the leader. He also gave a presentation outlining current areas of research and research highlights funded from that office. Dr. Bob Hwang, a detailee from Sandia National Laboratory-California was asked to describe one of the highlights concerning research performed by his group.

Dr. Paul Smith, also from OBES, acting team leader of the Molecular Processes and Geosciences Team (Chemical Sciences, Biosciences and Geosciences Division), described the materials-related projects funded by his team, indicating a few research highlights.

Dr. Gottschall suggested instituting a mechanism so that events of interest to others in EMaCC (e.g., on-site reviews or presentations) could be passed along. It was agreed that anyone knowing of events of interest would email the information to Dr. Varma, who would pass them along to the rest of the committee.

Tuesday, March 13, 2001, 10:15 A.M.-12:00 P.M., Room GH-035/GTN

Dr. Steve Johnson, Lawrence Berkeley National Laboratory, presented an overview of the Solid State Lighting Initiative and its cross-link to other DOE activities, including an update on the two dominant technologies, light-emitting diodes (LEDs) and organic light-emitting diodes (OLEDs).

Dr. Jerry Simmons, Sandia National Laboratory, made a presentation on LEDs, including a summary of the impact study, "A Market Diffusion and Energy Impact Model for Solid-State Lighting," and the white paper, "Inorganic LEDs for General Illumination."

Discussion followed on the application of these technologies.

Tuesday, June 12, 2001, 10:15 A.M.-12:05 P.M., Room E-114/GTN

Dr. Todd Allen from the Office of Nuclear Energy Sciences (NE) presented an overview of the programs within NE that deal with materials science. Dr. Allen is a detailee from Argonne National Laboratory and presented an outline of their organization and some examples of the materials research they are funding.

Dr. Larry James from the Office of Biological and Environmental Research (OBER) presented an overview of the programs within OBER. He also gave a presentation outlining current areas of research and research highlights funded from that office. Particular emphasis was placed on the materials research supported by OBER.

Dr.Uday Rao from the National Energy Technology Laboratory and Dr. Rod Judkins from Oak Ridge National Laboratory, representing the Office of Fossil Energy (FE), gave an overview of the advanced materials program, indicating a few research highlights.

The fifth EMaCC meeting for 2000-2001 was scheduled for September 11, 2001.

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 2000 and describes the materials research programs of various offices and divisions within the Department.

The EMaCC Chair for FY 2000 was Dr. Charles Sorrell. The compilation of this report was performed by Dr. David Hamilton, EMaCC Executive Secretary for FY 2001, with the assistance of the RAND Corporation.

Dr. Matesh Varma
Office of Science
EMaCC Chair, FY 2001

TABLE 1
ENERGY MATERIALS COORDINATING COMMITTEE MEMBERSHIP LIST

ORGANIZATION	REPRESENTATIVE	PHONE NO.
ENERGY EFFICIENCY AND RENEWABLE ENERGY		
Building Technology, State and Community Programs		
Building Research and Standards	Arun Vohra, EE-41	202/586-2193
Industrial Technologies		
Aluminum Vision Team	Sara Dillich, EE-22	202/586-7925
Industrial Materials of the Future	Charlie Sorrell, EE-23	202/586-1514
Transportation Technologies		
Advanced Automotive Technologies	Patrick Davis, EE-32	202/586-8061
	Joseph Carpenter, EE-32	202/586-1022
	Ray Sutula, EE-32	202/586-8064
	JoAnn Milliken, EE-32	202/586-2480
Heavy Vehicle Technologies	Sidney Diamond, EE-34	202/586-8032
Power Technologies		
Solar Energy Technologies	Richard King, EE-11	202/586-4198
Wind and Geothermal Technologies	Raymond LaSala, EE-12	202/586-1693
Hydrogen and Superconductivity Technologies	James Daley, EE-15	202/586-1165

ORGANIZATION	REPRESENTATIVE	PHONE NO.
SCIENCE		
Basic Energy Sciences		
Materials Sciences and Engineering	Pat Dehmer, SC-10	301/903-3081
	Iran L. Thomas, SC-13	301/903-3427
Metals, Ceramics and Engineering	Robert J. Gottschall, SC-13	301/903-3428
	Yok Chen, SC-13	301/903-3428
	Helen Kerch, SC-13	301/903-3428
Condensed Matter 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
	Robert S. Marianelli, SC-14	301/903-5808
Chemical Sciences, Geosciences and Biosciences	Nick Woodward, SC-14	301/903-4061
Advanced Scientific Computing Research		
Technology Research	Walter M. Polansky, SC-32	301/903-5995
	David Koegel, SC-32	301/903-3159
Fusion Energy Sciences		
Facilities and Enabling Technologies	Sam Berk, SC-52	301/903-4171
Biological and Environmental Research		
Medical Sciences	Larry James, SC-73	301/903-7481
Laboratory Operations and Environment, Safety and Health		
Environment, Safety and Health	Ted Tomczak, SC-83	301/903-6916
ENVIRONMENTAL RESTORATION AND WASTE MANAGEMENT		
Integration and Disposition		
Technical Program Integration	Doug Tonkay, EM-22	301/903-7212
Science and Technology		
Basic and Applied Research	Chet Miller, EM-52	202/586-3952

ORGANIZATION	REPRESENTATIVE	PHONE NO.
NUCLEAR ENERGY, SCIENCE AND TECHNOLOGY		
Technology and International Cooperation	Todd Allen, NE-20 William Van Dyke, NE-20	301/903-1647 301/903-4201
Nuclear Facilities Management	John Warren, NE-40 Bob Lange, NE-40	301/903-6491 301/903-2915
Space and Defense Power Systems	John Dowicki, NE-50	301/903-7729
NATIONAL NUCLEAR SECURITY ADMINISTRATION		
Naval Reactors	David I. Curtis, NR-1 Tom Kennedy, NR-1	202/781-6141 202/781-6124
Defense Programs		
Defense Science	Bharat Agrawal, DP-133	301/903-2057
CIVILIAN RADIOACTIVE WASTE MANAGEMENT		
Waste Acceptance and Transportation	Jim Carlson, RW-40	202/586-5321
FOSSIL ENERGY		
Advanced Research	Fred M. Glaser, FE-25	301/903-2786

ORGANIZATION OF THE REPORT

The FY 2000 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 2000 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 2000 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 2000 BUDGET SUMMARY OF DOE MATERIALS ACTIVITIES

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

	FY 2000
OFFICE OF BUILDING TECHNOLOGY, STATE AND COMMUNITY PROGRAMS	$955,000
Office of Building Systems	$955,000
OFFICE OF INDUSTRIAL TECHNOLOGIES	$21,438,373
Office of Industrial Strategies	11,282,000
Aluminum Vision Team	7,852,000
Forest and Paper Products Vision Team	300,000
Metal Casting Vision Team	1,900,000
Mining Vision Team	1,230,000
Office of Crosscut Technologies	10,156,373
Industrial Materials for the Future (IMF) Program	9,703,000
Financial Assistance Program	453,373
Inventions and Innovation	453,373
National Industrial Competitiveness Through Energy, Environment and Economic ($NICE^3$)	0
OFFICE OF TRANSPORTATION TECHNOLOGIES	$41,568,000
Office of Advanced Automotive Technologies	24,671,000
Transportation Materials Program	21,565,000
Automotive Propulsion Materials	3,110,000
Lightweight Vehicle Materials	18,455,000
Electric Drive Vehicle Technologies	3,106,000
Advanced Battery Materials	3,106,000
Office of Heavy Vehicle Technologies	16,897,000
Transportation Materials Technology	10,947,000
Heavy Vehicle Propulsion System Materials	10,947,000
High Strength Weight Reduction Materials	5,950,000
OFFICE OF POWER TECHNOLOGIES	$60,583,000
Office of Solar Energy Technologies	28,286,000
Office of Wind and Geothermal Technologies	897,000
Office of Hydrogen and Superconductivity Technologies	31,400,000

FY 2000 BUDGET SUMMARY OF DOE MATERIALS ACTIVITIES (Continued)

	FY 2000
OFFICE OF SCIENCE	$448,224,217
Office of Basic Energy Sciences	402,281,000
Division of Materials Science and Engineering	402,281,000
Office of Advanced Scientific Computing Research	37,343,217
Division of Technology Research	37,343,217
Laboratory Technology Research Program	4,152,000
Small Business Innovation Research Program	31,549,098
Small Business Technology Transfer Research Program	1,642,119
Office of Fusion Energy Sciences	8,600,000
OFFICE OF ENVIRONMENTAL MANAGEMENT	$3,260,572
OFFICE OF NUCLEAR ENERGY, SCIENCE AND TECHNOLOGY	$13,915,323
Office of Space and Defense Power Systems	2,871,000
Space and National Security Programs	2,871,000
Office of Technology and International Cooperation	11,044,323
Nuclear Energy Plant Optimization	3,985,011
Nuclear Energy Research Initiative	7,059,312
NATIONAL NUCLEAR SECURITY ADMINISTRATION	$116,511,000
Office of Naval Reactors	74,500,000[1]
Office of Defense Programs	42,011,000
The Weapons Research, Development and Test Program	42,011,000
Sandia National Laboratories	15,432,000
Los Alamos National Laboratory	19,951,000
Lawrence Livermore National Laboratory	6,628,000
OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT	$29,121,295
OFFICE OF FOSSIL ENERGY	$10,751,000
Office of Advanced Research	10,751,000
Fossil Energy Advanced Research Materials Program	6,751,000
Advanced Metallurgical Processes Program	4,000,000
TOTAL	**$746,327,780**

[1]This excludes $49.9 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.

TABLE 2
DISTRIBUTION OF FUNDS BY OFFICE

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	$7,972,000	$9,614,373	$3,852,000	$0	$21,438,373
Office of Transportation Technologies	$25,597,000	$12,155,000	$2,516,000	$1,300,000	$41,568,000
Office of Power Technologies	$44,180,000	$13,482,000	$1,584,000	$1,337,000	$60,583,000
Office of Science	$363,333,000	$51,500,000	$33,291,217	$100,000	$448,224,217
Office of Environmental Management	$1,834,333	$50,000	$1,359,572	$16,667	$3,260,572
Office of Nuclear Energy, Science and Technology	$7,397,983	$3,998,779	$2,518,561	$0	$13,915,323
National Nuclear Security Administration	$116,511,000	$0	$0	$0	$116,511,000
Office of Civilian Radioactive Waste Management	$29,121,295	$0	$0	$0	$29,121,295
Office of Fossil Energy	$9,172,000	$1,104,000	$475,000	$0	$10,751,000
TOTALS	**$606,073,611**	**$91,904,152**	**$45,596,350**	**$2,753,667**	**$746,327,780**

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 2000
OFFICE OF BUILDING TECHNOLOGY, STATE AND COMMUNITY PROGRAMS	$955,000
Office of Building Systems	$955,000
OFFICE OF INDUSTRIAL TECHNOLOGIES	$21,438,373
Office of Industrial Strategies	11,282,000
Aluminum Vision Team	7,852,000
Forest and Paper Products Vision Team	300,000
Metal Casting Vision Team	1,900,000
Mining Vision Team	1,230,000
Office of Crosscut Technologies	10,156,373
Industrial Materials for the Future (IMF) Program	9,703,000
Financial Assistance Program	453,373
Inventions and Innovation	453,373
National Industrial Competitiveness Through Energy, Environment and Economic ($NICE^3$)	0
OFFICE OF TRANSPORTATION TECHNOLOGIES	$41,568,000
Office of Advanced Automotive Technologies	24,671,000
Transportation Materials Program	21,565,000
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Office of Heavy Vehicle Technologies	16,897,000
Transportation Materials Technology	10,947,000
Heavy Vehicle Propulsion System Materials	10,947,000
High Strength Weight Reduction Materials	5,950,000
OFFICE OF POWER TECHNOLOGIES	$60,583,000
Office of Solar Energy Technologies	28,286,000
Office of Wind and Geothermal Technologies	897,000
Office of Hydrogen and Superconductivity Technologies	31,400,000

OFFICE OF BUILDING TECHNOLOGY, STATE AND COMMUNITY PROGRAMS

	FY 2000
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	30,000
Non-HCFC Closed-Cell Foam Insulation	250,000
Conventional Materials Performance	125,000
Hygrothermal Property Measurements	225,000
Sub-Ambient Pipe Insulation Materials and Systems	175,000
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**
   $30,000
   DOE Contact: Arun Vohra (202) 586-2193
   ORNL Contact: Ken Wilkes (865) 574-5931

This project is to continue long term aging 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. **CONVENTIONAL MATERIALS PERFORMANCE**
   $125,000
   DOE Contact: Arun Vohra (202) 586-2193
   ORNL Contact: Ken Wilkes (865) 574-5931

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. **HYGROTHERMAL PROPERTY MEASUREMENTS**
   $255,000
   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 moisture transfer in building envelopes.

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

5. **SUB-AMBIENT PIPE INSULATION MATERIALS AND SYSTEMS**
   $175,000
   DOE Contact: Arun Vohra (202) 586-2193
   ORNL Contact: Bill Miller (865) 574-2013

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 are 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

6. **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

7. **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 2000
OFFICE OF INDUSTRIAL TECHNOLOGIES - GRAND TOTAL	$21,438,373
OFFICE OF INDUSTRIAL STRATEGIES	$11,282,000
ALUMINUM VISION TEAM	$7,852,000
DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING	$5,104,000
Innovative Vertical Floatation Melter (VFM)	600,000
Inert Metal Anode Life in Low Temperature Aluminum Reduction Process	500,000
Advanced Anodes and Cathodes Utilized in Energy Efficient Aluminum Production Cells	347,000
Intelligent Potroom Operation	362,000
Development of a Novel Non-Consumable Anode for Electrowinning Primary Aluminum	409,000
Potlining Additives	679,000
Reduction of Oxidative Melt Loss of Aluminum	645,000
Selective Adsorption of Salts from Molten Aluminum	211,000
Aluminum Carbothermic Technology	679,000
Wetted Cathodes for Low Temperature Smelting	368,000
High Efficiency Low Dross Combustion System	304,000
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING	$401,000
Semi Solid Aluminum Alloys	155,000
Integrated Numerical Methods and Design Provisions for Aluminum Structures	90,000
Textures in Aluminum Alloys	156,000
MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING	$2,347,000
Recycling Aluminum Salt Cake	702,000
Processing and Recycling of Aluminum Wastes	399,000
Wettable Ceramic-based Drained Cathode Technology for Aluminum Electrolysis Cells	500,000
Spray Rolling Aluminum Strip	202,000
Modeling Optimization of Direct Chill Casting	544,000
FOREST AND PAPER PRODUCTS VISION TEAM	$300,000
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING	$300,000
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	0

OFFICE OF INDUSTRIAL TECHNOLOGIES (continued)

	FY 2000
OFFICE OF INDUSTRIAL STRATEGIES (CONTINUED)	
METAL CASTING VISION TEAM	$1,900,000
MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING	$281,000
Creep Resistant Zinc Alloy Development	132,000
Development of Surface Engineered Coatings for Die Casting Dies	149,000
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING	$1,619,000
Clean Cast Steel: 1) Machinability of Cast Steel; 2) Accelerated Transfer of Clean Steel Technology	332,000
Clean Metal Processing (Aluminum)	255,000
Advanced Lost Foam Casting Technology	325,000
Mechanical Properties Structure Correlation for Commercial Specification of Cast Particulate Metal Matrix Components	208,000
Ferrite Measurements in Duplex Stainless Steel Castings	70,000
Technology for the Production of Clean, Thin Wall, Machinable Gray and Ductile Iron Castings	215,000
Mold Materials for Permanent Molding of Aluminum Alloys	92,000
Systematic Microstructural and Corrosion Performance Evaluation of High Molybdenum Stainless Steel Casting	50,000
Development of a Fatigue Properties Data Base for Use in Modern Design Methods	72,000
MINING VISION TEAM	$1,230,000
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING	$260,000
Drilling and Blasting Optimization Using Seismic Analysis and X-ray Fluorescence Spectroscopy	260,000
DEVICE OR COMPONENT FABRICUATION, BEHAVIOR OR TESTING	$495,000
Application of High Temperature Superconductors to Underground Communications	357,000
Development of a Mine Compatible LIBS Instrument for Ore Grading	138,000
MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING	$475,000
Hydride Fuel Cell Mining Vehicles	275,000
Mining Byproduct Recovery	200,000

OFFICE OF INDUSTRIAL TECHNOLOGIES (continued)

	FY 2000
OFFICE OF CROSSCUT TECHNOLOGIES	$10,156,373
INDUSTRIAL MATERIALS FOR THE FUTURE (IMF) PROGRAM	$9,703,000
MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING	$3,050,000
Intermetallic Alloy Development and Technology Transfer of Intermetallic Alloys	570,000
Development of Advanced Metallic/Intermetallic Alloys	570,000
Composites and Coatings Through Reactive Metal Infiltration	300,000
Conducting Polymers: Synthesis and Industrial Applications	150,000
Membrane Systems for Efficient Separation of Light Gases	300,000
Plasma Processing - Advanced Materials for Corrosion and Erosion Resistance	250,000
Uniform Droplet Processing	350,000
Advanced Materials/Processes	560,000
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING	$3,480,000
Materials Development for the Forest Products Industry	780,000
Metals Processing Laboratory User (MPLUS) Facility	400,000
Continuous Fiber Ceramic Composites (CFCC) Supporting - Technologies	2,300,000
DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING	$3,173,000
Selective Inorganic Thin Films	200,000
Materials for High Temperature Filtration/Thermochemical Modeling	53,000
Continuous Fiber Ceramic Composites (CFCC) - Industrial - Technologies	2,920,000
FINANCIAL ASSISTANCE PROGRAM	$453,373
INVENTIONS AND INNOVATION	$453,373
DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING	$453,373
Laser Sensor for Optimization of Compressor Stations and Refinery Operations	0
Titanium Matrix Composite Tooling Material for Enhanced Manufacture of Aluminum Die Castings	0
An Insoluble Titanium-Lead Anode for Sulfate Electrolytes	0
Development of an Innovative Energy Efficient High Temperature Natural Gas Fired Furnace	0
A New High Temperature Coating for Gas Turbines	0
Tough-Coated Hard Powders (TCHPs): A New Paradigm in Mining and Machining Tool Materials	0
A New Energy Saving Method of Manufacturing Ceramic Products from Waste Glass	0
Distillation Column Flooding Predictor	0
Energy Saving Lightweight Refractory	0
High Intensity Silicon Vertical Multi-Junction Solar Cells	0
Fabrication and Testing of a Prototype Ceramic Furnace Coil	0
Germanium Compounds as Highly Selective Fluorination Catalysts	0

OFFICE OF INDUSTRIAL TECHNOLOGIES (continued)

	FY 2000
OFFICE OF CROSSCUT TECHNOLOGIES (CONTINUED)	
FINANCIAL ASSISTANCE PROGRAM (CONTINUED)	
INVENTIONS AND INNOVATION (CONTINUED)	
DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING (CONTINUED)	
Development of Phosphors for Use in High-Efficiency Lighting and Displays	0
Novel Ceramic Composition for Hall-Heroult Cell Anode Application	0
Functionally Graded Materials for Improved High Temperature Performance of Nd-Fe-B-Based Permanent Magnets	0
Improved Alkylation Contractor	0
Low Cost Synthesis and Consolidation of TiC	0
Development of Aluminum Iron Alloys for Magnetic Applications	0
Novel Frequency-Selective Solar Glazing System	0
A Ceramic Composite for Metal Casting	0
Electrochemical Method for Extraction of Oxygen From Air	0
Energy Saving Method for Producing Ethylene Glycol and Propylene Glycol	0
Improved Refractories Using Engineered Particles	0
Enabling Tool for Innovative Glass Applications	0
Distributed Optical Sensors for Continuous Liquid Level Tank Gauging	174,284
A Low Energy Alternative to Commercial Silica-Based Glass Fibers	199,089
Cromer Cycle Air Conditioning	40,000
Anaerobic Bioleaching Technology for Metals Release	40,000
NATIONAL INDUSTRIAL COMPETITIVENESS THROUGH ENERGY, ENVIRONMENT AND ECONOMICS (NICE^3)	**$0**
DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING	**$0**
Demonstration o: a Three-Phase Rotary Separator Turbine	0
Ceramic Turbine Wheel Technology To Provide Economic, Efficiency and Environmental Enhancements to Microturbines	0
Precision Irrigation Technologies for the Agricultural Industry	0
Energy Conserving Tool for Combustion Dependent Industries	0
Energy-Saving Regeneration of Hydrochloric Acid Pickling Liquor	0
Supercritical Fluid Purification of Combi-Chem Libraries	0
Full-Scale 100 Ton/Hr Demonstration of Magnetic Elutriation Technology for Clean and Efficient Processing of Iron Ore	0
Reducing Foundry Emissions and Green Sand Waste Via Integrated Advanced Oxidation-Underwater Plasma Processing	0

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

8. **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. Recycled aluminum accounts for more than one third of the total U.S. aluminum supply. Aluminum recycling results in significant energy savings, lower emissions and an increase in metal yield. Typically, aluminum scrap is cleaned/decoated and then melted in gas reverberatory furnaces that have low thermal efficiencies (20%) and generate substantial emissions. The vertical floatation melter is an innovative design that decoats, preheats and melts in one operation. The pilot demonstrated design provides a thermal efficiency of 58 percent. Not only is energy saved, but also the emissions are significantly reduced and more metal is recovered. The design provides a higher metal yield (dross reduction) because of lower gas temperature, lower residence time, lower oxygen content and no direct flame impingement on the metal. The VFM is a versatile design that can be integrated with indirect-fired controlled-atmosphere rotating kilns (IDEX™). This integration provides additional savings, with thermal efficiencies of over 75 percent in recovering aluminum scrap. This process also has applications in the glass and steel industries. A pilot scale unit capable of processing 1,000 pounds per hour of aluminum has been designed, constructed and successfully tested. Pilot operations have demonstrated a thermal efficiency (the ratio of heat going into scrap aluminum to that of the total energy used) of more than 2.5 times that of a conventional furnace, lower emissions and improved metal recovery (dross reduced by more than half). This project has now entered the planning, site preparation and field-testing phase that will demonstrate the VFM's commercial use.

Keywords: Floatation Melter, Aluminum Scrap

9. **INERT METAL ANODE LIFE IN LOW TEMPERATURE ALUMINUM REDUCTION PROCESS**
   $500,000
   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

10. **ADVANCED ANODES AND CATHODES UTILIZED IN ENERGY EFFICIENT ALUMINUM PRODUCTION CELLS**
$347,000
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

11. **INTELLIGENT POTROOM OPERATION**
$362,000
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

12. **DEVELOPMENT OF A NOVEL NON-CONSUMABLE ANODE FOR ELECTROWINNING PRIMARY ALUMINUM**
$409,000
DOE Contact: Simon Friedrich (202) 586-6759

Ohio State University assisted by Gas Research Institute, Kaiser Aluminum, 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

13. **POTLINING ADDITIVES**
$679,000
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 Virginia, Inc., EMEC Consultants, the NSA Division of Southwire Company and SGL Carbon Corporation.

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

14. **REDUCTION OF OXIDATIVE MELT LOSS OF ALUMINUM**
$645,000
DOE Contact: Tom Robinson (202) 586-0139

Fabrication of virtually all finished aluminum products requires melting. During the melting process, an average of 4 percent of the input material is lost to oxidation. The lost material takes three forms in the furnace: 1) dross, a mixture of aluminum oxide compounds and aluminum metal typically skimmed from the surface of the melt; 2) inclusions entrained in the molten metal removed by filtration; and 3) oxide sludge found at the bottom of the melt. In the U.S., an annual energy loss of approximately 70 trillion Btu results from oxidative melt loss of over 960 million pounds of aluminum. This project will target practices to significantly reduce these losses. The melt loss project will identify aluminum melting practices that will increase energy efficiency and decrease material losses. The project will lower the cost of aluminum products, reduce energy consumption, reduce industrial emissions, and significantly increase the recycling capability of the aluminum industry. An increased fundamental understanding of the oxidation of molten aluminum will be developed to be a cross-section of the aluminum industry. Project partners include Secat, Inc., Commonwealth Aluminum, Hydro Aluminum, IMCO Recycling Inc., NSA Division of Southwire Co., Alcan Aluminum Corp., ARCO Aluminum Inc., McCook Metals LLC, Albany Research Co., Argonne National Laboratory, Oak Ridge National Laboratory, and University of Kentucky.

Keywords: Dross, Aluminum Melting, Oxide Sludge

15. **SELECTIVE ADSORPTION OF SALTS FROM MOLTEN ALUMINUM**
$211,000
DOE Contact: Tom Robinson (202) 586-0139

Selee Corp. and Alcoa are project partners for the development of this Selective Adsorption technology. Primary aluminum is produced by the reduction of alumina in electrolytic cells. Cells contain a molten cryolite bath in which the alumina is dissolved. When an electric current is applied, aluminum is released and settles to the bottom of the cell. Molten aluminum is withdrawn to holding furnaces, and alumina is added to the bath as it is consumed. In normal production, a small portion of the bath is carried over with the molten aluminum. Most of the bath carry-over can be removed by careful skimming and good transfer practices. However, some carry-over of the bath to the metal holding furnace is common. Cryolite bath contains sodium and small amounts of calcium and lithium. These metal salts must be removed from aluminum in the holding furnace to produce metal of commercial value. Chlorine is used to remove these salts. Bath carry-over is undesirable because it adds significantly to the time required and the amount of chlorine used to make commercial aluminum. A new microporous material has been demonstrated to selectively adsorb salts from molten aluminum in holding furnace operations. This project will evaluate the potential of adapting these microporous materials to remove carry-over salts. Successful removal of these salts will result in significant reductions of energy, chlorine and metal loss.

Keywords: Alumina, Microporous Materials, Cryolite, Primary Aluminum

16. **ALUMINUM CARBOTHERMIC TECHNOLOGY**
$679,000
DOE Contact: Tom Robinson (202) 586-0139

Alcoa Technical Center, Elkem Aluminum Division, and Carnegie Mellon University are project partners for the development of the advanced reactor process (ARP). ARP is a new process for the production of aluminum by carbothermic reduction. This technology has been proposed as an alternative to the current Hall-Héroult electrolytic reduction process. ARP has the potential to produce primary aluminum at a power consumption in the range of 8.5 kWh/kg at an estimated 25 percent reduction in manufacturing cost. Although the carbothermic process involves the generation of carbon-based greenhouse gases (GHG), the total GHG reduction from power plant to metal should be substantial due to the significantly reduced power consumption, the elimination of perfluorocarbon emissions, and the elimination of carbon anode baking furnace emissions. The estimated capital investment required for ARP will be about 50 percent less than that for Hall-Héroult cell technology. The labor required for plant operation will also be reduced. ARP is a multi-step high temperature chemical reaction that produces aluminum by reduction of alumina with carbon. Optimization for reaction products requires a multi-zone furnace operating at temperatures in excess of 2,000°C. A significant portion of the aluminum is in the gas phase at these temperatures. A continuously operating furnace capable of producing the high temperatures required and recovering the molten and gas phase products is critical for the development of this technology. This is Phase I of a multi-phase effort to develop an ACT reactor based on advanced, high temperature, electric-arc furnace technology and improved understanding of the process reactions.

Keywords: Aluminum Carbothermic Reduction, Advanced Reactor Process, Alumina

17. **WETTED CATHODES FOR LOW TEMPERATURE SMELTING**
$368,000
DOE Contact: Tom Robinson (202) 586-0139

Wetted cathodes and inert anodes have potentially significant advantages over the century old Hall-Héroult cell used today for worldwide aluminum production. Wetted cathodes allow for decreased anode-cathode distances accompanied by reduced voltages and energy consumption. Inert anode replacement of conventional carbon anodes will eliminate the emission of greenhouse gases associated with the production of primary aluminum (e.g., CO, CO_2 and perfluoro-carbons) and with the manufacture of the carbon anodes. The use of wettable cathodes with inert anodes could reduce the energy needed for primary aluminum production by 25 to 30 percent. The adoption of these advanced electrodes has been hindered by their rapid corrosion, particularly of the cathode, when operating at a conventional temperature of 950°C. A low temperature electrolysis (LTE) cell that operates about 200°C lower than a conventional cell offers a more benign environment for advanced electrodes. This project will extend the knowledge of wetted cathode operation and failure mechanisms. It will prepare and screen various wetted cathode materials for aluminum LTE cells and develop techniques to measure and evaluate the aluminum film on the wetted cathode. Successful development of this technology will lower both capital and operating costs and offer many advantages in energy and environmental conservation. Project partners include Northwest Aluminum Technologies, assisted by Advanced Refractory Technologies, Material Modification Inc., Electrochemical Technology Corp., Brooks Rand Limited, and Pacific Northwest National Laboratory.

Keywords: Low Temperature Electrolysis, Inert Anode, Wetted Cathode

18. **HIGH EFFICIENCY LOW DROSS COMBUSTION SYSTEM**
$304,000
DOE Contact: Tom Robinson (202) 586-0139

Over 70 percent of 2.3 million tons of secondary aluminum recovered from scrap is processed in reverberatory furnaces. These furnaces are widely used because of their versatility and low capital cost. Despite their benefits, reverberatory furnaces exhibit uneven surface temperature and exposure to oxygen that promotes the production of dross on the surface of the molten aluminum. Dross formation lowers aluminum productivity and insulates the molten aluminum thereby lowering energy efficiency. This project will develop and demonstrate a high-efficiency low-dross combustion system for secondary aluminum natural gas-fired reverberatory furnaces. Oxygen enrichment is key to improving burner efficiency and has been demonstrated in many industries. Oxygen enriched flames are hotter than air-fired flames and can promote dross formation. However, new burners and controls allow for the control of the flame shape and distribution of oxygen within the flame. Controlling the flame with a fuel rich zone on the flame bottom ensures that the molten aluminum has minimal exposure to oxygen and minimizes dross formation. At the same time, control of the flame shape ensures that the surface is evenly heated. Upon successful completion, this project will decrease energy requirements, improve economics, and decrease gaseous and solid emissions from the remelting of aluminum. This technology can also be retrofitted to existing reverberatory furnaces. Project partners include Gas Technology Institute, assisted by Wabash Alloys, LLC, Eclipse Combustion Inc., and University of Illinois Chicago.

Keywords: Reverberatory Furnace, Low-Dross Combustion, Secondary Aluminum

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

19. SEMI SOLID ALUMINUM ALLOYS
$155,000
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
$90,000
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

21. TEXTURES IN ALUMINUM ALLOYS
$156,000
DOE Contact: Tom Robinson (202) 586-0139

Aluminum sheets made by continuous strip casting provide energy savings of greater than 26 percent and cost savings of more than 19 percent compared to sheets made from ingot casting and rolling. Sheet formability is among the most important characteristics of aluminum sheet. Formability depends on the crystal grain structure and is a result of the casting method and processing sequences used to produce the sheet. The demand for aluminum sheets is increasing particularly in the transportation industry where they are used to produce lighter, more fuel-efficient vehicles. As more complex forms are required, improved process controls are needed. Industry currently relies on post-processing testing to determine formability characteristics of finished sheet. The on-line monitoring of the continuously cast sheet production process will allow simultaneous control of important forming parameters. Crystallographic texture is related to the mechanical anisotropy/formability of metallic sheets. University of Kentucky and Commonwealth Aluminum will determine if there is a quantitative relationship between crystallographic texture measurements at processing temperatures and aluminum sheet formability. Data will be collected from two different spectroscopic measuring devices. This data will then be analyzed to determine if these instruments can produce measurements of the formability characteristics. The instrument proven to be most effective for measuring texture and formability at processing temperatures will be installed on-line in a production facility to demonstrate the ability to measure and control formability in continuous strip production.

Keywords: Textures in Aluminum Alloys, Crystallographic, Continuous Casting

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

22. **RECYCLING ALUMINUM SALT CAKE**
$702,000
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

23. **PROCESSING AND RECYCLING OF ALUMINUM WASTES**
$399,000
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

24. **WETTABLE CERAMIC-BASED DRAINED CATHODE TECHNOLOGY FOR ALUMINUM ELECTROLYSIS CELLS**
$500,000
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

25. **SPRAY ROLLING ALUMINUM STRIP**
$202,000
DOE Contact: Ramesh Jain (202) 586-2381
INEEL Contact: Kevin McHugh (208) 525-5713

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 percent 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

26. **MODELING OPTIMIZATION OF DIRECT CHILL CASTING**
$544,000
DOE Contact: Tom Robinson (202) 586-0139

The direct chill (DC) casting process is used for 68 percent of the aluminum ingots produced in the U.S. Ingot scrap from stress cracks and butt deformation account for a 5 percent loss in production. The basic process of DC casting is straightforward. However, the interaction of process variables is too complex to analyze by intuition or practical experience. The industry is moving toward larger ingot cross sections, higher casting speeds, and an increasing array of mold technologies to increase overall productivity. Control of scrap levels is important both in terms of energy usage and cost savings. Predictive modeling and increasing the general knowledge of the interaction effects should lower production losses to 2 percent. This reduction in scrap could result nationally in an estimated annual energy savings of over six trillion Btu and cost savings of over $550 million by 2020. The DC casting model project focuses on developing a detailed model of heat conditions, microstructure evolution, solidification, strain/stress development, and crack formation during DC casting of aluminum. This model will provide insights into the mechanisms of crack formation, butt deformation, and aid in optimizing DC process parameters and ingot geometry. Project partners include Secat Inc., assisted by Alcan Aluminum Corp., ARCO Aluminum Inc., Logan Aluminum Inc., McCook Metals, LCC, Wagstaff Inc., Albany Research Co., Argonne National Laboratory, Oak Ridge National Laboratory, and University of Kentucky.

Keywords: Aluminum Ingot, Direct Chill Casting, Aluminum Scrap

FOREST AND PAPER PRODUCTS VISION TEAM

The DOE works in partnership with the forest products industry through the American Forest and Paper Association to develop cleaner, more energy-efficient technologies and processes to boost the productivity and profitability of the forest and paper products industry. The goals of the program are to reduce net purchased electricity to zero by 2020, reduce the average water effluent by 35 percent by 2015 and to reduce the recovered paper utilization rate to 50 percent by 2010. The DOE Forest and Paper Products Team contact is Valri Robinson (202) 586-0937

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

27. **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

28. **SELECTION AND DEVELOPMENT OF REFRACTORY STRUCTURAL MATERIALS FOR BLACK LIQUOR GASIFICATION**
$0
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

METAL CASTING VISION TEAM
The DOE Metal Casting program manager is Harvey Wong (202) 586-9235

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

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

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

30. **DEVELOPMENT OF SURFACE ENGINEERED COATINGS FOR DIE CASTING DIES**
$149,000
DOE Contact: Ehr Ping HuangFu (202) 586-1493
Colorado School of Mines Contact: John Moore (303) 273-3770

The objective of this research project is to develop a coating system that minimizes premature die failure (heat checking, erosive and corrosive heat), and extends die life. No single (monolithic) coating is likely to provide the optimum system for any specific die casting application that will require its own specially designed "coating system." An optimized coating system will require a multi-layer "architecture" within which each layer provides a specific function, e.g. adhesion to the substrate, accommodation of thermal and residual stresses, wear and corrosion/oxidation resistance and non-wettability with the molten metal. The initial research project will concentrate on developing a coating system for dies used in die casting aluminum alloys. The measured outcomes from this research program will quantify comparisons of current aluminum die casting practice with the measured results using the newly developed coating systems. A comparison of cost/performance will also be determined for the new coating systems using current cost data as the baseline.

Keywords: Surface Coatings, Multi-Layered Surface Coatings, Die Casting, Die Casting Dies

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

31. **CLEAN CAST STEEL: 1) MACHINABILITY OF CAST STEEL; 2) ACCELERATED TRANSFER OF CLEAN STEEL TECHNOLOGY**
$332,000
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

32. **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

33. **ADVANCED LOST FOAM CASTING TECHNOLOGY**
$325,000
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

34. **MECHANICAL PROPERTIES STRUCTURE CORRELATION FOR COMMERCIAL SPECIFICATION OF CAST PARTICULATE METAL MATRIX COMPONENTS**
$208,000
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

35. **FERRITE MEASUREMENTS IN DUPLEX STAINLESS STEEL CASTINGS**
$70,000
DOE Contact: Ehr Ping Huang Fu (202) 586-1493
University of Tennessee Contact: Carl Lundin (423) 974-5310

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

Keywords: Metalcasting, Calibration, Duplex Stainless Steel

36. **TECHNOLOGY FOR THE PRODUCTION OF CLEAN, THIN WALL, MACHINABLE GRAY AND DUCTILE IRON CASTINGS**
$215,000
DOE Contact: Ehr Ping HuangFu (202) 586-1493
University of Alabama - Birmingham Contact: Charles Bates (205) 975-8011

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

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

37. **MOLD MATERIALS FOR PERMANENT MOLDING OF ALUMINUM ALLOYS**
$92,000
DOE Contact: Ehr Ping Huang Fu (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

38. **SYSTEMATIC MICROSTRUCTURAL AND CORROSION PERFORMANCE EVALUATION OF HIGH MOLYBDENUM STAINLESS STEEL CASTING**
$50,000
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

39. **DEVELOPMENT OF A FATIGUE PROPERTIES DATA BASE FOR USE IN MODERN DESIGN METHODS**
$72,000
DOE Contact: Ehr Ping HuangFu (202) 586-1493
Climax Research Services Contact: Jim DeLao (248) 489-0720

The objective of the project is to develop a comprehensive database of strain-life fatigue data for graphite cast irons suitable for modern design techniques (specifically, the structural grades of gray iron, ductile iron, austempered ductile iron and compacted graphitic iron). Each grade will be evaluated to two cast section sizes for comparison. The project will combine data obtained from the open literature with unpublished data contributed by cast iron producers and end-users. This information will be supplemented with strain-life testing to fill the gaps in the data.

Keywords: Metalcasting, Fatigue Properties, Casting Design

MINING VISION TEAM
The DOE Mining Team contact is Toni Marechaux, (202) 586-8051

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

40. **DRILLING AND BLASTING OPTIMIZATION USING SEISMIC ANALYSIS AND X-RAY FLUORESCENCE SPECTROSCOPY**
$260,000
DOE Contact: Toni Marechaux (202) 586-8501
Lawrence Berkeley National Laboratory Contact: Deborah Hopkins (510) 486-4922

This project examines 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

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

41. **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 develops 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)

42. **DEVELOPMENT OF A MINE COMPATIBLE LIBS INSTRUMENT FOR ORE GRADING**
$138,000
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, can 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

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

43. **HYDRIDE FUEL CELL MINING VEHICLES**
$275,000
DOE Contact: Toni Marechaux (202) 586-8501
Savannah River Technology Center: Contact: Ed Danko (803) 725-4264

This project develops optimized hydride materials for underground hydrogen storage for mining vehicles. 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

44. **MINING BYPRODUCT RECOVERY**
$200,000
DOE Contact: Toni Marechaux (202) 586-8501
Oak Ridge National Laboratory: Contact:
Jan Berry (865) 241-1939

This project develops 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

OFFICE OF CROSSCUT TECHNOLOGIES

INDUSTRIAL MATERIALS FOR THE FUTURE (IMF) 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 Industrial Materials for the Future program is a crosscutting program with emphasis on industrial needs of the Industries of the Future effort and of crosscutting industries including carbon products, forging, heat treating, and welding. Efforts in FY 2000 were focused on partnerships between industry and the National Laboratories for commercialization of new materials and processes. The DOE program managers are Charles A. Sorrell (202) 586-1514 and Mike Soboroff (202) 586-4936.

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

45. **INTERMETALLIC ALLOY DEVELOPMENT AND TECHNOLOGY TRANSFER OF INTERMETALLIC ALLOYS**
$570,000
DOE Contact: Charles A. Sorrell (202) 586-1514
ORNL Contacts: M. L. Santella (423) 574-4805
and V. K. Sikka (423) 574-5112
University of Tennessee, G. M. Pharr
(865) 974-8202

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 2000 included: (1) an ASTM specification was obtained for cast Ni_3Al compositions (A1002-99); this is the first SASTM specification for an intermetallic alloy; (2) a new technology was developed for joining nickel aluminide tubes with trunnion, and (3) a study of the long term phase stability of cast and welded Ni_3Al specimens was initiated.

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

46. **DEVELOPMENT OF ADVANCED METALLIC/INTERMETALLIC ALLOYS**
$570,000
DOE Contact: Charles A. Sorrell (202) 586-1514
ORNL Contact: P. J. Maziasz (423) 574-5082,
M. L. Santella (423) 574-4805 and V. K. Sikka
(423) 574-5112; C. T. Liu (423) 574-4459

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 2000 include; (1) the intermediate temperature ductility and fabricability of Ni_3Si alloys was improved, and (2) the behavior of FeAl in carburizing environments, and the joining of FeAl was evaluated.

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

47. **COMPOSITES AND COATINGS THROUGH REACTIVE METAL INFILTRATION**
$300,000
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 FY2000: (1) development of the technique was continued and materials evaluated included $MoSi_2$ and other compounds and (2) the collaboration was continued with National Refractories and Minerals Corporation.

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

48. **CONDUCTING POLYMERS: SYNTHESIS AND INDUSTRIAL APPLICATIONS**
$150,000
DOE Contact: Mike Soboroff (202) 586-4936
Los Alamos National Laboratory Contact:
S. Gottesfeld (505) 667-0853

In FY 2000, 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 2000, development of the oxygen polarized chlor-alkali cells was continued.

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

49. **MEMBRANE SYSTEMS FOR EFFICIENT SEPARATION OF LIGHT GASES**
$300,000
DOE Contact: Mike Soboroff (202) 586-4936
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 2000, the CRADA with BP Amoco was continued. Specimens of membranes were tested in various chemical environments.

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

50. **PLASMA PROCESSING- ADVANCED MATERIALS FOR CORROSION AND EROSION RESISTANCE**
$250,000
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, thermo-dynamically stable, and adherent coatings on die materials used to cast aluminum and other metals. Low temperature organometallic chemical vapor deposition combined with immersion ion processing are being developed as the coating technology. In FY 2000: (1) a CRADA between LANL and Pratt and Whitney was continued (2) Nitride and oxycarbide based coatings were produced on various substrates and evaluated.

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

51. **UNIFORM DROPLET PROCESSING**
$350,000
DOE: Contact: Charles A. Sorrell (202) 586-1514
ORNL Contact: Craig A. Blue (423) 574-4351 and Vinod Sikka (423) 574-5123
Massachusetts Institute of Technology Contact:
J-H Chun (617) 253-1759
Northeastern University Contact: T. Ando
(617) 373-3811

The purpose of this project is to adapt the uniform droplet process to higher melting materials, e.g., intermetallic alloys, stainless, steel, superalloys; to provide superior metal powders for the powder metallurgy industry and to develop methods for spray coating or casting of high temperature materials, including aluminide intermetallics. Spray forming of metallic systems is being investigated. Participants in the research include Oak Ridge National Laboratory, Massachusetts Institute of Technology, Northeastern University and powder metal companies. In FY 2000 the effort was completed with efforts at focusing on alternate methods of obtaining uniform spheres of various high temperature materials including Magnesium. Additional effort was continued in working with a licensee of the uniform droplet process, Uniform Metals Technologies to enhance the capabilities to produce uniform metallic spheres.

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

52. **ADVANCED MATERIALS/PROCESSES**
$560,000
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 and materials processing methods. 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 2000: (1) R&D utilizing the new 300,000 W high intensity infrared heating system and processing system continued. The surface of mullite refractory bricks were able to be fused thus decreasing the possible flow alkali bearing gaseous species into the refractory (2) wear resistant coatings were able to be fused onto various types of metallic substrates, and (3) thermally sprayed coating were successfully fused and metallurgically bonded to substrate materials.

Keywords: Intermetallic Alloys, Metalcasting, Glass, Alloys, Welding, Corrosion Resistance, Infrared Heating, Coatings, Refractories, WC, Thermal Spray

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

53. **MATERIALS DEVELOPMENT FOR THE FOREST PRODUCTS INDUSTRY**
$780,000
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 2000, recommendations regarding minimizing or eliminating floor tube cracking were made including: (a) for cooling water not to contact the boiler floor until the temperature drops below 150 degrees Celsius (b) minimize thermal fluctuations of the floor, and (c) substitute 825/CS or 625/CS coextruded or Alloy 625 weld overlaid or chromized carbon steel tubes for 304L/CS floor tubes. Various companies have currently installed or retrofitted parts of floors with the new materials. Additional efforts on evaluating cracking of air port tubes were performed. Temperature measurements showed that air ports with tube cracking experience more frequent and higher magnitude temperature fluctuations. 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

54. **METALS PROCESSING LABORATORY USER (MPLUS) FACILITY**
$400,000
DOE Contact: Charles A. Sorrell (202) 586-1514
Oak Ridge National Laboratory Contact:
P. Angelini (865) 574-4565

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 2000, Over 140 proposals were received with over 50 MPLUS projects having been completed. Projects crosscut all of the industries in the Industries of the Future effort and other supporting industries including forging, heat treating, welding.

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

55. **CONTINUOUS FIBER CERAMIC COMPOSITES (CFCC) SUPPORTING - TECHNOLOGIES**
$2,300,000
DOE Contact: Mike Soboroff (202) 586-4936
ORNL Contact: Peter Angelini (865) 574-4565

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

Keywords: Ceramic Composites, Materials Characterization, Test Methods, Life Prediction

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

56. **SELECTIVE INORGANIC THIN FILMS**
$200,000
DOE Contact: Mike Soboroff (202) 586-4936
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 FY2000, the R&D continued with advancements made in the fabricability of more robust membranes systems.

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

57. **MATERIALS FOR HIGH TEMPERATURE FILTRATION/THERMOCHEMICAL MODELING**
$53,000
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 1000C. In FY 2000: (1) the filtration efforts were completed showing that various materials survived the high temperature exposures of up to 1000 h periods in thermal oxidizer simulated environments and (2) the thermodynamics of molten smelt was continued to be evaluated.

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

58. **CONTINUOUS FIBER CERAMIC COMPOSITES (CFCC) - INDUSTRIAL - TECHNOLOGIES**
$2,920,000
DOE Contact: Mike Soboroff (202) 586-4936
ORNL Contact: Peter Angelini (865) 574-4565

The Continuous Fiber Ceramic Composites (CFCC) activity operates as a collaborative effort between industry, national laboratories, universities, and the government to develop advanced ceramic composite materials to a point at which industry will assume full risk of further development. There are currently five industrial teams developing industrial applications. National laboratories, along with universities, are developing supporting technologies (e.g., materials design, processing methods, and sensing technologies) and conducting performance based evaluations.

Keywords: Continuous Fiber Ceramic Composites, Materials Processing

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. 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 INNOVATION
DOE Contact Lisa Barnett (202) 586-2212

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

59. **LASER SENSOR FOR OPTIMIZATION OF COMPRESSOR STATIONS AND REFINERY OPERATIONS**
$0[1]
DOE Contact: Gibson Asuquo (303) 275-4910
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 per year.

Keywords: Laser, Leak Detection, Natural Gas, Pipeline

60. **TITANIUM MATRIX COMPOSITE TOOLING MATERIAL FOR ENHANCED MANUFACTURE OF ALUMINUM DIE CASTINGS**
$0[1]
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 percent.

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

61. **AN INSOLUBLE TITANIUM-LEAD ANODE FOR SULFATE ELECTROLYTES**
$0[1]
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 percent.

Keywords: Electrowinning, Anodes

62. **DEVELOPMENT OF AN INNOVATIVE ENERGY EFFICIENT HIGH TEMPERATURE NATURAL GAS FIRED FURNACE**
$0[1]
DOE Contact: Keith Bennett (303) 275-4905
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 percent of natural gas fuel and achieve a higher combustion efficiency for a given combustion gas discharge temperature.

Keywords: Heat Treating, Gas-fired Furnaces

63. **A NEW HIGH TEMPERATURE COATING FOR GAS TURBINES**
$0[1]
DOE Contact: Roxanne Danz (303) 275-4706
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

[1]Prior year funding

savings will be derived from reducing one of the two traditional coating steps and extending component life.

Keywords: Coatings, Gas Turbines

64. **TOUGH-COATED HARD POWDERS (TCHPs): A NEW PARADIGM IN MINING AND MACHINING TOOL MATERIALS**
$0[1]
DOE Contact: Gibson Asuquo (303) 275-4910
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

65. **A NEW ENERGY SAVING METHOD OF MANUFACTURING CERAMIC PRODUCTS FROM WASTE GLASS**
$0[1]
DOE Contact: Gibson Asuquo (303) 275-4910
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 35-50% by sintering glass powder instead of using traditional ceramic materials.

Keywords: Cullet, Ceramic, Sintering Glass Powder

66. **DISTILLATION COLUMN FLOODING PREDICTOR**
$0[1]
DOE Contact: Gibson Asuquo (303) 275-4910
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

67. **ENERGY SAVING LIGHTWEIGHT REFRACTORY**
$0[1]
DOE Contact: Gibson Asuquo (303) 275-4910
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

68. **HIGH INTENSITY SILICON VERTICAL MULTI-JUNCTION SOLAR CELLS**
$0[1]
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

69. **FABRICATION AND TESTING OF A PROTOTYPE CERAMIC FURNACE COIL**
$0[1]
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%

[1]Prior year funding

leading to substantial energy savings and increased productivity.

Keywords: Ceramic Tubes, Furnace Coils, Ethylene Production

70. **GERMANIUM COMPOUNDS AS HIGHLY SELECTIVE FLUORINATION CATALYSTS**
$0[1]
DOE Contact: Gibson Asuquo (303) 275-4910
Starmet Corporation Contact:
Dr. Matthew Stephens (978) 369-5410

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

71. **DEVELOPMENT OF PHOSPHORS FOR USE IN HIGH-EFFICIENCY LIGHTING AND DISPLAYS**
$0[1]
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

72. **NOVEL CERAMIC COMPOSITION FOR HALL-HEROULT CELL ANODE APPLICATION**
$0[1]
DOE Contact: Keith Bennett (303) 275-4905
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 percent, 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

73. **FUNCTIONALLY GRADED MATERIALS FOR IMPROVED HIGH TEMPERATURE PERFORMANCE OF Nd-Fe-B-BASED PERMANENT MAGNETS**
$0[1]
DOE Contact: Keith Bennett (303) 275-4905
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

74. **IMPROVED ALKYLATION CONTACTOR**
$0[1]
DOE Contact: Gibson Asuquo (303) 275-4910
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 percent, 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

[1]Prior year funding

75. **LOW COST SYNTHESIS AND CONSOLIDATION OF TiC**
$0[1]
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

76. **DEVELOPMENT OF ALUMINUM IRON ALLOYS FOR MAGNETIC APPLICATIONS**
$0[1]
DOE Contact: Keith Bennett (303) 275-4905
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 percent and a 15-25 percent increase in motor efficiency may be realized.

Keywords: Powder Metallurgy, Aluminum Iron Alloys, Magnets

77. **NOVEL FREQUENCY-SELECTIVE SOLAR GLAZING SYSTEM**
$0[1]
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

78. **A CERAMIC COMPOSITE FOR METAL CASTING**
$0[1]
DOE Contact: Keith Bennett (303) 275-4905
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

79. **ELECTROCHEMICAL METHOD FOR EXTRACTION OF OXYGEN FROM AIR**
$0[1]
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

80. **ENERGY SAVING METHOD FOR PRODUCING ETHYLENE GLYCOL AND PROPYLENE GLYCOL**
$0[1]
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

[1]Prior year funding

production consuming 33 trillion Btu and 4 billion gallons of water. The proposed process could reduce energy and water consumption by 20%.

Keywords: Glycol Production, Ethylene Glycol, Propylene Glycol

81. **IMPROVED REFRACTORIES USING ENGINEERED PARTICLES**
$0[1]
DOE Contact: Gibson Asuquo (303) 275-4910
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

82. **ENABLING TOOL FOR INNOVATIVE GLASS APPLICATIONS**
$0[1]
DOE Contact: Keith Bennett (303) 275-4905
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

83. **DISTRIBUTED OPTICAL SENSORS FOR CONTINUOUS LIQUID LEVEL TANK GAUGING**
$174,284
DOE Contact: Keith Bennett (303) 275-4905
Project Contact: Joram Hopenfeld (301) 340-1625

The grant will be used to develop a Noverflo multi-point tank gauging device that will be compact, sensitive, and manufactured inexpensively in large quantities. The sensor will not require special signal conditioning to interface with host computers and will save energy by reducing power requirements, optimizing fuel utilization, and reducing fuel leaks.

Keywords: Tank Gauging, Transportation, Tank Overfill Protection

84. **A LOW ENERGY ALTERNATIVE TO COMMERCIAL SILICA-BASED GLASS FIBERS**
$199,089
DOE Contact: Gibson Asuquo (303) 275-4910
MO-SCI Corporation Contact: Ted Day (573) 364-2338

The grant will be used to develop high strength, iron phosphate glass fibers for composites and other products in the transportation, aircraft and chemical industries. Iron phosphate glasses have a chemical durability that exceeds many commercial silica-based glasses and can be melted 3 to 20 times faster at temperatures 400-600°C lower than commercial boro-alumino-silicate glass.

Keywords: Glass, Iron Phosphate Glass Fibers, Silica-Based Glass Fibers

85. **CROMER CYCLE AIR CONDITIONING**
$40,000
DOE Contact: Keith Bennett (303) 275-4905
Solar Engineering Co. Contact: Charles Cromer (407) 638-1445

The grant will be used to develop the Cromer Cycle Air Conditioner that uses a desiccant to move moisture from the outlet duct to the inlet duct. This has the thermodymanic effect of reducing the overall energy consumption of the air conditioner and increasing the moisture removal capacity of the air conditioner coil resulting in a 16% reduction in energy consumption and a 47% improvement in EER.

Keywords: Air Conditioner, Desiccant, Moisture Removal

[1]Prior year funding

86. **ANAEROBIC BIOLEACHING TECHNOLOGY FOR METALS RELEASE**
$40,000
DOE Contact: Keith Bennett (303) 275-4905
Geo-Microbial Technologies, Inc. Contact:
Donald Hitzman (918) 535-2281

The grant will be used to develop a method (Anaerobic Denitrification Bio-leaching) to recover additional metal values from low grade and recalcitrant ores cost effectively reducing toxic chemical and acid waste streams. The proposed anaerobic bio-leaching process extends an anaerobic biosystem that has been used to remove Ni and Mo metal contaminates from spent furl catalysts.

Keywords: Anaerobic Denitrification, Anaerobic Bio-leaching, Mining, Low Grade Ore

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

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

87. **DEMONSTRATION OF A THREE-PHASE ROTARY SEPARATOR TURBINE**
$0[1]
DOE Contact: Chris Cockrill (816) 873-3299
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

88. **CERAMIC TURBINE WHEEL TECHNOLOGY TO PROVIDE ECONOMIC, EFFICIENCY AND ENVIRONMENTAL ENHANCEMENTS TO MICROTURBINES**
$0[1]
DOE Contact: Chris Cockrill (816) 873-3299
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

89. **PRECISION IRRIGATION TECHNOLOGIES FOR THE AGRICULTURAL INDUSTRY**
$0[1]
DOE Contact: Cathy Ghandehari (303) 275-4805
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

[1]Prior year funding

90. **ENERGY CONSERVING TOOL FOR COMBUSTION DEPENDENT INDUSTRIES**
$0[1]
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

91. **ENERGY-SAVING REGENERATION OF HYDROCHLORIC ACID PICKLING LIQUOR**
$0[1]
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

92. **SUPERCRITICAL FLUID PURIFICATION OF COMBI-CHEM LIBRARIES**
$0[1]
DOE Contact: Joe Barrett (215) 656-6957
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

93. **FULL-SCALE 100 TON/HR DEMONSTRATION OF MAGNETIC ELUTRIATION TECHNOLOGY FOR CLEAN AND EFFICIENT PROCESSING OF IRON ORE**
$0[1]
DOE Contact: Brian Olsen (312) 353-8579
Minnesota Department of Public Service Contact: Janet Streff (651) 297-2545
5R Research Contact: John McGaa (651) 730-4526

The Minnesota Department of 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 percent 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

[1]Prior year funding

94. **REDUCING FOUNDRY EMISSIONS AND GREEN SAND WASTE VIA INTEGRATED ADVANCED OXIDATION-UNDERWATER PLASMA PROCESSING**
$0[1]
DOE Contact: Joe Barrett (215) 656-6957
Pennsylvania Department of Environmental Protection Contact: Calvin Kirby (717) 783-9981
Advanced Cast Productions, Inc. Contact: William Franz (814) 724 2600

The Pennsylvania Department 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

[1]Prior year funding

OFFICE OF TRANSPORTATION TECHNOLOGIES

	FY 2000
OFFICE OF TRANSPORTATION TECHNOLOGIES - GRAND TOTAL	**$41,568,000**
OFFICE OF ADVANCED AUTOMOTIVE TECHNOLOGIES	**$24,671,000**
TRANSPORTATION MATERIALS PROGRAM	**$21,565,000**
AUTOMOTIVE PROPULSION MATERIALS	**$3,110,000**
TECHNOLOGY TRANSFER AND MANAGEMENT COORDINATION	**$270,000**
Technical Project Management	270,000
DEVICE OR COMPONENT FABRICATION, BEHAVIOR, OR TESTING	**$2,840,000**
POWER ELECTRONICS AND ELECTRIC MACHINES	**$880,000**
Carbon Foam Thermal Management Materials for Electronic Packaging	175,000
High-Temperature Capacitors for PNGV Power Electronics	220,000
Mechanical Reliability of Electronic Ceramics and Electronic Ceramic Devices	125,000
Low-Cost, High Energy Product Permanent Magnets	310,000
Characterization of Permanent Magnets	50,000
ADVANCED COMBUSTION AND EMISSION CONTROL	**$830,000**
Microwave-Regenerated Diesel Engine Exhaust Particulate Filter Technology	330,000
Ultralow-Friction Coatings for CIDI Fuel Injection Systems Components	150,000
Rapid Surface Modifications of Aluminum Engine Block Bores for Weight Reduction	150,000
Material Support for Nonthermal Plasma Diesel Engine Exhaust Emission Control	200,000
FUEL CELLS FOR TRANSPORTATION	**$1,130,000**
Nanopore Inorganic Membranes as Electrolytes in Fuel Cells	215,000
Inorganic Polymer Electrolyte Membrane Electrode/support Development	140,000
Low-Friction Coatings for Fuel Cell Air Compressors	175,000
Microstructural Characterization of Pem Fuel Cells	150,000
Carbon Foam for Radiators for Fuel Cells	75,000
Nanofluids for Thermal Management Applications	75,000
Carbon Composite Bipolar Plates for Pem Fuel Cells	200,000
Cost-Effective Metallic Bipolar Plates Through Innovative Control of Surface Chemistry	100,000

OFFICE OF TRANSPORTATION TECHNOLOGIES (continued)

	FY 2000
OFFICE OF ADVANCED AUTOMOTIVE TECHNOLOGIES (CONTINUED)	
TRANSPORTATION MATERIALS TECHNOLOGY (CONTINUED)	
LIGHTWEIGHT VEHICLE MATERIALS	$18,455,000
DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING	$18,455,000
Low-Cost High Performance Wrought Aluminum Components for Automotive Applications	1,800,00
Low-Cost High Performance Cast Light Metals for Automotive Applications	1,900,000
Advanced Materials and Processes for Automotive Applications	1,875,000
Automotive-Related Graduate Fellowships	100,000
Materials and Processes for Propulsion System Applications	450,000
Technology Assessment and Evaluation	1,400,000
Reinforced Composite Materials-joining, Durability, and Enabling Technologies	2,950,000
USAMP Cooperative Agreement	3,400,000
Development of Low Cost Carbon Fiber	2,400,000
Development of Low-cost Lightweight Metals And Alloys	900,000
Recycling	600,000
Structural Reliability of Lightweight Glazing Alternatives	380,000
High Rate Processing Technologies For Composite Materials	300,000
ELECTRIC DRIVE VEHICLE TECHNOLOGIES PROGRAM	$3,106,000
ADVANCED BATTERY MATERIALS	$3,106,000
OPTIMIZED LI-ION SYSTEM	$917,000
MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING	$202,000
Optimization of Cathode Materials	127,000
Development of Novel Electrolytes	75,000
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING	$715,000
Reactivity and Safety Aspects of Carbonaceous Anodes	160,000
Optimized Lithium-Ion Electrolyte and Binder	75,000
SEI Layer Formation on Carbon Anodes	70,000
Electrode Surface Layers	70,000
Carbon Electrochemistry	205,000
Corrosion of Lithium Batteries	135,000

OFFICE OF TRANSPORTATION TECHNOLOGIES (continued)

	FY 2000
OFFICE OF ADVANCED AUTOMOTIVE TECHNOLOGIES (CONTINUED)	
ELECTRIC DRIVE VEHICLE TECHNOLOGIES PROGRAM (CONTINUED)	
ADVANCED BATTERY MATERIALS (CONTINUED)	
HIGH-PERFORMANCE NON-FLAMMABLE ELECTROLYTES	$234,000
MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING	$234,000
Non-Flammable Electrolytes	82,000
Development of Non-flammable Electrolytes	82,000
Non-Flammable Electrolytes	70,000
NON-CARBONACEOUS ANODE MATERIALS	$130,000
MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING	$130,000
Non-Carbonaceous Anode Materials	100,000
Non-Carbon Anodes	30,000
NOVEL CATHODE MATERIALS	$430,000
MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING	$430,000
New Cathode Materials Based on Layered Structures	70,000
Novel Cathode Materials	70,000
Novel Cathode Structures	215,000
New Cathode Materials: Aerogels	75,000
ADVANCED SOLID POLYMER ELECTROLYTES	$675,000
MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING	$135,000
Composite Polymer Electrolytes	70,000
Highly Conductive Polyelectrolyte-Containing Rigid Polymers	65,000
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING	$475,000
Lithium-Polymer Electrolyte Interface	70,000
Advanced Solid Polymer Electrolytes	255,000
Advanced Solid Polymer Electrolytes	150,000

OFFICE OF TRANSPORTATION TECHNOLOGIES (continued)

	FY 2000
OFFICE OF ADVANCED AUTOMOTIVE TECHNOLOGIES (CONTINUED)	
ELECTRIC DRIVE VEHICLE TECHNOLOGIES PROGRAM (CONTINUED)	
ADVANCED BATTERY MATERIALS (CONTINUED)	
MATERIALS STRUCTURE AND COMPOSITION	$65,000
Modeling of Lithium/Polymer Electrolytes	65,000
ADVANCED DIAGNOSTIC METHODS	$245,000
MATERIALS STRUCTURE AND COMPOSITION	$245,000
Diagnostics: Electrode Surface Layers	120,000
Battery Materials: Structure and Characterization	125,000
IMPROVED ELECTROCHEMICAL MODELS	**$335,000**
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING	$285,000
Improved Electrochemical Models	235,000
Thermal Modeling/Thermal Management	50,000
MATERIALS STRUCTURE AND COMPOSITION	$50,000
Microstructural Modeling of Highly Porous Fibrous and Particulate Electrodes	50,000
NOVEL ELECTRODE COUPLES	$140,000
DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING	$140,000
New Couples: Lithium/Sulfur Cells	140,000
OFFICE OF HEAVY VEHICLE TECHNOLOGIES	$16,897,000
TRANSPORTATION MATERIALS TECHNOLOGY	$16,897,000
HEAVY VEHICLE PROPULSION SYSTEM MATERIALS	$10,947,000
MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING	$2,977,000
Cost-Effective Smart Materials For Diesel Engine Applications	400,000
Cost-Effective Sintering	162,000
Low Cost, High Toughness Ceramics	350,000
Intermetallic-bonded Cermets	100,000
Diesel Particulate Trap Development	100,000

OFFICE OF TRANSPORTATION TECHNOLOGIES (continued)

	FY 2000
OFFICE OF HEAVY VEHICLE TECHNOLOGIES (CONTINUED)	
TRANSPORTATION MATERIALS TECHNOLOGY (CONTINUED)	
HEAVY VEHICLE PROPULSION SYSTEM MATERIALS (CONTINUED)	
MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING (CONTINUED)	
Insulating Structural Ceramics For High Efficiency, Low Emission Engines	300,000
Thick Thermal Barrier Coatings (TTBCS) For Low Emissions, High Efficiency Diesel Engine Components	200,000
Materials For Low Emissions, High Efficiency Diesel Engine Components	518,000
Materials For Low Emissions, High Efficiency Diesel Engine Components	300,000
R&D For Advanced Ceramics And Cermets	400,000
Development of Low-cost, Cast Engine Materials With Enhanced Reliability	75,000
Carbon Foams For Heat Transfer	72,000
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING	**$6,557,000**
The High Temperature Materials Laboratory User Program	5,500,000
Diesel Exhaust Catalyst Characterization	200,000
Life Prediction Verification	200,000
High Temperature Tensile Testing	155,000
NDE/C Technology for Heavy Duty Diesel Engines: Fuel Delivery and Insulating Materials	25,000
International Exchange Agreement (IEA)	150,000
Standard Reference Materials	150,000
Mechanical Property Standardization	100,000
Reliable Joining Techniques for Advanced Diesel Engine Valves	37,000
Raman and Fluorescence Spectroscopic Characterization of Ceramic Materials: Stress, Phase, and Temperature	40,000
TECHNOLOGY TRANSFER AND MANAGEMENT COORDINATION	**$500,000**
Technical Project Management	500,000
DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING	**$913,000**
Durability of Diesel Engine Component Materials	200,000
Advanced Machining/manufacturing	225,000
NDE Development for Ceramic Valves for Diesel Engines	175,000
Cylindrical Wire Electron Discharge Machining Process	40,000
Quantifying the Environmental Effects on the Mechanical Properties of Advanced Silicon Nitride Materials for Diesel Engine Applications	23,000
Development of No_x Sensors for Heavy Vehicle Applications	250,000

OFFICE OF TRANSPORTATION TECHNOLOGIES (continued)

	FY 2000
OFFICE OF HEAVY VEHICLE TECHNOLOGIES (CONTINUED)	
TRANSPORTATION MATERIALS TECHNOLOGY (CONTINUED)	
HIGH STRENGTH WEIGHT REDUCTION MATERIALS	$5,950,000
DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING	$5,950,000
Design, Analysis and Development of Lightweight Frames for Truck and Bus Applications	1,150,000
Development of a Casting Process for Producing Ultra-large Components	1,300,000
Development of Advanced Casting Technologies for Production of High Integrity Truck Components	900,000
Technology Development for Lightweight Engines	100,000
Advanced Forming Technologies for Lightweight Alloys	600,000
Development of Carbon Monoliths for Safe, Low Pressure Adsorption Storage and Release Natural Gas	200,000
Improved Materials for Heavy Vehicle Brake and Friction Applications	400,000
High Conductivity Carbon Foams for Thermal Management	100,000
Technology Assessment and Evaluation	1,200,000

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 intiative 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 development effort to triple the fuel efficiency of today's automobile by the year 2004.

The Automotive Propulsion Materials program is an integral partner with the Power Electronics, the Advanced Combustion and Emissions Control, and the Fuel Cells for Transportation R&D programs. Projects within the Automotive Propulsion Materials program address materials concerns that directly impact the critical technical barriers in each of these programs—barriers such as thermal management, emissions reduction, and reduced manufacturing costs. 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.

AUTOMOTIVE PROPULSION MATERIALS

TECHNOLOGY TRANSFER AND MANAGEMENT COORDINATION

95. **TECHNICAL PROJECT MANAGEMENT**
    $270,000
    DOE Contact: P. B. Davis (202) 586-8061
    ORNL Contact: D. P. Stinton
    (865) 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

POWER ELECTRONICS AND ELECTRIC MACHINES

96. **CARBON FOAM THERMAL MANAGEMENT MATERIALS FOR ELECTRONIC PACKAGING**
    $175,000
    DOE Contact: P. B. Davis (202) 586-8061
    ORNL Contact: D. P. Stinton (865) 574-4556
    ORNL Contact: J. W. Klett (865) 574-5220

The objective of this work is to collaborate with automotive partners to develop carbon foam heat exchanger and heat sink designs for high-power electronics that dissipate 30 W/cm^2 using conventional cooling fluids. A test facility was fabricated that has been used to evaluate the performance of various carbon foam heat sink designs. The facility proved to be very effective in comparing various heat sink designs. Novel carbon foam heat sinks were fabricated that proved to be much more efficient (an order of magnitude increase in heat transfer coefficient) than conventional copper or aluminum heat sinks. These carbon foam heat sinks appear to be able to cool electronics adequately with less than half the water flow rates used in conventional designs. The increased efficiency will be realized in weight savings because the heat sinks will be smaller, they will utilize less cooling water, and carbon foam is much lighter than copper or aluminum.

Keywords: Carbon Foam, Heat Sinks, Heat Transfer, Power Electronics, Thermal Management

97. **HIGH-TEMPERATURE CAPACITORS FOR PNGV POWER ELECTRONICS**
$220,000
DOE Contact: P. B. Davis (202) 586-8061
ORNL Contact: D. P. Stinton (865) 574-4556
SNL Contact: B. A. Tuttle (505) 845-8026

The objective of this work is to develop a high-temperature polymer dielectric film technology that has dielectric properties technically superior to those of aluminum electrolytic dc buss capacitors and is comparable or smaller in size. A plan was developed for large-scale commercialization of polymer film dc buss capacitors with AVX/TPC, GM, and Sandia National Laboratory. New polymer film dielectrics were fabricated at SNL during the year that demonstrated a 100% increase in dielectric constant compared with industry standards, while maintaining reasonable electric field and dielectric loss stability of 0.5 MV/cm. Further molecular engineering investigation and electrical testing are necessary to make the slight improvements necessary to meet both voltage and temperature requirements for commercialization.

Keywords: Capacitors, Dielectrics, Polymer Films, Power Electronics

98. **MECHANICAL RELIABILITY OF ELECTRONIC CERAMICS AND ELECTRONIC CERAMIC DEVICES**
$125,000
DOE Contact: P. B. Davis (202) 586-8061
ORNL Contact: D. P. Stinton (865) 574-4556
ORNL Contact: H.-T. Lin (865) 576-8857

The objectives of this task are to develop testing algorithms that can be used to assess electronic ceramic (EC) and electronic ceramic device (ECD) mechanical reliability, and to mechanically characterize EC and ECD alternatives that are less expensive and that can be used to promote device miniaturization. The mechanical reliability of multilayer capacitors (MLCs) has been evaluated from measurements of strength and thermal properties and by numerical analysis of the residual stresses. This information is currently being used by MLC manufacturers to quantitatively predict the maximum allowable thermal excursions that can be tolerated without producing thermal fracture.

Keywords: Electronics, Failure Analysis, Life Prediction, Mechanical Properties, Multilayer Capacitors

99. **LOW-COST, HIGH ENERGY PRODUCT PERMANENT MAGNETS**
$310,000
DOE Contact: P. B. Davis (202) 586-8061
ORNL Contact: D. P. Stinton (865) 574-4556
ANL Contact: T. M. Mulcahy (630) 252-6141

The objective of this work is to develop a low-cost process for the fabrication of high-strength NdFeB permanent magnets to enable significant size and weight reductions of traction motors for hybrid electric vehicles. For the first time, a facility has been established for pressing permanent magnets in the high fields (9 T) of a superconducting solenoid. The solenoid better aligns the magnetic domains of NdFeB powder during pressing into green compacts. The energy product (MGOe) and remnant field Br(kG) of magnets produced in this facility showed a strong dependence on the magnitude of the alignment field H(T). Improvements in permanent magnet strength of 25% were found by increasing the alignment field to 8 T from the 2 T typically used in industry. The 8 T magnet strengths are comparable to those obtained in industry. Characterization of the magnets attempted to quantify the relationship between processing parameters and the crystal chemistry and microstructure of NdFeB permanent magnets fabricated at Argonne National Laboratory and by commercial suppliers. Improvements of alignment in the higher fields of the superconducting solenoid will be evaluated next.

Keywords: NdFeB, Permanent Magnets, Superconducting Solenoids, Traction Motors

100. **CHARACTERIZATION OF PERMANENT MAGNETS**
$50,000
DOE Contact: P. B. Davis (202) 586-8061
ORNL Contact: D. P. Stinton (865) 574-4556
ANL Contact: E. A. Payzant (865) 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: NdFeB, Permanent Magnets

ADVANCED COMBUSTION AND EMISSION CONTROL

101. **MICROWAVE-REGENERATED DIESEL ENGINE EXHAUST PARTICULATE FILTER TECHNOLOGY**
$330,000
DOE Contact: P. B. Davis (202) 586-8061
ORNL Contact: D. P. Stinton (865) 574-4556
Industrial Ceramic Solutions Contact:
R. Nixdorf (865) 482-7552

The objective of this work is to develop a Diesel Particulate Filter that demonstrates greater than 75% capture efficiency and can be regenerated to within 90% of the new filter condition with the use of microwave energy. During the year a microwave regeneration system was designed and built that is capable of performing on a PNGV-type diesel engine. The microwave filter system was first tested on a 1.2-L DIATA diesel at the Ford Motor Company's Scientific Research Laboratory. A second engine test was performed at Oak Ridge National Laboratory on a 1.9-L Volkswagen engine. A third test was performed on a much larger 7.3-L International engine at the University of Tennessee. The results from the three engine tests demonstrated a 85-95% particulate removal efficiency and a 95-100% regeneration efficiency. The microwave filter system fuel penalty, as calculated from these three test results, was an impressively low 0.3%.

Keywords: Carbon Particulates, Diesel, Filters, Microwave Regeneration

102. **ULTRALOW-FRICTION COATINGS FOR CIDI FUEL INJECTION SYSTEMS COMPONENTS**
$150,000
DOE Contact: P. B. Davis (202) 586-8061
ORNL Contact: D. P. Stinton (865) 574-4556
ANL Contact: G. R. Fenske (630) 252-5190

The objective of this work is to evaluate the performance of amorphous carbon coatings on the reliability and durability of critical fuel system components for diesel engines. The durability of near-frictionless carbon (NFC) coatings was examined with a high-frequency reciprocating test rig using a ball-on-flat contact geometry. Tests were conducted with uncoated steel balls sliding on coated flats. The three variations of NFC coatings evaluated all reduced the wear of both the ball and flat specimens substantially (more than 10 times) compared with other hard coatings and uncoated surfaces. Scuffing resistance was also evaluated with a reciprocating pin-on-flat configuration. Scuffing tests were conducted at different constant contact loads and with a step-increase in sliding speed until scuffing occurred. The scuffing tests demonstrated two features: first, the scuffing resistance of the synthetic fuel is less than that of conventional diesel fuel with 500 ppm sulphur; and second, use of the NFC coating increased the scuffing resistance by approximately one order of magnitude.

Keywords: Carbon, Friction, Fuel Injection Systems, Near Frictionless Coating, Wear

103. **RAPID SURFACE MODIFICATIONS OF ALUMINUM ENGINE BLOCK BORES FOR WEIGHT REDUCTION**
$150,000
DOE Contact: P. B. Davis (202) 586-8061
ORNL Contact: D. P. Stinton (865) 574-4556
ORNL Contact: C. Blue (865) 574-5112

Innovative, rapid, high-density surface modification processes are being used to develop a new, durability-enhancing coating for automotive applications such as aluminum engine block cylinder bores, compressor housings, fuel pumps, and sealing surfaces. Coatings will be characterized through metallurgical analysis and tribology and, ultimately, in real-world environments. Coatings were produced by fusing fine WC and Cr_2C_3 particulates in copper- and nickel-based binders directly onto aluminum surfaces using a high-density radiant heating process. Metallography and hardness testing have quantified the quality of this coating. A second plasma-assisted deposition process has been developed which is capable of depositing hard, 390 aluminum overlays onto soft 319 aluminum. Metallurgical analysis and wear and hardness testing have verified the wear resistance of the hard 390 aluminum coating.

Keywords: Aluminum, Cost Reduction, Engines, Hard Coatings, Wear

104. **MATERIAL SUPPORT FOR NONTHERMAL PLASMA DIESEL ENGINE EXHAUST EMISSION CONTROL**
$200,000
DOE Contact: P. B. Davis (202) 586-8061
ORNL Contact: D. P. Stinton (865) 574-4556
ORNL Contact: S. D. Nunn (865) 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, proprietary component designs for use in nonthermal plasma reactors (NTP) for the treatment of diesel exhaust gases. Gelcast ceramic components for the NTP reactor were fabricated and shipped to PNNL for evaluation and testing. It was concluded that the gelcasting process was probably not amenable to high-volume commercial production and would, therefore, be too costly. An alternative fabrication process was identified and the ceramic components were redesigned to accommodate the new process. Trial components were fabricated using the new process and shipped to PNNL for examination.

Keywords: Aftertreatment, Ceramics, Diesel, Gelcasting, Nonthermal Plasma

FUEL CELLS FOR TRANSPORTATION

105. **NANOPORE INORGANIC MEMBRANES AS ELECTROLYTES IN FUEL CELLS**
$215,000
DOE Contact: P. B. Davis (202) 586-8061
ORNL Contact: D. P. Stinton (865) 574-4556
U. of Wisconsin Contact: M. A. Anderson (608) 262-2674

The objective of this work is to collaborate with Oak Ridge National Laboratory to develop microporous inorganic membranes of TiO_2, with high proton conductivity that are capable of operating at temperatures above 100°C with minimal water management problems. Inorganic PEMs represent a fundamental departure from the polymer-based PEMs currently used in hydrogen fuel cells. Therefore, fuel cells built using inorganic PEMs will require a significantly different fabrication method. In particular, inorganic PEMs are not free standing, but rather need to be supported on a strong, porous substrate because the membranes are inherently ultra-thin and brittle. Inorganic membranes were developed that demonstrated high proton conductivity, both as self-standing monoliths and as supported thin films. Supported membranes were fabricated and are currently being tested for permeability and crossover across the assembly. Prototype inorganic microporous MEAs have also been produced and shipped to Los Alamos National Laboratory for testing.

Keywords: Fuel Cells, Inorganic Membranes, Proton Conductivity, PEM

106. **INORGANIC POLYMER ELECTROLYTE MEMBRANE ELECTRODE/SUPPORT DEVELOPMENT**
$140,000
DOE Contact: P. B. Davis (202) 586-8061
ORNL Contact: D. P. Stinton (865) 574-4556
ORNL Contact: M. A. Janney (865) 574-4281

The goal of this effort is to develop electrically conducting electrodes/supports and catalytically active ceramic sandwich layers for use in inorganic microporous PEM membranes based on nanoparticles of TiO_2 and Al_2O_3. The materials developed in this project will be used as substrates at the University of Wisconsin for the fabrication of microporous inorganic proton exchange membranes. A process was developed to fabricate electrically conducting, porous nickel materials that will be initially used as substrates (carbonaceous materials will be developed after preliminary testing). After successful development of the substrates, a second process was devised to deposit microporous titania with carefully controlled particle size and permeability onto the substrate. Sandwich layers of microporous titania on porous nickel were fabricated and shipped to the University of Wisconsin. The nickel/titania sandwich material was found to be an appropriate surface upon which to deposit the nanoparticle membrane.

Keywords: Ceramics, Fuel Cells, Membranes, Titanium Oxide

107. **LOW-FRICTION COATINGS FOR FUEL CELL AIR COMPRESSORS**
$175,000
DOE Contact: P. B. Davis (202) 586-8061
ORNL Contact: D. P. Stinton (865) 574-4556
ANL Contact: G. R. Fenske (630) 252-5190

The objective of this work is to develop and evaluate the friction and wear performance of low-friction coatings for fuel cell air compressor/expander systems. The impact of the near-frictionless carbon (NFC) coating on the scuffing performance of steel surfaces under dry contact condition was evaluated in laboratory bench top tests using a reciprocating sliding-contact configuration. NFC-coated steel surfaces showed very good tribological behavior in terms of reduced friction, reduced wear, and improved scuffing resistance compared with the uncoated surface. Therefore, this material is indeed a good candidate for application in fuel cell compressor/expander components. Four sets of turbocompressor air bearings were NFC-coated and are being tested.

Keywords: Air Compressors, Carbon, Friction, Near Frictionless Coating, Scuffing, Wear

108. **MICROSTRUCTURAL CHARACTERIZATION OF PEM FUEL CELLS**
$150,000
DOE Contact: P. B. Davis (202) 586-8061
ORNL Contact: D. P. Stinton (865) 574-4556
ORNL Contact: L. F. Allard (865) 574-4981

The objectives of this effort are to optimize the catalyst microstructure and distribution in membrane electrode assemblies (MEAs) for low cost and high performance, and to understand the effects of microstructure and microchemical composition on the performance and aging characteristics of the fuel cell. A new specimen preparation technique has been developed and demonstrated that produces thin cross-sections of PEM fuel cell MEAs suitable for microstructural and microchemical characterization in a TEM. Initial observations of precious metal catalyst content and distribution indicate that the microstructure of the catalyst layer is far from optimized in a commercially available PEM MEA. Negligible performance degradation was observed in the initial, 325 hour aging studies, however, microstructural and chemical composition changes were found at the interface of the PEM and the cathode catalyst layer.

Keywords: Catalysts, Fuel Cells, Platinum Membrane Electrode Assemblies, TEM Characterization

109. **CARBON FOAM FOR RADIATORS FOR FUEL CELLS**
$75,000
DOE Contact: P. B. Davis (202) 586-8061
ORNL Contact: D. P. Stinton (865) 574-4556
ORNL Contact: J. W. Klett (865) 574-5220

The purpose of this work is to develop compact, lightweight, and more efficient radiators for fuel-cell-powered vehicles utilizing Oak Ridge National Laboratory's unique, high-conductivity carbon foam. High-conductivity, high-surface-area carbon foam presents a unique solution to the thermal management problems that face fuel-cell vehicles. Novel carbon foam radiators of several different designs were fabricated and tested. The initial design produced an extremely high heat transfer coefficient (~2 orders of magnitude greater than those of conventional radiators), but created an unacceptable pressure drop. Alternative designs eliminated the pressure drop, but the heat-transfer coefficients were reduced to less than half of the original value. High-conductivity carbon foam appears to have great promise for use in fuel-cell radiators; however, innovative designs that take advantage of the unique properties of the foam need to be developed.

Keywords: Carbon Foam, Heat Exchangers, Heat Transfer, Radiators

110. **NANOFLUIDS FOR THERMAL MANAGEMENT APPLICATIONS**
$75,000
DOE Contact: P. B. Davis (202) 586-8061
ORNL Contact: D. P. Stinton (865) 574-4556
ANL Contact: S. Choi (630) 252-6439

The objective of this work is to exploit the unique properties of nanoparticles to develop high-thermal-conductivity heat transfer fluids. Improved nanofluid coolants could then be utilized to increase the efficiency of radiators for fuel-cell vehicles. More efficient radiators would translate into smaller, lighter, and more compact radiators. Thermal conductivity and heat transfer experiments were performed using commercial and developmental coolants. Enhanced thermal properties have been obtained with a variety of liquids that contained nanoparticles.

Keywords: Heat Transfer, Nanofluids, Nanoparticles, Radiators

111. **CARBON COMPOSITE BIPOLAR PLATES FOR PEM FUEL CELLS**
$200,000
DOE Contact: JoAnn Milliken (202) 586-2480
ORNL Contact: D. P. Stinton (865) 574-4556
ORNL Contact: T. M. Besmann (865) 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. During the year, the process used to fabricate single-sided bipolar plates was modified and improved to permit fabrication of double-sided plates. The molding of the flow field and other features into slurry-molded preforms was demonstrated for both one- and two-sided bipolar plates. This process resulted in components that replicated the mold and that were easily prepared for the CVI step. Corrosion testing over a 60-day span revealed little effect on the material—its performance was superior to that of the material supplied by Poco

Graphite. Freeze/thaw testing of the components revealed no detrimental effect. A number of single-sided and double-sided bipolar plates were fabricated and shipped to potential fuel-cell manufacturers for testing and evaluation. Discussions were held with companies interested in manufacturing plates of this design.

Keywords: Bipolar Plates, Carbon Composites, Fuel Cells, Manufacturing

112. **COST-EFFECTIVE METALLIC BIPOLAR PLATES THROUGH INNOVATIVE CONTROL OF SURFACE CHEMISTRY**
$100,000
DOE Contact: JoAnn Milliken (202) 586-2480
ORNL Contact: D. P. Stinton (865) 574-4556
ORNL Contact: M. P. Brady (865) 574-5153

The objective of this work is to develop a titanium-containing bipolar plate alloy that will form an electrically conductive and corrosion-resistant TiN surface layer during thermal nitridation. The alloy must meet DOE cost/performance goals related to the $10/kW bipolar plate target. A series of Ni-Ti, Fe(Ni)-Ti, and Ni(Cu)-Ti based alloys were nitrided and metallographically evaluated. Two protection schemes were identified: (1) a discrete TiN surface layer and (2) an inward-growing nitrogen gradient zone. The discrete TiN surface layer was found to be highly amenable to the formation of TiN coatings, but it can be sensitive to surface defects and, therefore, corrosion. The inward-growing nitrogen gradient zone is formed on alloys with high nitrogen permeability. Because of the inward nature of the growth front, these coatings are less sensitive to surface defects and corrosion. A series of nitrided coupons were fabricated and shipped to Los Alamos for testing. The electrical conductivity and corrosion resistance of the inward-growing scales met or surpassed the DOE targets.

Keywords: Bipolar Plates, Coatings, Corrosion Resistance, Fuel Cells, Nitride

LIGHTWEIGHT VEHICLE MATERIALS

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

113. **LOW-COST HIGH PERFORMANCE WROUGHT ALUMINUM COMPONENTS FOR AUTOMOTIVE APPLICATIONS**
$1,800,00
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 and PNNL
University Partners: University of Michigan, Michigan Technological University (MTI) and University of Stuttgart (IFU)
Industry Partners: Alcoa, Erie Press Systems, Imageware, AutoDie International, Advanced Technology Associates, Reynolds Metals Company and Commonwealth Aluminum

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

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

114. **LOW-COST HIGH PERFORMANCE CAST LIGHT METALS FOR AUTOMOTIVE APPLICATIONS**
$1,900,000
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 and ANL
Industry Partners: USAMP (Ford, GM, Chrysler), LEP (Ford, GM, Chrysler) and 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, Automotive, Die Life, Die Wear, Die Castings

115. **ADVANCED MATERIALS AND PROCESSES FOR AUTOMOTIVE APPLICATIONS**
$1,875,000
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 and ORNL
University Partner: University of Wisconsin-Milwaukee
Industry Partners: USAMP (Ford, GM, Chrysler), The Electric Power Research Institute (EPRI), Alcoa and 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

116. **AUTOMOTIVE-RELATED GRADUATE FELLOWSHIPS**
$100,000
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 Masters 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, Masters Degree, Ph.D. Degree, Lightweight Materials, Research, Automotive Applications, Characterization Techniques

117. **MATERIALS AND PROCESSES FOR PROPULSION SYSTEM APPLICATIONS**
$450,000
DOE Contact: Joseph Carpenter (202) 586-1022
ORNL Contact: Phil Sklad (865) 574-5069
Laboratory Partner: SNL
Industry Partner: 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

118. **TECHNOLOGY ASSESSMENT AND EVALUATION**
$1,400,000
DOE Contact: Joseph Carpenter (202) 586-1022
ORNL Contact: 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

119. **REINFORCED COMPOSITE MATERIALS-JOINING, DURABILITY, AND ENABLING TECHNOLOGIES**
$2,950,000
DOE Contact: Joseph Carpenter (202)586-1022
ORNL Contact: Dave Warren (865) 574-9693
Laboratory Partners: LBNL, LLNL, ORNL
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 and University of Nottingham
Industry Partners: USAMP/Automotive Composites Consortium Oak Ridge Institute of Science and Technology, Goodrich, Baydur Adhesives and Dow

The objective of this effort is to develop critical enabling technologies necessary for the implementation of advanced structural composite materials. In cooperation with the ACC Energy Management working group, develop material and component level 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 anc material models which can be used in designing automotive components. Specific technology thrust areas include the development of test methods, creep, fracture, fatigue and environmental durability using carbon fiber reinfoced composites. This work includes the characterization of bulk adhesives, sheet composite, sheet metals and adhesive-adherend pairs. Models are being developed 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. NDE technology is being developed to evaluate bonded joint integrity of automotive assemblies, such as a body-in-white.

Keywords: Polymer, Composites, Joining, Fracture, Durability, Automotive, Adhesives, Nondestrucive Inspection, Environmental Degradation

120. **USAMP COOPERATIVE AGREEMENT**
$3,400,000
DOE Contact: Joseph Carpenter (202) 586-1022
ORO Contact: Mary Rawlins (865) 576-0823
University Partners: University of Tulsa, University of Michigan, University of Santa Barbara, University of Cincinnati, Wayne State University, Stanford University, University of Nottingham
Industry Partners: US Automotive Materials Partnership (DaimlerChrysler, Ford, GM), Goodrich, Baydur Adhesives, Dow, Westmoreland, EKK, Entelechy, American Foundryman's Society, Mascotech, Stackpole Ltd., Valimet and Aluminum Consultant's Group

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, P4 Preforming, ACC Focal Project II and ACC Focal Project III. Projects are 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

121. **DEVELOPMENT OF LOW COST CARBON FIBER**
$2,400,000
DOE Contact: Joseph Carpenter (202) 586-1022
ORNL Contact: Dave Warren (865) 574-9693
Laboratory Partner: ORNL
University Partners: North Carolina State University, Clemson University, Virginia Technological University, Penn State University and Michigan State University
Industry Partners: USAMP/Automotive Composites Consortium, AKZO Fortafil Fibers, Amoco Cornerstone Technologies, Westvaco and Hexcel Corporation

The objective is to conduct materials research to lead to the development of low cost carbon fiber for automotive applications. Research includes investigation of alternate energy deposition methods, and alternate precursors for producing carbon fiber as well as the development of improved thermal processing methods and equipment for fiber manufacture. This work examines the fiber architecture and manufacturing issues associated with carbon fiber usage to take advantage of this material's high strength and modulus while minimizing the effects of its low strain to failure. The ultimate goal of this effort is to reduce the cost of commodity grade carbon fiber to $3-5 per pound.

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

122. **DEVELOPMENT OF LOW-COST LIGHTWEIGHT METALS AND ALLOYS**
$900,000
DOE Contact: Joseph Carpenter (202) 586-1022
ORNL Contact: Phil Sklad (865) 574-5069
PNNL Contact: Russ Jones (509) 376-4276
Laboratory Partner: PNNL
University Partner: Boston University
Industry Partners: Alcoa, EIMEx, LLC and Santa Fe Alloys

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

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

123. **RECYCLING**
$600,000
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 and Albany Research Laboratory
Industry Partners: Aluminum Association, Garfield Alloys and 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

124. **STRUCTURAL RELIABILITY OF LIGHTWEIGHT GLAZING ALTERNATIVES**
$380,000
DOE Contact: Joseph Carpenter (202)586-1022
ORNL Contact: Phil Sklad (865) 574-5069
PNNL Contact: M. A. Khaleel (509) 375-2438
Laboratory Partner: PNNL
Industry Partner: 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

125. **HIGH RATE PROCESSING TECHNOLOGIES FOR COMPOSITE MATERIALS**
$300,000
DOE Contact: Joseph Carpenter (202)586-1022
ORNL Contact: Dave Warren (865) 574-9693
Laboratory Partners: ORNL and PNL
Industry Partners: USCAR (DaimlerChrysler, Ford, General Motors), Delphi and 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

ELECTRIC DRIVE VEHICLE TECHNOLOGIES PROGRAM

ADVANCED BATTERY MATERIALS

OPTIMIZED LI-ION SYSTEM

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

126. **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. The effect of doping elements in modifying the structure and performance of the multi-element doped cathode was investigated. The beneficial effects of doping elements to eliminate the phase change and to improve performance are as the following: Ti>Al>Ga>Mg>Ca.

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

127. **DEVELOPMENT OF NOVEL ELECTROLYTES**
$75,000
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 a homologous series of sulfone cross-linked PEO solvents was completed.

Keywords: Intercalation Electrodes, Rechargeable Batteries

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

128. **REACTIVITY AND SAFETY ASPECTS OF CARBONACEOUS ANODES**
$160,000
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. A novel passive film, phosphonated polymer was developed which prevents electrolyte decomposition and enhances the safety aspects of the graphitic anodes.

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

129. **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. Studies of non-flammable binder and its compatibility with lithiated graphite and high voltage cathodes (lithium nickelate based) were completed.

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

130. **SEI LAYER FORMATION ON CARBON ANODES**
$70,000
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. Experimental measurements of the electrochemical reduction potentials of all carbonate solvents of interest in Li-ion batteries were completed.

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

131. **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. A determination of the structure, compactness, and chemical nature of the SEI formed on electron-beam deposited carbon was completed.

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

132. **CARBON ELECTROCHEMISTRY**
$205,000
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. The analysis of the relationship between the ICL and the physical properties of natural flake graphite was completed. This study was conducted in collaboration with Hydro-Quebec.

Keywords: Carbon Electrode, Rechargeable Batteries

133. **CORROSION OF LITHIUM BATTERIES**
$135,000
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 physical and electrochemical properties of passive film formed on carbonaceous anode using *in situ* electrochemical techniques. An extensive study of the passive layer on carbon anodes and Li de/intercalation in various candidate electrolytes (solvent/salt combinations) has been carried out using the Electrochemical Quartz Crystal Microbalance (EQCM) and other techniques, especially ellipsometry and cyclic voltammetry.

Keywords: Current Collector, Rechargeable Batteries

HIGH-PERFORMANCE NON-FLAMMABLE ELECTROLYTES

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

134. **NON-FLAMMABLE ELECTROLYTES**
$82,000
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. Results obtained by proton NMR studies of the thermal reaction products from EC/DMC/$LiPF_6$ suggested that polyether carbonates $(CH_2CH_2O)_m(COO)_n$ are formed during decomposition of 1M $LiPF_6$ in a mixture of 1:1 ethylene carbonate/dimethyl carbonate (EC/DMC).

Keywords: Non-flammable Electrolyte, Rechargeable Batteries

135. **DEVELOPMENT OF NON-FLAMMABLE ELECTROLYTES**
$82,000
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. Accelerated Rate Calorimetry (ARC) studies were conducted to investigate the thermal stability of the over-charged $LiNi_{0.8}Co_{0.2}O_2$ cathode in an electrolyte containing a flame retardant (FR) material, hexa-methoxy-tri-aza-phosphazene ($N_3P_3[OCH_2CH_3]_6$). It is clear that the presence of the FR additive shifts the onset of the exothermic peaks to higher temperatures.

Keywords: Non-flammable Electrolyte, Rechargeable Batteries

136. **NON-FLAMMABLE ELECTROLYTES**
$70,000
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. The fluorinated esters failed to meet the non-flammable criteria, therefore the project was re-directed to effort on ionic liquids.

Keywords: Non-flammable Electrolyte, Rechargeable Batteries

NON-CARBONACEOUS ANODE MATERIALS

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

137. **NON-CARBONACEOUS ANODE MATERIALS**
$100,000
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 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. Lithium-indium-antimony products having overall compositions $Li_zIn_{1-z/3}Sb$ (z=0, 1.2, 1.5, 2.0, 3.0) were prepared. These intermetallic electrodes have excellent electronic conductivity at all states of charge and discharge, thereby providing cells with a high rate capability.

Keywords: Non-carbon Electrodes, Rechargeable Batteries

138. **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 feasibility study of using manganese oxides as anodes was completed.

Keywords: Non-carbon Electrodes, Rechargeable Batteries

NOVEL CATHODE MATERIALS

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

139. **NEW CATHODE MATERIALS BASED ON LAYERED STRUCTURES**
$70,000
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. Vanadium oxygen pillars can be incorporated between the manganese oxide layers and that these materials appear to retain their structure over a range of cycling rates unlike the pure Li_xMnO_2.

Keywords: Intercalation Electrodes, Rechargeable Batteries

140. **NOVEL CATHODE MATERIALS**
$70,000
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. An improvement in techniques to stabilize layered $LiMO_2$ electrode materials, in which M is predominantly Mn, that do not convert to spinel on electrochemical cycling will have been made. Electrode materials will have been prepared, characterized and evaluated in electrochemical cells.

Keywords: Intercalation Electrodes, Rechargeable Batteries

141. **NOVEL CATHODE STRUCTURES**
$215,000
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. Electrochemical experiments to determine discharge profiles, and rate studies of $Li_xTi_yMn_{1-y}O_2$ series in polymer and liquid electrolyte cells were completed.

Keywords: Intercalation Electrodes, Rechargeable Batteries

142. **NEW CATHODE MATERIALS: AEROGELS**
$75,000
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. Work on manganese oxides has been completed. We have shifted emphasis to new methods to prepare intermetallic alloys as negative electrodes for Li batteries.

Keywords: Intercalation Electrodes, Rechargeable Batteries

ADVANCED SOLID POLYMER ELECTROLYTES

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

143. **COMPOSITE POLYMER ELECTROLYTES**
$70,000
DOE Contact: Ray Sutula (202) 586-8064
North Carolina State University/Michigan State University Contacts:
S. A. Khan (919) 515-4519 and
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 on different silica type and concentration on full-cell with $LiMn_2O_4$ were completed.

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

144. **HIGHLY CONDUCTIVE POLYELECTROLYTE-CONTAINING RIGID POLYMERS**
$65,000
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 indicate that PVICOX is not chemically stable when in contact with Li metal; the resistance of the cell increases by more than an order of magnitude in the first few hours due to.formation of the layer between PVICOX and Li.

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

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

145. **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. The FTIR analysis of SEI layer formed on Li electrode in oligoether electrolyte, THF/PEGDM, was completed.

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

146. **ADVANCED SOLID POLYMER ELECTROLYTES**
$255,000
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. A comparison of the conductivities of propanediol (PEPExPx) polymers with comb branch and linear polymers that contain only ethylene oxide units was determined. The PEPExPx samples show higher conductivity at low temperatures, which is consistent with lowering the barrier to Li ion movement from one solvation site to another.

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

147. **ADVANCED SOLID POLYMER ELECTROLYTES**
$150,000
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. A cell was fabricated to determine transport parameters in electrodes and preliminary measurements using NMR methods on composite electrodes were performed.

Keywords: Intercalation Electrodes, Rechargeable Batteries, Polymer Electrolyte

MATERIALS STRUCTURE AND COMPOSITION

148. **MODELING OF LITHIUM/POLYMER ELECTROLYTES**
$65,000
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. Extensive ab-initio calculations have been completed, showing the importance of ion-pairing effects in reducing ionic conductivity of the Li cation in both molten salts and polymer electrolytes. Control of this ion pairing by selection of the structure and electronegativity behavior of the anion has been demonstrated.

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

ADVANCED DIAGNOSTIC METHODS

MATERIALS STRUCTURE AND COMPOSITION

149. **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. The relationships between $LiMn_2O_4$ cathode history, electrolyte composition, electrode surface properties, and temperature for a model thin-film electrode structure were determined.

Keywords: Thin Films, Surface Studies

150. **BATTERY MATERIALS: STRUCTURE AND CHARACTERIZATION**
$125,000
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. Studies of the effects of stoichiometry of $LiMn_2O_4$ on phase behavior and cycling of $LiMn_2O_4$ were completed.

Keywords: X-ray Studies, Electrode Materials

IMPROVED ELECTROCHEMICAL MODELS

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

151. **IMPROVED ELECTROCHEMICAL MODELS**
$235,000
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. The measurements of transference numbers and diffusion coefficients on the LiTFSI/PEMO (lithium trifluorosulfonylimide in oxymethylene linked PEO) system to the salt concentration range of 0.03 to 3.16 M were completed.

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

152. **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. A web page devoted to the Thermal Modeling/Thermal Management Task was established.

Keywords: Thermal Management, Rechargeable Batteries

MATERIALS STRUCTURE AND COMPOSITION

153. **MICROSTRUCTURAL MODELING OF HIGHLY POROUS FIBROUS AND PARTICULATE ELECTRODES**
$50,000
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 fiber/particle mechanics and damage simulations for Li-ion cells were completed.

Keywords: Modeling, Microstructural Characterization

NOVEL ELECTRODE COUPLES

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

154. **NEW COUPLES: LITHIUM/SULFUR CELLS**
$140,000
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

OFFICE OF HEAVY VEHICLE TECHNOLOGIES

TRANSPORTATION MATERIALS PROGRAM

HEAVY VEHICLE PROPULSION SYSTEM MATERIALS

The Office of Heavy Vehicle Technologies (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.

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

155. **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

156. **COST-EFFECTIVE SINTERING**
$162,000
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

157. **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_{Ic}), 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 ongoing.

Keywords: Composites, Intermetallics, Nickel Aluminide, Toughened Ceramics

158. **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

159. **DIESEL PARTICULATE TRAP DEVELOPMENT**
$100,000
DOE Contact: Sidney Diamond (202) 586-8032
ORNL Contact: D. R. Johnson (865) 576-6832
ORNL Contact: R. D. Ott (865) 574-5172

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

160. **INSULATING STRUCTURAL CERAMICS FOR HIGH EFFICIENCY, LOW EMISSION ENGINES**
$300,000
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

161. **THICK THERMAL BARRIER COATINGS (TTBCS) FOR LOW EMISSIONS, HIGH EFFICIENCY DIESEL ENGINE COMPONENTS**
$200,000
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

162. **MATERIALS FOR LOW EMISSIONS, HIGH EFFICIENCY DIESEL ENGINE COMPONENTS**
$518,000
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

163. **MATERIALS FOR LOW EMISSIONS, HIGH EFFICIENCY DIESEL ENGINE COMPONENTS**
$300,000
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

164. **R&D FOR ADVANCED CERAMICS AND CERMETS**
$400,000
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

165. **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

166. **CARBON FOAMS FOR HEAT TRANSFER**
$72,000
DOE Contact: Sidney Diamond (202) 586-8032
ORNL Contact: D. R. Johnson (865) 576-6832
ORNL Contact: J. W. Klett (865) 574-5220

The purpose of this work is to develop carbon foams for heat transfer removal from the air side of heavy vehicle radiators.

Keywords: Carbon, Components, Heat Transfer

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

167. **THE HIGH TEMPERATURE MATERIALS LABORATORY USER PROGRAM**
$5,500,000
DOE Contact: Sidney Diamond (202) 586-8032
ORNL Contact: D. R. Johnson (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 microsturctural 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

168. **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 micro-structural changes to performance of diesel NOx reduction catalysts. The research is focussed on understanding these changes through TEM studies of experimental catalyst materials reacted in an ex situ catalyst reactor system especially constructed to allow appropriate control of the reaction conditions and the transfer of the sample between reactor and microscope.

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

169. **LIFE PREDICTION VERIFICATION**
$200,000
DOE Contact: Sidney Diamond (202) 586-8032
ORNL Contact: D. R. Johnson (865) 576-6832
ORNL Contact: H.-T. Lin (865) 576-6657

The first goal of this research program is the systematic study of candidate structural ceramics for internal combustion engine components as a function of temperature (< 900°C), environment, time, and machining conditions. The second goal 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

170. **HIGH TEMPERATURE TENSILE TESTING**
$155,000
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 objectives of this research are to understand the high-temperature mechanical performance (creep, fatigue) of self-reinforced silicon nitride ceramics; to understand environmental effects on the high-temperature mechanical behavior of self-reinforced ceramics, to understand the microstructure of silicon nitride ceramics, to understand the effects of surface engineering (coatings) on the mechanical properties of silicon nitride and environmental effects on ceramic systems performance, to investigate the effect of Partially Stabilized Zirconia (PSZ) thermal barrier coatings on diesel engine performance, and to use Finite Element Methodology (FEM) to understand the behavior of the various materials systems under investigation through modeling.

Keywords: Advanced Materials, Coatings, Creep, Diesel, Environmental Effects, Fatigue, Fracture, Microscopy, Silicon Nitride, Tensile Testing, Zirconia

171. **NDE/C TECHNOLOGY FOR HEAVY DUTY DIESEL ENGINES: FUEL DELIVERY AND INSULATING MATERIALS**
$25,000
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 is to develop enabling nondestructive evaluation/characterization (NDE/C) technology to support materials development related to lower-emission, higher-efficiency diesel engines for heavy vehicles. Specifically, the project addresses development of advanced NDE/C technology for advanced fuel delivery systems (including injector nozzles), and insulating materials for reduced heat loss in the combustion zone.

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

172. **INTERNATIONAL EXCHANGE AGREEMENT (IEA)**
$150,000
DOE Contact: Sidney Diamond (202) 586-8032
ORNL Contact: D. R. Johnson (865) 576-6832
and 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. Subtasks 11 (Techniques for the Measurement of Thermal and Mechanical Fatigue) and 12 (Characterizing Ceramic Powders) were initiated in October 1999. However, Subtask 12 research performed by NIST was transferred to the Versailles

Project on Advanced Materials and Standards (VAMAS) and is no longer a part of Annex II.

Keywords: IEA, Powder Characterization

173. **STANDARD REFERENCE MATERIALS**
$150,000
DOE Contact: Sidney Diamond (202) 586-8032
ORNL Contact: D. R. Johnson (865) 576-6832
NIST Contact: S. Jahanmir (301) 975-3671

The objective of IEA Subtask 10 was to establish the repeatability and reproducibility of test methods used for the characterization of ceramic powders through an international round-robin study. Due to continued interest by all countries participating in this activity, this project has been extended to further evaluate some of the test methods that require refinement, and plans have been developed for continuation of this work as Subtask 12. Subtask 12 has been transitioned to VAMAS, and plans will be established to initiate a new IEA activity focussed on test methods and standards for the assessment of reliability of advanced materials used for diesel-powered heavy vehicles.

Keywords: IEA, Reference Material, Powder Characterization

174. **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

175. **RELIABLE JOINING TECHNIQUES FOR ADVANCED DIESEL ENGINE VALVES**
$37,000
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. Low-cost techniques for joining of high-performance titanium aluminide engine valve heads to more-cost-effective valve stem materials are being evaluated.

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

176. **RAMAN AND FLUORESCENCE SPECTROSCOPIC CHARACTERIZATION OF CERAMIC MATERIALS: STRESS, PHASE, AND TEMPERATURE**
$40,000
DOE Contact: Sidney Diamond (202) 586-8032
ORNL Contact: D. R. Johnson (865) 576-6832
and 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

TECHNOLOGY TRANSFER AND MANAGEMENT COORDINATION

177. **TECHNICAL PROJECT MANAGEMENT**
$500,000
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

178. **DURABILITY OF DIESEL ENGINE COMPONENT MATERIALS**
$200,000
DOE Contact: Sidney Diamond (202) 586-8032
ORNL Contact: D. R. Johnson (865) 576-6832
and 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

179. **ADVANCED MACHINING/MANUFACTURING**
$225,000
DOE Contact: Sidney Diamond (202) 586-8032
ORNL Contact: D. R. Johnson (865) 576-6832
and 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

180. **NDE DEVELOPMENT FOR CERAMIC VALVES FOR DIESEL ENGINES**
$175,000
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 work is to evaluate several nondestructive evaluation (NDE) techniques to detect defects/damage in structural ceramic valves for diesel engines. There are four tasks: (1) establish correlation of NDE data with mechanical properties for fatigue/wear-damaged samples (2) develop NDE techniques for ceramic-metal joints (3) conduct NDE studies of full-sized engine valves, and (4) finalize correlation of NDE results to machining damage.

Keywords: Computed Tomography, Joining, Machining, Nondestructive Evaluation, Structural Ceramics

181. **CYLINDRICAL WIRE ELECTRON DISCHARGE MACHINING PROCESS**
$40,000
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

182. **QUANTIFYING THE ENVIRONMENTAL EFFECTS ON THE MECHANICAL PROPERTIES OF ADVANCED SILICON NITRIDE MATERIALS FOR DIESEL ENGINE APPLICATIONS**
$23,000
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

183. **DEVELOPMENT OF NO_x SENSORS FOR HEAVY VEHICLE APPLICATIONS**
$250,000
DOE Contact: Sidney Diamond (202) 586-8032
ORNL Contact: D. R. Johnson (865) 576-6832
and T. A. Armstrong (865) 574-7996

The objective of this program is to develop a zirconia-based NO_x sensor for improved engine and exhaust diagnostics in class 1-8 truck engines.

Keywords: Characterization, Components, Electrochemistry, Fabrication, Zirconia

HIGH STRENGTH WEIGHT REDUCTION MATERIALS

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

184. **DESIGN, ANALYSIS AND DEVELOPMENT OF LIGHTWEIGHT FRAMES FOR TRUCK AND BUS APPLICATIONS**
$1,150,000
DOE Contact: Sid Diamond (202) 586-8032
ORNL Contact: Phil Sklad (865) 574-5069
Laboratory Partner: ORNL
Industry Partners: Autokinetics, DaimlerChrysler, Ford, Budd Company, Alcan, Alcoa and 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, MMCs, and polymer matrix composites.

Keywords: Frames, Manufacturing, Lightweight, Trucks, Buses

185. **DEVELOPMENT OF A CASTING PROCESS FOR PRODUCING ULTRA-LARGE COMPONENTS**
$1,300,000
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

186. **DEVELOPMENT OF ADVANCED CASTING TECHNOLOGIES FOR PRODUCTION OF HIGH INTEGRITY TRUCK COMPONENTS**
$900,000
DOE Contact: Sid Diamond (202) 586-8032
ORNL Contact: Phil Sklad (865) 574-5069
Laboratory Partners: ORNL, PNNL, Albany Research Labs
Industry Partners: Thompson Aluminum Casting, Tennessee Tool and Engineering-Die Casting, Freightliner, PACCAR and Alcoa

The objectives of this project are 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; to develop the necessary understanding and technology to cast large structural components for Class 8 truck cabs; and to develop modeling and design capabilities for optimizing steel castings for heavy vehicle applications to reduce weight without sacrificing performance.

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

187. **TECHNOLOGY DEVELOPMENT FOR LIGHTWEIGHT ENGINES**
$100,000
DOE Contact: Sid Diamond (202) 586-8032
ORNL Contact: Phil Sklad (865) 574-5069
Laboratory Partner: ORNL
Industry Partner: Cummins Engine Co.

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

188. **ADVANCED FORMING TECHNOLOGIES FOR LIGHTWEIGHT ALLOYS**
$600,000
DOE Contact: Sid Diamond (202) 586-8032
ORNL Contact: Phil Sklad (865) 574-5069
Laboratory Partners: LANL, PNNL, INEEL and ORNL

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

189. **DEVELOPMENT OF CARBON MONOLITHS FOR SAFE, LOW PRESSURE ADSORPTION STORAGE AND RELEASE NATURAL GAS**
$200,000
DOE Contact: Sid Diamond (202) 586-8032
ORNL Contact: Phil Sklad (865) 574-5069
Laboratory Partner: ORNL

The objective of this project is to develop and test monolithic carbon adsorbant 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

190. **IMPROVED MATERIALS FOR HEAVY VEHICLE BRAKE AND FRICTION APPLICATIONS**
$400,000
DOE Contact: Sid Diamond (202) 586-8032
ORNL Contact: Phil Sklad (865) 574-5069
Laboratory Partner: ORNL
Industry Partner: Honeywell

The objective of these activities is to investigate the nature of changes on surfaces of materials during braking, develop understanding of the role of friction films in braking, to evaluate advanced materials for heavy vehicle brake application, and to develop reliable, cost-effective, laboratory-scale friction tests to select and rank new materials and surface treatments for engine components.

Key words: Brakes, Friction Materials, Friction Films

191. **HIGH CONDUCTIVITY CARBON FOAMS FOR THERMAL MANAGEMENT**
$100,000
DOE Contact: Sid Diamond (202) 586-8032
ORNL Contact: Phil Sklad (865) 574-5069
Laboratory Partner: ORNL
Industry Partners: Caterpillar, Modine and Peterbilt

The objective of this activity is to evaluate the use of conductive carbon foam materials as a highly efficient and lightweight heat exchanger for heavy vehicle cooling needs such as radiators, etc. Focus is on determining basic material properties, defining acceptable operating limits, and fabrication of the core structures which can operate in a Class 7-8 vehicle.

Keywords: Carbon Foam, Heat Exchanger, Heavy Vehicle

192. **TECHNOLOGY ASSESSMENT AND EVALUATION**
$1,200,000
DOE Contact: Sid Diamond (202) 586-8032
ORNL Contact: Phil Sklad (865) 574-5069
Laboratory Partner: 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 2000
OFFICE OF POWER TECHNOLOGIES - GRAND TOTAL	$60,583,000
OFFICE OF SOLAR ENERGY TECHNOLOGIES	$28,286,000
MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING	$16,577,000
Amorphous Silicon for Solar Cells	4,787,000
Polycrystalline Thin-film Materials for Solar Cells	8,418,000
Film Silicon for Solar Cells	1,907,000
Deposition of Solar Grade Silicon	302,000
Deposition of III-V Semiconductors for High-efficiency Solar Cells	1,163,000
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING	$4,913,000
Materials and Device Characterization	4,913,000
MATERIALS STRUCTURE AND COMPOSITION	$3,830,000
Structure of Photovoltaic and Photoelectrochemical Materials	3,830,000
DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING	$2,966,000
High-efficiency Crystalline Silicon Solar Cells	2,966,000
OFFICE OF WIND AND GEOTHERMAL TECHNOLOGIES	$897,000
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING	$897,000
Corrosion Characteristics of Clad and Thermal Sprayed NiCrMo Alloys	125,000
Coatings and Concrete Mix Design for Prevention of MIC in Cooling Towers	120,000
Remediation of Deformed Well Casing	167,000
High Performance Polymer Coating Systems	90,000
Thermally Conductive Composites	185,000
CaP Cements	150,000
Adhesive Sealants	45,000
Evaluation of Bearing Elastomers	15,000
OFFICE OF HYDROGEN AND SUPERCONDUCTIVITY TECHNOLOGIES	$31,400,000
HIGH TEMPERATURE SUPERCONDUCTIVITY FOR ELECTRIC SYSTEMS	$31,400,000
DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING	$31,400,000
The Superconductivity Partnership Initiative	14,000,000
The 2nd Generation Wire Initiative	10,000,000
Strategic Research	7,400,000

OFFICE OF POWER TECHNOLOGIES

OFFICE OF SOLAR ENERGY TECHNOLOGIES

The National Photovoltaics Program sponsors research and development with the goal of making terrestrial solar photovoltaic power a significant and commercially viable part of the national energy mix. From such efforts, private enterprise can choose options for further development and competitive application in U.S. and foreign electric power markets. Approximately 70 percent of the domestic product is exported to developing countries. The objective of materials research is to overcome the technical barriers that limit the efficiency and cost-effectiveness of photovoltaic cells. Conversion efficiency of photovoltaic (PV) cells is limited by the spectral response of the cell's semiconductor material (dependent on bandgap), and by device engineering factors such as junction depth, reflection coefficient, parasitic resistances (i.e., series resistance in the metallization and contacts, shunt resistance through the thickness of the cell), and material imperfections that support dark recombination of excess photogenerated carriers. Manufacturing cost is affected by the expense of semiconductor material growth, the complexity of junction formation and cell fabrication, and the fabrication requirements of final module assembly. While most photovoltaics in the U.S. have (historically) been intended for remote stand-alone applications, an increasing number of domestic deployments are intended for a grid-tied (net metering) environment. Anticipated world-wide production in CY 2000 is approximately 255 MW, with about 80 MW made in the U.S.

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

193. **AMORPHOUS SILICON FOR SOLAR CELLS**
$4,787,000
DOE Contact Jeffrey Mazer (202) 586-2455
NREL Contact: Bolko von Roedern
(303) 384-6480

These projects perform research on the deposition and characterization of amorphous silicon thin films to improve solar cell conversion efficiency and high-throughput manufacturability. Efficient conversion is hindered by unintended impurities or undesired structure in the deposited films and by poor uniformity of the films over large (4000 cm^2) areas. The films are deposited by plasma enhanced chemical vapor deposition (glow discharge), thermal chemical vapor deposition, and sputtering. The long-term goal 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 Silicon, Amorphous Materials, Coatings and Films, Semiconductors, Chemical Vapor Deposition, Sputtering, Solar Cells

194. **POLYCRYSTALLINE THIN-FILM MATERIALS FOR SOLAR CELLS**
$8,418,000
DOE Contact: Jeffrey Mazer (202) 586-2455
NREL Contact: Harin Ullal (303) 384-6486

These projects perform applied research on the deposition of CuIn(Ga,S)Se$_2$ (CIGSS) 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 CIGSS and CdTe films, by controlling interlayer diffusion and lattice matching in heterojunction structures, and by controlling the uniformity of deposition over large (4000 cm^2) areas. The films are deposited by chemical and physical vapor deposition, electrodeposition, 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

195. **FILM SILICON FOR SOLAR CELLS**
$1,907,000
DOE Contact: Jeffrey Mazer (202) 586-2455
NREL Contact: Ted Ciszek (303) 384-6569

These projects perform applied research on the high-throughput deposition of relatively thin crystalline silicon (50-100 microns). Methods include recrystallization of silicon powder on inexpensive ceramic substrates, and are amenable to rapid thermal annealing (RTA) and integrated module manufacturing techniques. The goal is to develop highly cost-effective crystalline silicon modules, with conversion efficiencies in the 12-14 percent range.

Keywords: Semiconductors, Crystalline Silicon, Recrystallization, Rapid Thermal Annealing, Solar Cells, Film Silicon

196. **DEPOSITION OF SOLAR GRADE SILICON**
$302,000
DOE Contact: Jeffrey Mazer (202) 586-2455
NREL Contact: Ted Ciszek (303) 384-6569

This project has the goal of achieving a low-cost (~$15/kilogram) crystalline silicon feed stock material suitable for commercial solar cell production. The method involves the refining of liquid metallurgical grade silicon. Such material could prove critical to photovoltaic commercial expansion in the event that large quantities of reject electronic-grade feed stock from the integrated circuit industry become unavailable.

Keywords: Solar Grade Silicon, Solar Cells, Crystalline Silicon Solar Cells

197. **DEPOSITION OF III-V SEMICONDUCTORS FOR HIGH-EFFICIENCY SOLAR CELLS**
$1,163,000
DOE Contact: Jeffrey Mazer (202) 586-2455
NREL Contact: Sarah Kurtz (303) 384-6475

These projects perform applied research on the deposition and conduction properties of III-V semiconductors for super-high-efficiency concentrator solar cells. Research is focused on precise deposition of layers, studying the properties of the interfacial regions, and understanding the conduction-limiting mechanisms of the materials. Conduction-limiting mechanisms are particularly severe in the case of GaInAsN, an otherwise ideal material for use in a four-junction super-high-efficiency concentrator cell. The materials are deposited by metal organic chemical vapor deposition (MOCVD), liquid phase epitaxy, and molecular beam epitaxy. The long-term goal is to develop three- and four-junction III-V-based cells that achieve 38 percent efficiency under high-ratio concentration.

Keywords: Semiconductors, Chemical Vapor Deposition, Solar Cells, MOCVD

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

198. **MATERIALS AND DEVICE CHARACTERIZATION**
$4,913,000
DOE Contact: Jeffrey Mazer (202) 586-2455
NREL Contact: Angelo Mascarenhas (303) 384-6608

These projects measure and characterize material and device properties. Methods include 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, scanning transmission electron microscopy, and Auger spectroscopy.

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

MATERIALS STRUCTURE AND COMPOSITION

199. **STRUCTURE OF PHOTOVOLTAIC AND PHOTOELECTROCHEMICAL MATERIALS**
$3,830,000
DOE Contact: Jeffrey Mazer (202) 586-2455
NREL Contact: Alex Zunger (303) 384-6672

These projects support the fundamental and exploratory research needed for advancement of PV technologies in the long term, i.e., five to ten years and beyond. Projects include collaboration with the Office of Science (SC). Topics include material structure of quaternary III-V materials such as GaInAsN, and structure of photoelectrochemical materials.

Keywords: Semiconductors, Band Structure, Solar Cells

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

200. HIGH-EFFICIENCY CRYSTALLINE SILICON SOLAR CELLS

$2,966,000
DOE Contact: Jeffrey Mazer (202) 586-2455
NREL Contact: John Benner (303) 384-6496

These projects perform applied research on crystalline silicon devices to improve conversion efficiency. Methods employ new and improved dopant profiles, advanced back-surface fields, and silicon nitride and other bulk passivation treatments to reduce carrier 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, Multicrystalline Silicon

OFFICE OF WIND AND 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 PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

201. CORROSION CHARACTERISTICS OF CLAD AND THERMAL SPRAYED NiCrMo ALLOYS

$125,000
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 alloys investigated included Inconel 625, Incoloy 825, and Hastelloy C-276. 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 in synthetic hypersaline brine and solutions of different chloride concentrations to investigate corrosion characteristics of the different materials. Critical pitting temperature studies were also performed. The clad versions of Inconel 625 and Incoloy 825 consistently exhibited greater susceptibility to corrosion than the wrought materials under the experimental conditions used. The reasons for the difference in corrosion behavior were investigated using microstructural and EDAX analyses. It was determined that the surface microstructure and chemical composition for the clad materials differs from that of the wrought alloys and this results in increased corrosion rates. Wrought and clad Hastelloy C-276 tended to have similar corrosion characteristics. The thermal-sprayed Inconel 625 had the highest corrosion rate of all materials tested due to the coating porosity. Of the materials tested, wrought Inconel 625 and Hastelloy C-276 gave the best performance based on corrosion potential and corrosion current density. Whether the observed differences in behavior of clad and wrought alloys will significantly affect corrosion resistance and mechanisms under operating conditions in a geothermal system needs to be investigated further.

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

202. COATINGS AND CONCRETE MIX DESIGN FOR PREVENTION OF MIC IN COOLING TOWERS

$120,000
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. Initial work focused on performance comparison of commercially available concrete repair and protection materials have been selected for performance comparison. This was supplemented by studies of the resistance of different concrete types to microbiologically influenced corrosion (MIC). The repair materials tested included three epoxy coatings, an epoxy sealant, an epoxy-modified cement mortar, a latex-modified mortar and a calcium aluminate mortar. The influence of partial replacement of cement with silica fume or ground granulated blast furnace slag on the performance of concrete was determined. Coated and uncoated concrete panels were exposed to sulphur oxidizing bacteria (*Thiobacillus ferrooxidans*) at 40°C for a period of 60 days. The coatings, mortars and different concretes 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 followed by the calcium aluminate mortar. Replacement of cement with 10 percent silica fume improved the resistance of bare concrete to MIC. The concrete mix with 40 percent replacement of cement with blast furnace slag also exhibited enhanced durability. However, increasing the slag content to 60% resulted in decreased resistance. Specimens of coated concrete, calcium aluminate mortar and different concrete mix proportions were sent to Unocal in Indonesia for long-term field testing. The field performance will be compared with that obtained under laboratory conditions and used to make recommendations for dealing with the problem of MIC.

Keywords: Microbiologically Influenced Corrosion, Concrete, Epoxy Coatings, Calcium Aluminate, Silica Fume, Blast Furnace Slag, Repair, Mortars, Cooling Towers, Durability

203. **REMEDIATION OF DEFORMED WELL CASING**
$167,000
DOE Contact: R. LaSala (202) 586-4198
BNL Contacts: M. L. Berndt (631) 344-3060 and A. J. Philippacopoulos (631) 344-6090

Deformation surveys conducted in geothermal fields have shown that geothermal wells can experience excessive deformation. Formation movement, which in turn, is associated with 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. This involves milling of the deformed casing and cementing a liner into place. The objective of this project is to develop and analyze optimum cement formulations for well casing remediation. 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. Cement slurries considered to date include standard Class G-silica flour, latex-modified, low density perlite-modified and glass fiber reinforced. The cements have been tested for compressive properties under unconfined and triaxial loading, flexural and tensile strength, elastic modulus, Poisson's ratio, thermal conductivity and coefficient of thermal expansion.

In addition to the material development, numerical modeling is performed to investigate the cement patch/formation interaction. The loads under consideration include pressure and temperature. The finite element models used for this purpose incorporate the liner and the various cement formulations developed under this program. In addition, all existing casing as well as the surrounding formation are incorporated into the models. A series of analyses were performed to take into account parametrically different materials and loading conditions. The project initially utilized two-dimensional models. Subsequently, three-dimensional models were used in order to ascertain the validity of the assumptions used in the analysis. In both loading conditions, the stress field has high values in the vicinity of the remediation. Due to the nature of the configuration and loads, high tensile stresses are developed in the system. While the cements deform plastically at higher strains under compression, their tensile capability needs to be increased in order to respond to the demand shown by the analysis. Furthermore, material modeling will be focused on yield surface characterization of the cement materials and subsequent failure analysis. Laboratory testing and finite element analysis are carried out interactively to achieve optimization. It is planned to extend the research to cover broader issues of cement design criteria and structural response analysis for completion as well as remediation cements.

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

204. **HIGH PERFORMANCE POLYMER COATING SYSTEMS**
$ 90,000
DOE Contact: Raymond LaSala (202) 586-4198
BNL Contact: Toshifumi Sugama (631) 344-4029

This project is for the development of organic, inorganic, and organometallic polymer coating systems consisting of primer and topcoating layers that mitigate corrosion, oxidation, and abrasive wear in tubing, heat exchanger, piping, vent gas blower, cooling condenser, and plant structure components made from different metals. The key factors for successful coating systems include low ionic conductivity, anti-oxidation properties, superior surface hardness, low surface-energy, excellent adherence of the coatings to metals, and great durability of interfacial bonds. Coated test panels are evaluated in short-term exposures in an autoclave at brine temperatures up to 200°C. Once potential coating systems are identified, test panels coated with these systems will be send to geothermal power plants for long-term performance tests.

Keywords: Polymer Coating, Anti-corrosion, Anti-oxidation, Abrasive Wear Resistance, Metal, Hot Brine

205. **THERMALLY CONDUCTIVE COMPOSITES**
$185,000
DOE Contact: Raymond LaSala (202) 586-4198
BNL Contact: Toshifumi Sugama (631) 344-4029

This project is to formulate thermally conductive polyphenylenesulfide-based composites for use as a lining material of the internal surfaces for inexpensive carbon steel-heat exchanger tubes. The task also includes developing state-of-the-art lining process technologies suitable for composite materials. The lining materials fabricated have excellent thermal conductivity, high-temperature stability and anti-corrosion and anti-fouling characteristics. Tubes with these linings were sent to geothermal binary cycle power plants operated with brine temperatures up to 160°C for long-term field validation tests at plant's site. Post-test analyses will be conducted on these tubes to determine the rate of scale deposits and the degree of corrosion of the underlying steel, as well as to assess any damage to the liners incurred during hydroblasting, which is used to clean the tubes before reuse.

Keywords: Thermally Conductive Composite, Polyphenylenesulfide, Heat Exchanger Tube, Anti-corrosion, Anti-fouling, Liner

206. **CaP CEMENTS**
$150,000
DOE Contact: Raymond LaSala (202) 586-4198
BNL Contact: Toshifumi Sugama (631) 344-4029

This project is designed to synthesize and characterize cost-effective acid-resistant calcium aluminate polyphosphate (CaP) cementitious material used to support casing pipes, and to inhibit their corrosion in CO_2-rich geothermal wells at brine temperatures up to 300°C and a pH of 1.8. The synthesized CaP cements were applied to geothermal wells in Indonesia, Japan, and the United States to evaluate their full-scale technical feasibility. Long-term monitoring tests are being conducted to determine the magnitude of cement's susceptibility to acid, their ability to mitigate corrosion of pipes, and also their aging characteristics including phase transitions and changes in mechanical properties.

Keywords: Calcium Aluminate Polyphosphate Cement, Acid-resistance, Corrosion, Casing Pipe, Synthesis

207. **ADHESIVE SEALANTS**
$45,000
DOE Contact: Raymond LaSala (202) 586-4198
BNL Contact: Toshifumi Sugama (631) 344-4029

This project is for the development of the sealing materials that protect the blade-fit area of turbine rotors against corrosion. Poly(dimethylmethyphenyl-methoxy)siloxane-based silicon was synthesized and formulated to meet the following five criteria. These are: (1) ability to wick readily into a very narrow interstice, (2) excellent adherence to alloy steel rotors and stainless steel blades, (3) resistance to acidic brine at 180°C, (4) curable in moist surroundings at room temperature; and (5) good elastomeric properties. Long-term durability tests will be needed to ensure that this sealing material adequately protects the bladed turbine rotors.

Keywords: Sealants, Corrosion, Silicon, Turbine Rotor, Synthesis

208. **EVALUATION OF BEARING ELASTOMERS**
$15,000
DOE Contact: Raymond LaSala (202) 586-4198
BNL Contact: Toshifumi Sugama (631) 344-4029

The objective of this task is to gain a fundamental understanding of the mechanisms of hydrothermal degradation and stabilization of fluoro- and nitrile-based bearing elastomers used in down-hole pumps. These pumps extract the energy resource from geothermal brine reservoirs at 150°C. This information will not only provide a prediction of their useful lifespan, but also impart to us better ways to retard and inhibit the degree of degradation of these elastomers.

Keywords: Bearing Elastomers, Hydrothermal Degradation, Down-hole Pumps

OFFICE OF HYDROGEN AND SUPERCONDUCTIVITY TECHNOLOGIES

HIGH TEMPERATURE SUPERCONDUCTIVITY FOR ELECTRIC SYSTEMS

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

209. **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 that 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:

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 and the unit has been relocated to Los Alamos National Laboratory (LANL) for tests designed to optimize its performance.

LANL Contact: Dean Peterson (505) 665-3030

1,000 hp and 5,000 hp Motors - The project, led by Rockwell Automation, led to the demonstration of a 1,000 horsepower (hp) motor in late 2000. Rockwell's Reliance Electric division assembled the motor, which incorporates HTS coils fabricated and wound by American Superconductor. The motor continues to undergo load testing. Design analysis and preliminary system component testing for a 5,000 hp unit has also begun. 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

Cold Dielectric Superconducting Transmission Cable - Southwire Company and Oak Ridge National Laboratory (ORNL) demonstrated a 30-meter, three-phase HTS cable feeding electricity to three Southwire manufacturing facilities. This effort included conductor fabrication, cable assembly including terminations and vacuum-insulated pipe, and the construction of a control building and switchyard. The cable was tested at full current and voltage as well as at off-design conditions. The cable was dedicated and began delivering power in early 2000, and has amassed over 5,000 hours of uninterrupted operation, a record for this technology.

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

Warm Dielectric Superconducting Transmission Cable - A team led by Pirelli Cables and Systems and including Detroit Edison, American Superconductor, and Los Alamos National Lab is continuing work on a two-phase project to design, fabricate, install, and test a 120-meter, 3-phase, room-temperature dielectric HTS power system. This cable project is distinct from the Southwire project in that its design involves a dielectric that is outside of the cable's thermal insulation, and the cable will be demonstrated in a retrofit application: supplying transformers in a Detroit Edison substation. The HTS cable will lead to smaller, more efficient electricity transmission lines in utility networks.

Pirelli Contact: Nathan Kelley (803) 356-7762

Flywheel Electricity System - This project 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 completed the design of a 3kW/10kWh system in 2000. Components of the system, including the superconducting bearings, motor/generator, and control systems, have been fabricated and are undergoing extensive testing. Construction of the rotor has also begun, and a drop test of a model flywheel spinning at 41,000 rpm was performed. The containment structure successfully absorbed the energy of the simulated system failure.

Boeing Contact: Mike Strasik (425) 237-7176

Reciprocating Magnetic Separator - This project 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 2000, 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

Transformer - Waukesha Electric Systems (WES) is leading a team that includes ORNL, IGC-SuperPower, and Rochester Gas and Electric to build and operate a 5/10 MVA alpha prototype cryocooled HTS power transformer on the Wisconsin Electric Power utility grid. The prototype will power WES' main transformer manufacturing plant. In 2000, the team advanced the conceptual design of the project, concentrating on limiting AC losses in the transformer's HTS coils and testing system components. The projected commissioning date for the transformer is in December 2001.

ORNL Contact: Bob Hawsey (865) 574-8057

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

210. **THE 2ND GENERATION WIRE INITIATIVE**
$10,000,000
DOE Contact: Jim Daley (202) 586-1165
Argonne National Laboratory Contact:
U. Balachandran (630) 252-4250
Brookhaven National Laboratory Contact:
David Welch (516) 282-3517
Los Alamos National Laboratory Contact:
Dean Peterson (505) 665-3030
National Renewable Energy Laboratory
Contact: Richard Blaugher (303) 384-6518
Oak Ridge National Laboratory Contact:
Robert Hawsey (865) 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 Superconducting Technology Contact:
Seung Hong (732) 541-1300
3M Contact: Arnold Funkenbusch (651) 733-5071
MicroCoating Technologies Contact:
Shara Shoup (678) 287-2478
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 2000, 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:

Collaborative R&D Projects - Metal-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 2000 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.

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 Laboratory 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).

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 2000. A variety of deposition and processing strategies were being investigated to develop a fundamental understanding of this deposition approach and to optimize film properties. Additionally, Sandia scientists worked on developing high-quality, solution-derived, 123-type superconducting films for coated conductor applications.

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

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

Process Technology - DOE partners worked toward developing and demonstrating process technology needed for epitaxial growth of buffer layers by metal-organic 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.

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

211. **STRATEGIC RESEARCH**
$7,400,000
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Brookhaven National Laboratory Contact:
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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:

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.

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 2000. Researchers at Stanford University investigated ion-beam assisted deposition of buffer layers and *in situ* deposition of YBCO by electron beam evaporation. The University of Wisconsin conducted research on BSCCO critical currents and microstructures, YBCO coated conductor microstructure, and pulse tube cryocooler technology. Finally, researchers at the University of Houston continued investigation of high-rate photon-assisted metal-organic chemical vapor deposition for YBCO onto buffered, textured metallic substrates.

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 2000, 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 2000
OFFICE OF SCIENCE - GRAND TOTAL	$448,224,217
OFFICE OF BASIC ENERGY SCIENCES	$402,281,000
DIVISION OF MATERIAL SCIENCES AND ENGINEERING	$402,281,000
Theoretical Condensed Matter Physics	17,624,000
Experimental Condensed Matter Physics	32,751,000
Materials Chemistry	27,390,000
Mechanical Behavior and Radiation Effects	18,211,000
Neutron and X-ray Scattering	24,659,000
Structure and Composition of Materials	24,372,000
Physical Behavior	16,494,000
Synthesis and Processing Sciences	15,448,000
Engineering Research	14,020,000
Experimental Program to Stimulate Competitive Research	6,815,000
National User Facilities (Materials Research)	204,497,000
OFFICE OF ADVANCED SCIENTIFIC COMPUTING RESEARCH	$37,343,217
DIVISION OF TECHNOLOGY RESEARCH	$37,343,217
LABORATORY TECHNOLOGY RESEARCH PROGRAM	$4,152,000
MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING	$2,578,000
High Performance Tailored Materials for Levitation and Permanent Magnet Technologies (ANL 97-02)	126,000
Atomic Scale Structure of Ultrathin Magnetic Multilayers and Correlation With Resistance, Giant Magnetoresistance, and Spin-Dependent Tunneling (ORL 97-03)	120,000
Improved Materials for Semiconductor Devices (PNL 98-17)	250,000
Development of High-Temperature Superconducting Wire Using RABiTS Coated Conductor Technologies (ORL 97-02)	110,000
Development of Bismuth-Based Superconducting Wire with Improved Current Carrying and Flux Pinning Properties (ANL 99-15)	229,000
Light Emission Processes and Dopants in Solid State Light Sources (LBL 97-13)	114,000
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)	207,000
Combinatorial Discovery and Optimization of Novel Materials for Advanced Electro Optical Devices (LBL 97-18)	100,000
Advanced Computational Models and Experiments for Deformation of Aluminum Alloys - Prospects for Design (PNL 99-07)	200,000
Near-Frictionless Carbon Coatings (ANL 98-03)	56,000
Smooth Diamond Films for Friction and Wear Applications and Chemically Protective Coatings (ANL 97-05)	100,000
Nanometer Characterization and Design of Molecular Lubrication for the Head-Disk Interface (LBL 98-10)	126,000

OFFICE OF SCIENCE (Continued)

	FY 2000
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)	
An Advanced Hard Carbon Plasma Deposition System with Application to the Magnetic Storage Industry (LBL 98-16)	250,000
Interfacial Properties of Electron Beam Cured Composites (ORNL 99-08)	220,000
Photocatalytic Metal Deposition for Nanolithography (ANL 99-13)	120,000
DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING	$1,574,000
Ionically Conductive Membranes for Oxygen Separation (LBL 97-03)	40,000
Advanced Separations Technology for Efficient and Economical Recovery and Purification of Hydrogen Peroxide (ANL 98-07)	229,000
Synthesis and Crystal Chemistry of Technologically Important Ceramic Membranes (ANL 97-06)	59,000
Catalytic Production of Organic Chemicals Based on New Homogeneously Catalyzed Ionic Hydrogenation Technology (BNL 97-05)	122,000
Highly Dispersed Solid Acid Catalysts on Mesoporous Silica (PNL 97-28)	215,000
Development of a High-Efficiency Rotary Magnetocaloric Refrigerator Prototype (AL 99-02)	200,000
Direct Casting of Titanium Alloy Wire for Low-Cost Aerospace and Automotive Fasteners (PNL 99-02)	187,000
Controlled Nonisothermal Hot Forging Using Infrared for Microstructural Control (ORL 98-08)	150,000
Nonconsumable Metal Anodes for Primary Magnesium Production (ANL 98-05)	5,000
Development of Electrolyte and Electrode Materials for Rechargeable Lithium Batteries (BNL 98-04)	201,000
Optimized Catalysts for the Cracking of Heavier Petroleum Feedstocks (LBL 99-01)	166,000
SMALL BUSINESS INNOVATION RESEARCH PROGRAM	$31,549,098
DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING	$18,350,421
PHASE I	$6,867,692
Fabrication of Non-Toxic and Thermally Conductive Ceramic Components	100,000
Non-Linear Optical Devices for High Performance Networking, Computing and Telecommunication Routing and Modulating	100,000
Resistive Temperature Device for Two Wire, Downhole, Temperature Measurement as a Function of Current	77,767
Advanced Geothermal Optical Transducer (AGOT)	99,800
Pixelized Scintillating Neutron Detector	99,963
Neutron Detection with Heavily Lithium-Doped Amorphous Selenium Solid-State Detector	100,000

OFFICE OF SCIENCE (continued)

OFFICE OF ADVANCED SCIENTIFIC COMPUTING RESEARCH (CONTINUED)

DIVISION OF TECHNOLOGY RESEARCH (CONTINUED)

SMALL BUSINESS INNOVATION RESEARCH PROGRAM (CONTINUED)

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING (CONTINUED)

PHASE I (CONTINUED)

	FY 2000
Position-Sensitive and Flight-Time Differentiable Single-Crystal Neutron Detector	99,770
Fast-Response, Two-Dimensional Detector for Epithermal Neutron Detection with Adjustable Shape	100,000
Improved, Position Sensitive Detectors for Thermal Neutrons	100,000
Focusing Neutrons Using Replicated Optics	99,369
Corrosion-Resistant Honeycomb Ceramics for Economical Membrane Separation of Individual Wastewater	100,000
Ceramic Appliques for the Production of Supported Thin-Film Catalytic Membrane Reactors	99,995
Low-Cost, High-Purity Ionic Transport Ceramic Oxygen Generator	100,000
Affinity Ceramic Membranes with Carbon Dioxide Transport Channel	100,000
Photocatalytic Membranes for Producing Ultrapure Water	99,922
Mercury-Binding Membranes for Flue Gas Cleanup	99,997
Novel Membrane Reactor for Fischer-Tropsch Synthesis	100,000
A Membrane Reactor for High-Density Hydrogen Production at 100 Percent Purity	99,995
Ultrasensitive Readout Devices for Protein Chips	99,826
Nanostructured Sensing Devices for Biomedical Applications	100,000
Ultra High-Resolution Positron-Emission Tomography Detector	98,453
Fast, Low-Noise Readout Chip for Avalanche Photodiode Arrays for Use in Positron-Emission Tomography Imaging	99,427
Miniature Electrochemical Carbon Dioxide Detector	100,000
An Innovative Ultramicroelectrode Array for Field-Deployable Trace Metal Analysis	100,000
Spark-Induced Breakdown Spectroscopy-Based Sensor for Mercury and Barium in Soils	99,904
Development of a Fiber-Optic Dissolved Oxygen Sensor for Continuous Monitoring of Groundwater	97,976
A Robotically-Deployed, High-Performance, Radiation Imaging Device for Characterization of Difficult-to-Access Locations	100,000
Novel Joining Technique for Oxide-Dispersion Strengthened Iron Aluminide Alloys	100,000
Compliant Metal Interconnects for Energy Systems	99,556
A Metallic Interconnect for Intermediate Temperature, Planar, Solid Oxide Fuel Cells	99,933
Tailorable, Inexpensive Carbon Foam Electrodes for High-Efficiency Fuel Cell and Electrochemical Applications	99,984
Fast-Response Plasmatron Fuel Converter for Diesel Reforming	100,000
Direct-Oxidation Solid Oxide Fuel Cell (SOFC) Anodes	100,000
Advanced Cathode Structure for Oxygen Reduction in Polymer Electrolyte Membrane Fuel Cells	100,000
New Cathode Electrodes for Low-Cost, High-Temperature, Atmospheric-Air-Operated, Proton Exchange Membrane Fuel Cells	100,000
Wire, Shaped, Semiconductor Light-Emitting Diodes for General-Purpose Lighting	99,771

OFFICE OF SCIENCE (continued)

OFFICE OF ADVANCED SCIENTIFIC COMPUTING RESEARCH (CONTINUED)

DIVISION OF TECHNOLOGY RESEARCH (CONTINUED)

SMALL BUSINESS INNOVATION RESEARCH PROGRAM (CONTINUED)

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING (CONTINUED)

PHASE I (CONTINUED)

	FY 2000
Efficient Incandescent Lighting Based on Selective Thermal Emitters	99,964
Optical Torque Sensor for Electric-Motor-Controller Feedback in a Hybrid Electric Vehicle	99,883
Micro-Electromechanical Systems: Fabrication of High-Energy Density, DC Bus Capacitors	99,964
"On Chip" Smart Sensor Array and Control Teleplatform for Thermophotovoltaic Cell Manufacturing Applications	99,995
Photonic Bandgap Surface Structures for Mechanically Rugged Thermovoltaic Emitters	99,814
Geometrically-Weighted, Frisch Grid Superconductor Radiation Detectors for Remote and Portable Gamma-Ray Spectroscopy	100,000
Improved Detection Capabilities of Cadmium Zinc Telluride for High-Resolution, Room-Temperature Radiation Detectors	100,000
Solid-State Continuous-Wave Ultraviolet Laser System	100,000
High-Speed Long-Wave Infrared Acousto-Optic Tuner	100,000
Infrared Focal Plane Array with Fast Shuttering	100,000
Linear Avalanche Photodiode Detector Arrays for Gated Spectroscopy with Single-Photon Sensitivity	100,000
Fast-Imaging Fabry Perot Filter	99,913
Development of a Large-Area Mercuric Iodide Photodetector for Scintillation Spectroscopy	97,873
Segmented, Deep-Sensitive-Depth Silicon Radiation Detectors	100,000
Micromachined Silicon, Large Area X-Ray Detector	100,000
Ultra-Sensitive Electrometer as Readout Electronics for Silicon Microstrip Detectors	99,968
Carbon Nanotube-Based Cathodes for High-Power Microwave Tubes	99,907
Highly-Stable, Diode-Pumped Titanium Sapphire Pulse Train Amplifier for Photoinjector Applications	99,198
Optimization of Carbon Nanotube Field Emitters	99,997
Development of Millimeter-Wave Accelerating Structures Using Precision Metal-Forming Technology	100,000
Cost-Reduction Techniques for Powder-in-Tube Niobium-Tin Superconductors	100,000
Flexible Niobium-Tin Cables Suitable to React-then-Wind Approach to Fabricating Accelerator Magnets	100,000
Using Cabled Niobium and Aluminum Wires as Precursor for Fabrication of Niobium Aluminum Wires	100,000
Ultra-Reliable Hybrid Film Capacitors	99,927
Ultra-High Resolution Microchannel Plates	100,000
Novel Avalanche Photodiode Arrays for Scintillating Fiber Readout	100,000
Micromachined VLSI (Very Large-Scale Integration) Three-Dimensional Electronics	100,000
Novel Radiation-Resistant Insulation Systems for Fusion Magnets	99,990

OFFICE OF SCIENCE (continued)

	FY 2000
OFFICE OF ADVANCED SCIENTIFIC COMPUTING RESEARCH (CONTINUED)	
DIVISION OF TECHNOLOGY RESEARCH (CONTINUED)	
SMALL BUSINESS INNOVATION RESEARCH PROGRAM (CONTINUED)	
DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING (CONTINUED)	
PHASE I (CONTINUED)	
New Generation Nb_3Sn Cable-In-Conduits with Improved Economy and Higher Performance	100,000
Using Cables Made of Co-Axial Copper-Niobium and Copper-Tin Wires as Precursor for Fabricating Niobium-Tin Wires	100,000
New Methods for Joining Beta"-Alumina to Niobium 1% Zirconium	99,982
Manufacturing of Robust Ceramic/Metal Joints for Alkali Metal Thermal-to-Electric Converters	100,000
PHASE II (FIRST YEAR)	$7,879,597
High-Temperature Oscillator and Digital Clock	373,618
Capacitors for Extreme Temperature Applications	375,000
A High Temperature MEMS Inclination Sensor for Geothermal Drilling	374,612
High Efficiency Thermoelectric Power Conversion Devices	375,000
Fast Repetitive Arc Free Current Limiting Circuit Breaker	374,894
A High Current Very Low Cost $Niobium_3$Tin Titanium Doped Conductor Utilizing A Novel Internal Tin Process, with Separate Stabilizing Elements Scalable To Modern Niobium Titanium Production Economics	300,000
Automated Diamond Turning Lathe for the Production of Copper Accelerator Cells	375,000
High Power Switch	313,798
Adiabatic Forming of Copper Accelerator Cells for the NLC	375,000
Low Cost Support Structures, With New Advanced Composite Materials Tailored For Ultra-Stable Particle Tracking Detectors	337,032
SQUID Susceptometers for Read Out of Magnetic Microcalorimeters	374,987
Electromagnetically Forming a Seamless Niobium Radio Frequency (RF) Superconducting Cavity	314,003
Development of High Power RF Windows for Next-Generation Superconducting and Normal Conducting Accerlerators	317,706
High Power RF Window and Its Input Coupler Technology	375,000
Mercury Cadmium Telluride Detectors for Near Infrared Applications	300,000
Development of III-Nitride UV Detectors	374,981
Low Temperature, High Altitude Humidity Sensor	374,643
A Diode Laser Sensor for High Precision Measurement of Terrestrial CO_2 Sources and Sinks	374,879
A Generic Approach to Improved Semi-Solid Forming of Metals	374,445
High-Strain-Rate Superplastic Forging of Aluminum Alloys	375,000
Three Dimensional Si Imaging Array For Cold Neutrons	375,000
Chemosensor Array for Detecting the Proliferation of Weapons of Mass Destruction	374,999

OFFICE OF SCIENCE (continued)

	FY 2000
OFFICE OF ADVANCED SCIENTIFIC COMPUTING RESEARCH (CONTINUED)	
DIVISION OF TECHNOLOGY RESEARCH (CONTINUED)	
SMALL BUSINESS INNOVATION RESEARCH PROGRAM (CONTINUED)	
DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING (CONTINUED)	
PHASE II (SECOND YEAR)	$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 TiO_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
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING	$1,677,971
PHASE I	$399,992
Low-Energy Separation of Azeotropes by Gel Absorption	99,992
Synthesis of Hydrogen from Hydrocarbons Using Electrically Activated Catalysts	100,000
Utilization of Hydrocarbon Fuels in Low-Temperature Solid Oxide Fuel Cells	100,000
Thin Alternatives to Braided Glass Insulation for Low-Temperature Superconducting Wire	100,000
PHASE II (FIRST YEAR)	$1,277,979
SunGuard: A Roofing Tile for Natural Cooling	374,950
High Performance Nb_3Sn (Ta) Wires by Tin Enrichment and Increased Filament Content	300,000
Development of New Lossy Material for Cryogenic and Ambient Applications	228,029
An Advanced Avalanche-Photodiode Based Spectroscopic Radiation Imager	375,000

OFFICE OF SCIENCE (continued)

	FY 2000
OFFICE OF ADVANCED SCIENTIFIC COMPUTING RESEARCH (CONTINUED)	
DIVISION OF TECHNOLOGY RESEARCH (CONTINUED)	
SMALL BUSINESS INNOVATION RESEARCH PROGRAM (CONTINUED)	
MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING	$11,520,706
PHASE I	$3,197,031
Metallization of AIN through Reactive Wetting	99,886
The Development and Demonstration of Reliable Adherent Metalization of AIN	100,000
Advanced Single Ion-Conducting Polymer Electrolytes for Lithium-Ion Batteries	99,997
New Lithium Salts for Safe Operation of High-Energy, High-Rate Lithium-Ion Batteries	99,996
Novel Lithium-Ion Conducting Polymer Electrolytes for Lithium-Ion Batteries	99,997
Low-Cost, Alkaline-Metal Salts for Rechargeable Lithium-Ion Batteries	98,753
Synthesis of New Solid Polymer Electrolytes	99,998
High-Selectivity Membranes for Olefin/Paraffin Separations	100,000
Membranes for Reverse Organic-Air Separations	100,000
Hydrogen Recovery Process Using New Membrane Materials	100,000
A Novel, Inorganic, Surface-Diffusion Membrane for Hydrogen Separations	100,000
Nanopore-Silica Reactive Adsorbent	99,997
Molecular Imprinting of Enzymes with Hydrophobic Compounds to Improve Catalytic Activity in Nonaqueous Media	100,000
Small-Molecule Tumor-Targeting [99mTc] Agents for Breast Cancer Imaging	100,000
New Boronated Amino Acids for Neutron Capture Therapy	98,455
Novel Membranes for Upgrading Natural Gas	100,000
Nanostructured Thermal Barrier Coatings	99,994
Nanoengineered Intermetallics for Energy Systems	99,970
Alternative Interconnect Materials for Improved Solid Oxide Fuel Cell Performance	100,000
A Rapid-Oxidation Stabilization Technique for the Post-Processing of Carbon Foams and Carbon Materials	100,000
Low-Cost Arc Process to Produce Single-Walled Nano-Tubes Using Coal-Based Starting Materials	100,000
Novel Catalyst for Carbon Monoxide Removal from Fuel Cell Reformate	100,000
Development of Improved Oxygen-Reduction Catalysts Using Combinatorial Electrochemistry	100,000
Phase-Corrective, Polymer-Coated, Lightweight Mirror	99,995
A Fast, High Light Output Scintillator for Gamma Ray and Neutron Detection	100,000
A New and Novel Method for Producing Niobium-Coated Copper Cavities	100,000
In-Situ Electron Beam Processing for Radio Frequency Cavities	100,000
An Innovative Fabrication Concept for Niobium-Tin Superconducting Wire	100,000
High-Performance Niobium-Tin-Tantalum Superconductors Formed by Mechanical Alloying and Near-Net Shape Tube Filling	100,000

OFFICE OF SCIENCE (continued)

	FY 2000
OFFICE OF ADVANCED SCIENTIFIC COMPUTING RESEARCH (CONTINUED)	
DIVISION OF TECHNOLOGY RESEARCH (CONTINUED)	
SMALL BUSINESS INNOVATION RESEARCH PROGRAM (CONTINUED)	
MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING (CONTINUED)	
PHASE I (CONTINUED)	
Niobium Aluminum Precursor Surface Modification for Improved Multifilamentary Bonding	100,000
Ceramic Insulation for Heavy Ion Fusion and other High-Radiation Magnets	99,993
Development of High-Fiber-Volume, Radiation-Resistant, High-Pressure Laminate for Cryogenic Applications	100,000
PHASE II (FIRST YEAR)	$5,023,756
Thermally Stable Catalysts for Methane Combustion	300,000
Improved Precursors for Oxygen-Selective Membranes in Practical Devices for Methane Conversion	375,000
Supported Flat Plate Thin Films for Oxygen Separation	374,996
A New Radiation Resistant Epoxy Resin System for Liquid Impregnation Fabrication of Composite Insulation	374,990
Advanced Heat Sink Materials for Fusion Energy Devices	375,000
Hybrid 3-D SiC/C High Thermal Conductivity Composites	375,000
Co-Processed Ceramic Insulation for High Field Accelerator Magnets	300,000
Improvement of High Field Performance and Reliability of Nb_3Sn Conductor by PIT Method	300,000
Functionally Graded, Nanocrystalline, Multiphase, Boron-and-Carbon-Based Superhard Coatings	374,961
Large Area Filtered Arc Deposition of Carbon and Boron Based Hard Coatings	374,967
Meter Length YBCO Coated Conductor Development	375,000
Novel Catalyst for CH_4-CO Conversion	375,000
Flame Retardant Electrolytes for Li-Ion Batteries	373,842
Nonflammable Lithium-Ion Battery Electrolytes	375,000
PHASE II (SECOND 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
Antennas in Magnetic Fusion Devices 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

OFFICE OF SCIENCE (continued)

	FY 2000
OFFICE OF ADVANCED SCIENTIFIC COMPUTING RESEARCH (CONTINUED)	
DIVISION OF TECHNOLOGY RESEARCH (CONTINUED)	
SMALL BUSINESS INNOVATION RESEARCH PROGRAM (CONTINUED)	
MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING (CONTINUED)	
PHASE II (SECOND YEAR) (CONTINUED)	
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
SMALL BUSINESS TECHNOLOGY TRANSFER RESEARCH PROGRAM	$1,642,119
DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING	$899,534
PHASE I	$399,534
Low-Cost Silicon Carbide Ceramic Membranes	100,000
Optimized Performance of Thin Film Polymer Light-Emitting Diodes Through Interface Layers	99,947
Development of High-Temperature Superconducting (HTS) Copper Current Leads with HTS Sections Operating in the Current-Sharing Mode	100,000
ZnO: Ga Single Crystal Scintillator	99,587
PHASE II (FIRST YEAR)	$250,000
Thin-Film Fiber Optic Sensors for Power Control and Fault Detection	250,000
PHASE II (SECOND YEAR)	$250,000
High Energy and Power Ultracapacitors Utilizing Novel Type III Polymers and Non-Aqueous Electrolytes	250,000
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR, TESTING	$493,737
PHASE I	$493,737
The Use of Recycled Plastics as Alternative Soil Amendments in the Culture of Plants	95,000
Improved Ternary Substituted, Powder Processed, Melt Quenched, Niobium-Aluminum Strand for High-Field Dipole Applications	100,000
Conceptual and Computational Design of Vanadium-Based Alloys for Fusion Reactor Structural Applications	98,755

OFFICE OF SCIENCE (continued)

	FY 2000
OFFICE OF ADVANCED SCIENTIFIC COMPUTING RESEARCH (CONTINUED)	
DIVISION OF TECHNOLOGY RESEARCH (CONTINUED)	
SMALL BUSINESS TECHNOLOGY TRANSFER RESEARCH PROGRAM (CONTINUED)	
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR, TESTING (CONTINUED)	
PHASE I (CONTINUED)	
Advanced Materials and Processing Methods for Magnetohydrodynamic Mitigation Coatings	99,992
Advanced Materials and Processing Methods for In-Situ Thermal Barrier Coating Repair	99,990
MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING	**$248,848**
PHASE II (SECOND YEAR)	**$248,848**
Boron Carbide Coatings for Enhanced Performance of Radio-Frequency Antennas in Magnetic Fusion Devices	248,848
OFFICE OF FUSION ENERGY SCIENCES	**$8,600,000**
Vanadium Alloy and Insulating Coatings Research	930,000
Irradiation Effects Modeling	50,000
Fusion Materials Research	3,880,000
Fusion Structural Materials Research	1,300,000
SiC/SiC Composite Irradiation Effects Research	50,000
Fusion Materials Fracture and Deformation Research	140,000
Fusion Materials Damage and Fundamentals Research	250,000
Plasma Facing Components Materials Research	2,000,000

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, Health and Environmental Research, High Energy and Nuclear Physics and Computational and Technology Research. The Director also advises the Secretary on DOE physical research programs, university-based education and training activities, grants and other forms of financial assistance.

The Office of Science mainly conducts materials research in the following offices and divisions:

Office of Basic Energy Sciences - Division of Materials Sciences and Engineering
Office of Advanced Scientific Computing Research - Division of Advanced Energy Projects and Technology Research
Office of Biological and Environmental Research - Medical Sciences Division
Office of Fusion Energy - Division of Advanced Physics and Technology

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

OFFICE OF BASIC ENERGY SCIENCES

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

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

DIVISION OF MATERIALS SCIENCES AND ENGINEERING

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 and Engineering 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. Description of research supported by various elements of the materials program is presented below.

THEORETICAL CONDENSED MATTER PHYSICS

The Theoretical Condensed Matter Physics program is a diverse program that provides theoretical support for all relevant parts of the Materials Science program. Research areas parallel those in the experimental CRA, including quantum dots, nanotubes and their properties, tribology at the atomic level, superconductivity, magnetism, and optics. A significant part of the portfolio consists of the development of advanced computer simulation algorithms, and fast codes to treat many particle systems. Research is conducted in 7 DOE laboratories, Ames, Argonne, Berkeley, Brookhaven, Los Alamos, the National Renewable Energy Lab., Oak Ridge and at 35 universities. An important component of the portfolio is the Computational Materials Science Network (CMSN) which brings together groups of scientists from DOE laboratories, universities, and to a lesser extent industry to solve materials problems requiring collaboration across disciplinary boundaries. The FY 2000 funding for this program is $17,624,000 and the DOE contact is Manfred Leiser, (301) 903-3426.

EXPERIMENTAL CONDENSED MATTER PHYSICS

The portfolio consists of a broad-based experimental program in condensed matter and materials physics research with selected emphases in the areas of electronic structure, surfaces/interfaces, and new materials. It includes the development and exploitation of advanced experimental techniques and methodology. The objective is to provide the understanding of the physical phenomena and processes underlying the properties and behavior of advanced materials. It provides the technology-base support in condensed matter physics to energy technologies and contributes to the generic knowledge base in condensed matter and materials physics. The portfolio and scope are determined by opportunities, National Laboratory research expertise, and unsolicited research applications, as modified by programmatic requirements including scientific impact, materials needs, and energy technology requirements. Presently, the portfolio includes specific research thrusts in magnetism, semiconductors, superconductivity, materials synthesis and crystal growth, and photoemission spectroscopy. The portfolio addresses well-recognized needs, including understanding magnetism and superconductivity, the control of electrons and photons in solids, understanding materials at reduced dimensionality, the physical properties of large, interacting systems, and the properties of materials under extreme conditions. The FY 2000 funding for this program is $32,751,000 and the DOE contact is Jerry Smith, (301) 903-3426.

MATERIALS CHEMISTRY

The program addresses basic research on the synthesis, characterization, and chemical properties of materials to gain a more fundamental understanding of the effects of chemical reactivity on the synthesis and behavior of novel materials and structures. The portfolio includes research with particular emphases on surface and interfacial chemistry, nanoscience, polymer and organic materials, and solid state chemistry which underpin many energy related areas such as batteries and fuel cells, catalysis, friction and lubrication, membranes, electronics and environmental chemistry. It includes investigations of novel materials including low-dimensional, self-assembled monolayers; cluster and nanocrystal-based materials; polymeric conductors; organic superconductors and magnets; complex fluids; biomolecular materials; and solid state neutron detectors. The research employs a wide variety of experimental techniques to characterize these materials including x-ray photoemission and other spectroscopies, scanning tunneling and atomic force microscopies, nuclear magnetic resonance (NMR), and x-ray and neutron reflectometry. The program also supports the development of new experimental techniques such as high-resolution magnetic resonance imaging (MRI) without magnets, neutron reflectometry, and atomic force microscopy of liquids. The FY 2000 funding for this program is $27,390,000 and the DOE contact is Richard Kelley, (301) 903-3426.

MECHANICAL BEHAVIOR AND RADIATION EFFECTS

This activity focuses on the understanding of the mechanical behavior of materials under static and dynamic stresses and the effects of radiation on materials properties. The objective is to understand the defect-property relationship at an atomic level. In the area of mechanical behavior, the research aims to advance understanding of deformation and fracture and to develop predictive models for design of materials having prescribed mechanical behavior. In the area of radiation effects, the research aims to advance understanding of mechanisms of amorphization (transition from crystalline to a non-crystalline phase), predict and suppress radiation damage, develop radiation-tolerant materials, and modify surfaces by ion implantation. The FY 2000 funding for this program is $18,211,000 and the DOE contact is Yok Chen, (301) 903-3428.

NEUTRON AND X-RAY SCATTERING

Basic research in condensed matter and materials physics using neutron and x-ray scattering capabilities primarily at major BES-supported user facilities. Research is aimed at achieving a fundamental understanding of the atomic, electronic, and magnetic structures and excitations of materials, and the relationship of these structures and excitations to the physical properties of materials. Both ordered and disordered materials are of interest as are strongly correlated electron systems, surface and interface phenomena and behavior under environmental variables such as temperature, pressure, and magnetic field. Development of neutron and x-ray instrumentation for next generation sources. The FY 2000 funding for this program is $24,659,000 and the DOE contact is Helen Kerch, (301) 903-3426.

STRUCTURE AND COMPOSITION OF MATERIALS

Structure and composition of materials includes research on the arrangement and identity of atoms and molecules in materials; specifically the development of quantitative characterization techniques, theories and models describing how atoms and molecules are arranged, and the mechanisms by which the arrangements are created and evolve. Increasingly important are the structure and composition of in homogeneities including defects and the morphology of interfaces, surfaces and precipitates. Advancing the state of the art of electron beam micro characterization methods and instruments is an essential element in this portfolio. Four electron beam user centers are operated at ANL, LBNL, ORNL, and the Frederick Seitz MRL at the University of Illinois. The FY 2000 funding for this program is $24,372,000 and the DOE contact is Robert Gottschall, (301) 903-3428.

PHYSICAL BEHAVIOR

Physical behavior refers to the electronic, chemical, microstructural or other response of a material to an applied stimulus. The research in this portfolio aims to understand, predict and control physical behavior of materials by developing scientifically rigorous models for the response of materials to environmental stimuli such as temperature, electromagnetic field, chemical environment, and proximity of surfaces or interfaces. Basic research topics supported include modeling of materials behaviors, electrochemistry and corrosion, high-temperature materials performance, superconductivity, photovoltaics and fuel cells, and more. The FY 2000 funding for this program is $16,494,000 and the DOE contact is Robert J. Gottschall, (301) 903-3428.

SYNTHESIS AND PROCESSING SCIENCES

Synthesis and Processing Science includes research on understanding and developing innovative ways to make materials with desired structure, properties or behavior. Examples include atomic and molecular self-assembly to create new materials; nanostructured materials that mimic the structure of natural materials; new approaches to the processing of materials to improve properties or behavior; and welding and joining of materials. Since this research often requires specialized, high-purity materials that are not commercially or otherwise available, the Materials Preparation Center at the Ames Laboratory is operated for the purposes of developing methods, fabricating research grade materials, and providing these materials to the research community. The FY 2000 funding for this program is $15,448,000 and the DOE contact is Robert J. Gottschall, (301) 903-3428.

ENGINEERING RESEARCH

Engineering Sciences includes research in the development of engineering principles to make scientific advances in materials practicable; in nanotechnology and microsystems; in multi-component fluid dynamics and heat transfer; and non-linear dynamic systems. The FY 2000 funding for this program is $14,020,000 and the DOE contact is Robert Price, (301) 903-3428.

EXPERIMENTAL PROGRAM TO STIMULATE COMPETITIVE RESEARCH

Basic research spanning the entire range of programmatic activities supported by the Department within the Office of Science in states that have historically received relatively less Federal research funding. The DOE designated EPSCoR states are Alabama, Alaska, Arkansas, Idaho, Kansas, Kentucky, Louisiana, Maine, Mississippi, Montana, Nebraska, Nevada, North Dakota, Oklahoma, South Carolina, South Dakota, Vermont, West Virginia, and Wyoming, and the Commonwealth of Puerto Rico. EPSCoR is managed in Materials Science and Engineering Division within BES. The FY 2000 funding for this program is $6,815,000 and the DOE contact is Matesh Varma, (301) 903-3209.

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. The FY 2000 funding for this program is $204,497,000.

OFFICE OF ADVANCED SCIENTIFIC COMPUTING RESEARCH

DIVISION OF TECHNOLOGY RESEARCH

LABORATORY TECHNOLOGY RESEARCH PROGRAM

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

212. **HIGH PERFORMANCE TAILORED MATERIALS FOR LEVITATION AND PERMANENT MAGNET TECHNOLOGIES (ANL 97-02)**
$126,000
DOE Contact: Walter M. Polansky (301) 903-5995
ANL Contact: George W. Crabtree (630) 252-5509

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

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

213. **ATOMIC SCALE STRUCTURE OF ULTRATHIN MAGNETIC MULTILAYERS AND CORRELATION WITH RESISTANCE, GIANT MAGNETORESISTANCE, AND SPIN-DEPENDENT TUNNELING (ORL 97-03)**
$120,000
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

214. **IMPROVED MATERIALS FOR SEMICONDUCTOR DEVICES (PNL 98-17)**
$250,000
DOE Contact: Walter M. Polansky (301) 903-5995
PNNL Contact: Suresh Baskaran (509) 375-6483

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

215. **DEVELOPMENT OF HIGH-TEMPERATURE SUPERCONDUCTING WIRE USING RABiTS COATED CONDUCTOR TECHNOLOGIES (ORL 97-02)**
$110,000
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

216. **DEVELOPMENT OF BISMUTH-BASED SUPERCONDUCTING WIRE WITH IMPROVED CURRENT CARRYING AND FLUX PINNING PROPERTIES (ANL 99-15)**
$229,000
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 $(Bi,Pb)_2Sr_2Ca_2Cu_3Oy$

217. **LIGHT EMISSION PROCESSES AND DOPANTS IN SOLID STATE LIGHT SOURCES (LBL 97-13)**
$114,000
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

218. **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 mm) $YBa_2Cu_3O_7$ involves heat treating $YBa_2Cu_3O_7$ precursor films in a moist atmosphere at high temperatures (>725° C), it is important to select a buffer layer material which does not interfere with the growth of $YBa_2Cu_3O_7$. In order to study this, the project has initially deposited a $YBa_2Cu_3O_7$ precursor film on a CeO_2 buffered single crystalline $LaAlO_3$ and heat treated it to form a $YBa_2Cu_3O_7$ layer on top of the CeO_2. Note that CeO_2 is a well-known buffer layer which is used in conjunction with pulsed laser deposition of $YBa_2Cu_3O_7$. Although a significant reaction takes place between the $YBa_2Cu_3O_7$ and CeO_2 layers if they are heat-treated above 750°C, the reaction appears to be sufficiently minimized by keeping the reaction temperature below 735°C. A further study is being conducted to see the extent of the reaction, and other possible candidates for the buffer materials are being examined. If this project is successful, the superconducting tapes will be used in electrical utility systems, greatly increasing the efficiency of power transmission. This project supports DOE's mission through increased energy efficiency.

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

219. **INTERPLAY BETWEEN INTERFACIAL AND DIELECTRIC AND FERROELECTRIC BEHAVIORS OF BARIUM STRONTIUM TITANATE THIN FILMS (PNL 99-08)**
$207,000
DOE Contact: Walter M. Polansky (301) 903-5995
PNNL 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

220. **COMBINATORIAL DISCOVERY AND OPTIMIZATION OF NOVEL MATERIALS FOR ADVANCED ELECTRO OPTICAL DEVICES (LBL 97-18)**
$100,000
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

221. **ADVANCED COMPUTATIONAL MODELS AND EXPERIMENTS FOR DEFORMATION OF ALUMINUM ALLOYS - PROSPECTS FOR DESIGN (PNL 99-07)**
$200,000
DOE Contact: Walter M. Polansky (301) 903-5995
PNNL 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

222. **NEAR-FRICTIONLESS CARBON COATINGS (ANL 98-03)**
$56,000
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

223. **SMOOTH DIAMOND FILMS FOR FRICTION AND WEAR APPLICATIONS AND CHEMICALLY PROTECTIVE COATINGS (ANL 97-05)**
$100,000
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

224. **NANOMETER CHARACTERIZATION AND DESIGN OF MOLECULAR LUBRICATION FOR THE HEAD-DISK INTERFACE (LBL 98-10)**
$126,000
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

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

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

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

226. **INTERFACIAL PROPERTIES OF ELECTRON BEAM CURED COMPOSITES (ORNL 99-08)**
$220,000
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

227. **PHOTOCATALYTIC METAL DEPOSITION FOR NANOLITHOGRAPHY (ANL 99-13)**
$120,000
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

228. **IONICALLY CONDUCTIVE MEMBRANES FOR OXYGEN SEPARATION (LBL 97-03)**
$40,000
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

229. **ADVANCED SEPARATIONS TECHNOLOGY FOR EFFICIENT AND ECONOMICAL RECOVERY AND PURIFICATION OF HYDROGEN PEROXIDE (ANL 98-07)**
$229,000
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

230. **SYNTHESIS AND CRYSTAL CHEMISTRY OF TECHNOLOGICALLY IMPORTANT CERAMIC MEMBRANES (ANL 97-06)**
$59,000
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

231. **CATALYTIC PRODUCTION OF ORGANIC CHEMICALS BASED ON NEW HOMOGENEOUSLY CATALYZED IONIC HYDROGENATION TECHNOLOGY (BNL 97-05)**
$122,000
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

232. **HIGHLY DISPERSED SOLID ACID CATALYSTS ON MESOPOROUS SILICA (PNL 97-28)**
$215,000
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

233. DEVELOPMENT OF A HIGH-EFFICIENCY ROTARY MAGNETOCALORIC REFRIGERATOR PROTOTYPE (AL 99-02)
$200,000
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

234. DIRECT CASTING OF TITANIUM ALLOY WIRE FOR LOW-COST AEROSPACE AND AUTOMOTIVE FASTENERS (PNL 99-02)
$187,000
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

235. **CONTROLLED NONISOTHERMAL HOT FORGING USING INFRARED FOR MICROSTRUCTURAL CONTROL (ORL 98-08)**
$150,000
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

236. **NONCONSUMABLE METAL ANODES FOR PRIMARY MAGNESIUM PRODUCTION (ANL 98-05)**
$5,000
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

237. **DEVELOPMENT OF ELECTROLYTE AND ELECTRODE MATERIALS FOR RECHARGEABLE LITHIUM BATTERIES (BNL 98-04)**
$201,000
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

238. **OPTIMIZED CATALYSTS FOR THE CRACKING OF HEAVIER PETROLEUM FEEDSTOCKS (LBL 99-01)**
$166,000
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

Fabrication of Non-Toxic and Thermally Conductive Ceramic Components - DOE Contact Samuel Barish (301) 903-2917; CC Components, LLC. Contact Jay Duke (214) 321-3054

Non-Linear Optical Devices for High Performance Networking, Computing and Telecommunication Routing and Modulating - DOE Contact George Seweryniak (301) 903-0071; Ionic Systems, Inc. Contact Constance Eve Teague (408) 885-0800

Resistive Temperature Device for Two Wire, Downhole, Temperature Measurement as a Function of Current - DOE Contact Raymond J. LaSala (202) 586-4198; Accusol, Inc. Contact Dr. David J. Anderson (847) 671-7295

Advanced Geothermal Optical Transducer (AGOT) - DOE Contact Raymond J. LaSala (202) 586-4198; LEL Corporation Contact Piedao H. Liucci (201) 569-8641

Pixelized Scintillating Neutron Detector - DOE Contact Helen Kerch (301) 903-3426; Biotraces, Inc. Contact Dr. Andrzej Drukier (703) 793-1550

Neutron Detection with Heavily Lithium-Doped Amorphous Selenium Solid-State Detector - DOE Contact Helen Kerch (301) 903-3426; EIC Laboratories, Inc. Contact Dr. R. David Rauth (781) 769-9450

Position-Sensitive and Flight-Time Differentiable Single-Crystal Neutron Detector - DOE Contact Helen Kerch (301) 903-3426; Millennia Ceramics, Inc. Contact Chris Marie Sayir (440) 835-2660

Fast-Response, Two-Dimensional Detector for Epithermal Neutron Detection with Adjustable Shape - DOE Contact Helen Kerch (301) 903-3426; Nova Scientific, Inc. Contact Dr. Paul L. White (508) 347-7679

Improved, Position Sensitive Detectors for Thermal Neutrons - DOE Contact Helen Kerch, (301) 903-3426; Nuclear Safeguards and Security Systems, LLC Contact Dr. Richard S. Seymour (865) 945-1223

Focusing Neutrons Using Replicated Optics - DOE Contact Helen Kerch (301) 903-3426; X-ray Optical Systems, Inc. Contact David Usher (518) 464-3334

Corrosion-Resistant Honeycomb Ceramics for Economical Membrane Separation of Individual Wastewater - DOE Contact Charlie Russomanno (202) 586-7543; Applied Ceramics, Inc. Contact Robert L. Mitchell (770) 448-6888

Ceramic Appliques for the Production of Supported Thin-Film Catalytic Membrane Reactors - DOE Contact Charlie Russomanno (202) 586-7543; Eltron Research, Inc. Contact Eileen E. Sammells (303) 530-0263

Low-Cost, High-Purity Ionic Transport Ceramic Oxygen Generator - DOE Contact Charlie Russomanno (202) 586-7543; Energy Research Company Contact Robert De Saro (718) 442-2725

Affinity Ceramic Membranes with Carbon Dioxide Transport Channel - DOE Contact Charlie Russomanno (202) 586-7543; Media and Process Technology, Inc. Contact Dr. Paul K.T. Liu (412) 826-3721

Photocatalytic Membranes for Producing Ultrapure Water - DOE Contact Charlie Russomanno (202) 586-7543; Technology Assessment & Transfer, Inc. Contact Sharon S. Fehrenbacher (410) 224-3710

Mercury-Binding Membranes for Flue Gas Cleanup - DOE Contact Charlie Russomanno (202) 586-7543; TPL, Inc. Contact James Lopez (505) 342-4471

Novel Membrane Reactor for Fischer-Tropsch Synthesis - DOE Contact Charlie Russomanno (202) 586-7543; CeraMem Corporation Contact Dr. Robert Goldsmith (781) 899-4495

A Membrane Reactor for High-Density Hydrogen Production at 100 Percent Purity - DOE Contact Charlie Russomanno (202) 586-7543; Reb Research and Consulting Contact Dr. Robert E. Buxbaum (248) 545-0155

Ultrasensitive Readout Devices for Protein Chips - DOE Contact Marvin Stodolsky (301) 903-4475; Biotraces, Inc. Contact Dr. Andrzej K. Drukier (703) 793-1550

Nanostructed Sensing Devices for Biomedical Applications - DOE Contact Dean Cole (301) 903-3268; Amsen Technologies Contact Dr. Ayyasamy Aruchamy (520) 546-6944

Ultra High-Resolution Positron-Emission Tomography Detector - DOE Contact Prem Srivastava (301) 903-4071; Constellation Technology Corporation Contact Charles Settgast (727) 547-0600

Fast, Low-Noise Readout Chip for Avalanche Photodiode Arrays for Use in Positron-Emission Tomography Imaging - DOE Contact Prem Srivastava (301) 903-4071; Nova R & D, Inc. Contact Raymond B. Pifer (909) 781-7332

Miniature Electrochemical Carbon Dioxide Detector - DOE Contact Roger Dahlman (301) 903-4951; Superior Sensing Solutions Contact Michael J. Newman (303) 702-1672

An Innovative Ultramicroelectrode Array for Field-Deployable Trace Metal Analysis - DOE Contact Paul Bayer (301) 903-5324; Lynntech, Inc. Contact Dr. G. Duncan Hitchens (979) 693-0017

Spark-Induced Breakdown Spectroscopy-Based Sensor for Mercury and Barium in Soils - DOE Contact Paul Bayer (301) 903-5324; Physical Sciences, Inc. Contact Dr. B. David Green (978) 689-0003

Development of a Fiber-Optic Dissolved Oxygen Sensor for Continuous Monitoring of Groundwater - DOE Contact Paul Bayer (301) 903-5324; YSI, Inc. Contact Barbara K. McQuiston (937) 767-7241

A Robotically-Deployed, High-Performance, Radiation Imaging Device for Characterization of Difficult-to-Access Locations - DOE Contact Ronald K. Staubly (304) 291-4991; Radiation Monitoring Devices, Inc. Contact Dr. Gerald Entine (617) 926-1167

Novel Joining Technique for Oxide-Dispersion Strengthened Iron Aluminide Alloys - DOE Contact Richard Read (412) 386-5721; Materials & Electrochemical Research (MER) Corp. Contact Dr. R.O. Loutfy (520) 574-1980

Compliant Metal Interconnects for Solid Oxide Fuel Cells - DOE Contact Wayne Surdoval (412) 386-6002; Ceramatec, Inc. Contact Dr. Ashok V. Joshi (801) 978-2143

A Metallic Interconnect for Intermediate Temperature, Planar, Solid Oxide Fuel Cells - DOE Contact Wayne Surdoval (412) 386-6002; Materials and Systems Research, Inc. Contact Dr. Dinesh K. Shetty (801) 530-4987

Tailorable, Inexpensive Carbon Foam Electrodes for High-Efficiency Fuel Cell and Electrochemical Applications - DOE Contact Richard Read (412) 386-5721; Touchstone Research Laboratory, Ltd. Contact Brian E. Joseph (304) 547-5800

Fast-Response Plasmatron Fuel Converter for Diesel Reforming - DOE Contact Bill Haslebacher (304) 285-5435; Hydrogen Microplasmatron Technologies, LLC Contact Dr. Alexander Rabinovich (781) 784-3865

Direct-Oxidation Solid Oxide Fuel Cell (SOFC) Anodes - DOE Contact Wayne Surdoval (412) 386-6002; ITN Energy Systems, Inc. Contact Janet L. Casteel (303) 285-5111

Advanced Cathode Structure for Oxygen Reduction in Polymer Electrolyte Membrane Fuel Cells - DOE Contact Ronald J. Fiskum (202) 586-9154; FuelCell Energy, Inc. Contact Dr. Hans Maru (203) 825-6006

New Cathode Electrodes for Low-Cost, High-Temperature, Atmospheric-Air-Operated, Proton Exchange Membrane Fuel Cells - DOE Contact Ronald J. Fiskum (202) 586-9154; Ion Power, Inc. Contact Dr. Stephen A. Grot (302) 832-9550

Wire, Shaped, Semiconductor Light-Emitting Diodes for General-Purpose Lighting - DOE Contact John Ryan (202) 586-9130; AstroPower, Inc. Contact Thomas J. Stiner (302) 366-0400

Efficient Incandescent Lighting Based on Selective Thermal Emitters - DOE Contact John Ryan (202) 586-9130; Foster-Miller, Inc. Contact Adi R. Guzdar (781) 684-4239

Optical Torque Sensor for Electric-Motor-Controller Feedback in a Hybrid Electric Vehicle - DOE Contact Jim Merritt (202) 586-0903; Karta Technologies, Inc. Contact Dr. G. P. Singh (210) 731-9187

Micro-Electromechanical Systems: Fabrication of High-Energy Density, DC Bus Capacitors - DOE Contact Jim Merritt (202) 586-0903; SatCon Technology Corporation Contact Dr. James L. Kirtley, Jr. (617) 349-0820

"On Chip" Smart Sensor Array and Control Teleplatform for Thermophotovoltaic Cell Manufacturing Applications - DOE Contact Alec Bulawka (202) 586-5633; ARSECO Contact Marine Boyadzhyan (818) 249-6362

Photonic Bandgap Surface Structures for Mechanically Rugged Thermovoltaic Emitters - DOE Contact Alec Bulawka (202) 586-5633; Ion Optics, Inc. Contact James C. Louney (781) 788-8777

Geometrically-Weighted, Frisch Grid Superconductor Radiation Detectors for Remote and Portable Gamma-Ray Spectroscopy - DOE Contact Carl Friesen (208) 526-1765; Radiation Safety Engineering, Inc. Contact Dr. Robert L. Metzger (480) 897-9459

Improved Detection Capabilities of Cadmium Zinc Telluride for High-Resolution, Room-Temperature Radiation Detectors - DOE Contact Carl Friesen (208) 526-1765; Yinnel Tech, Inc. Contact Dr. Longxia Li (219) 234-3488

Solid-State Continuous-Wave Ultraviolet Laser System - DOE Contact Eric Sander (202) 586-5852; Aculight Corporation Contact Karen Walls (425) 482-1100

High-Speed Long-Wave Infrared Acousto-Optic Tuner - DOE Contact Eric Sander (202) 586-5852; Aurora Associates Contact Phoebe Chang (408) 748-2960

Infrared Focal Plane Array with Fast Shuttering - DOE Contact Eric Sander (202) 586-5852; Princeton Scientific Instruments, Inc. Contact John L. Lowrance (732) 274-0774

Linear Avalanche Photodiode Detector Arrays for Gated Spectroscopy with Single-Photon Sensitivity - DOE Contact Eric Sander (202) 586-5852; Radiation Monitoring Devices, Inc. Contact Dr. Gerald Entine (617) 926-1167

Fast-Imaging Fabry Perot Filter - DOE Contact Eric Sander (202) 586-5852; Physical Sciences, Inc. Contact Dr. David B. Green (978) 689-0003

Development of a Large-Area Mercuric Iodide Photodetector for Scintillation Spectroscopy - DOE Contact Jehanne Simon-Gillo (301) 903-1455; Constellation Technology Corporation Contact Charles Settgast (727) 547-0600

Segmented, Deep-Sensitive-Depth Silicon Radiation Detectors - DOE Contact Jehanne Simon-Gillo (301) 903-1455; IntraSpec, Inc. Contact John Walter (865) 483-1394

Micromachined Silicon, Large Area X-Ray Detector - DOE Contact Jehanne Simon-Gillo (301) 903-1455; Physical Optics Corporation Contact Gordon Drew (310) 320-3088

Ultra-Sensitive Electrometer as Readout Electronics for Silicon Microstrip Detectors - DOE Contact Jehanne Simon-Gillo (301) 903-1455; Quantum Applied Science and Research Contact Dr. Andrew D. Hibbs (858) 535-9680

Carbon Nanotube-Based Cathodes for High-Power Microwave Tubes - DOE Contact Jerry Peters (301) 903-5228; Physical Sciences, Inc. Contact Dr. B. David Green (978) 689-0003

Highly-Stable, Diode-Pumped Titanium Sapphire Pulse Train Amplifier for Photoinjector Applications - DOE Contact Jerry Peters (301) 903-5228; Positive Light, Inc. Contact Jeremy Weston (408) 399-7744

Optimization of Carbon Nanotube Field Emitters - DOE Contact Jerry Peters (301) 903-5228; UHV Technologies, Inc. Contact Dr. Nalin Kumar (856) 608-0311

Development of Millimeter-Wave Accelerating Structures Using Precision Metal-Forming Technology - DOE Contact Jerry Peters (301) 903-5228; Dayton Reliable Tool & Mfg. Co. Contact Gary L. Van Gundy (937) 298-7391

Cost-Reduction Techniques for Powder-in-Tube Niobium-Tin Superconductors - DOE Contact Jerry Peters (301) 903-5228; Supercon, Inc. Contact Elaine Tarkiainen (508) 842-0174

Flexible Niobium-Tin Cables Suitable to React-then-Wind Approach to Fabricating Accelerator Magnets - DOE Contact Jerry Peters (301) 903-5228; Superconducting Systems, Inc. Contact Dr. Shanin Pourrahimi (781) 642-6702

Using Cabled Niobium and Aluminum Wires as Precursor for Fabrication of Niobium Aluminum Wires - DOE Contact Jerry Peters (301) 903-5228; Superconducting Systems, Inc. Contact Dr. Shanin Pourrahimi (781) 642-6702

Ultra-Reliable Hybrid Film Capacitors - DOE Contact Jerry Peters (301) 903-5228; Sigma Technologies International, Inc. Contact Dr. Angelo Yializis (520) 575-8013

Ultra-High Resolution Microchannel Plates - DOE Contact Michael P. Procario (301) 903-2890; Nanomaterials Research Corporation Contact Michael Newman (303) 702-1672

Novel Avalanche Photodiode Arrays for Scintillating Fiber Readout - DOE Contact Michael P. Procario (301) 903-2890; Radiation Monitoring Devices, Inc. Contact Dr. Gerald Entine (617) 926-1167

Micromachined VLSI (Very Large-Scale Integration) Three-Dimensional Electronics - DOE Contact Timothy E. Toohig (301) 903-4115; Nanosciences Corporation Contact Dr. John Steinbeck (717) 295-6639

Novel Radiation-Resistant Insulation Systems for Fusion Magnets - DOE Contact Warren Marton (301) 903-4958; Composite Technology Development, Inc. Contact Dr. Naseem A. Munshi (303) 664-0394

New Generation Nb_3Sn Cable-In-Conduits with Improved Economy and Higher Performance - DOE Contact Warren Marton (301) 903-4958; Superconducting Systems, Inc. Contact Dr. Shanin Pourrahimi (781) 642-6702

Using Cables Made of Co-Axial Copper-Niobium and Copper-Tin Wires as Precusor for Fabricating Niobium-Tin Wires - DOE Contact Warren Marton (301) 903-4958; Superconducting Systems, Inc. Contact Dr. Shahin Pourrahimi (781) 642-6702

New Methods for Joining Beta"-Alumina to Niobium 1% Zirconium - DOE Contact Lisa C. Herrera (301) 903-8218; Advanced Modular Power Systems, Inc. Contact Dr. Thomas K. Hunt (734) 677-4260

Manufacturing of Robust Ceramic/Metal Joints for Alkali Metal Thermal-to-Electric Converters - DOE Contact Lisa C. Herrera (301) 903-8218; Triton Systems, Inc. Contact Ross Haghighat (978) 250-4200

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

PHASE II (FIRST YEAR)

High-Temperature Oscillator and Digital Clock - DOE Contact Raymond J. LaSala (202) 586-4198; Linear Measurements, Inc. Contact Robert Hatch (619) 535-2172

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 John C. Cole (425) 391-8329

High Efficiency Thermoelectric Power Conversion Device - DOE Contact Jim Merritt (202) 586-0903; Hi-Z Technology, Inc. Contact Norbert Elsner (619) 695-6660

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

A High Current Very Low Cost $Niobium_3Tin$ Titanium 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 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 James W. Drain (805) 684-8307

High Power Switch - DOE Contact Jerry Peters (301) 903-5228; Diversified Technologies, Inc. Contact 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 Lennart J. Lindell (815) 758-3514

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 William O. Miller (505) 662-0080

SQUID Susceptometers for Read Out of Magnetic Microcalorimeters - DOE Contact Jehanne Simon-Gillo (301) 903-1455; Hypres, Inc. Contact Dr. Elie Track (914) 592-1190

Electromagnetically Forming a Seamless Niobium Radio Frequency (RF) Superconducting Cavity - DOE Contact Jehanne Simon-Gillo (301) 903-1455; Advanced Energy Systems, Inc. Contact Anthony Favale (516) 575-9345

Development of High Power RF Windows for Next-Generation Superconducting and Normal Conducting Accelerators - DOE Contact Jehanne Simon-Gillo (301) 903-1455; Advanced Energy Systems, Inc. Contact Anthony Favale (516) 575-9345

High Power RF Window and Its Input Coupler Technology- DOE Contact Jehanne Simon-Gillo (301) 903-1455; 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 Molly M. W. Kostelecky (303) 702-1672

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

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

Three Dimensional Si Imaging Array For Cold Neutrons - DOE Contact Helen Kerch (301) 903-3426; IntraSpec, Inc. Contact John Walter (423) 483-1859

Chemosensor Array for Detecting the Proliferation of Weapons of Mass Destruction - DOE Contact Carl Friesen (208) 526-1765; Intelligent Optical Systems, Inc. Contact Robert Lieberman (310) 530-7130

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

PHASE II (SECOND 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 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 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

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

PHASE I

Low-Energy Separation of Azeotropes by Gel Absorption - DOE Contact Charlie Russomanno (202) 586-7543; Foster-Miller, Inc. Contact Adi Guzdar (781) 684-4239

Synthesis of Hydrogen from Hydrocarbons Using Electrically Activated Catalysts - DOE Contact Bill Haslebacher (304) 285-5435; Nanomaterials Research Corporation Contact Dr. Tapesh Yadav (303) 702-1672

Utilization of Hydrocarbon Fuels in Low-Temperature Solid Oxide Fuel Cells - DOE Contact Wayne Surdoval (412) 386-6002; Applied Thin Films, Inc. Contact Derrick Calandra (847) 467-6877

Thin Alternatives to Braided Glass Insulation for Low-Temperature Superconducting Wire - DOE Contact Jerry Peters (301) 903-5228; Microcoating Technologies Contact Jeffrey Moore (678) 287-2400

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

PHASE II (FIRST YEAR)

SunGuard: A Roofing Tile for Natural Cooling - DOE Contact Terrence Logee (202) 586-1689; Powerlight Corporation Contact Thomas L. Dinwoodie (510) 540-0550

High Performance Nb_3Sn (Ta) Wires by Tin Enrichment and Increased Filament Content - DOE Contact Jerry Peters (301) 903-5228; Superconducting Systems, Inc. Contact Minou Mossavat (781) 642-6702

Development of New Lossy Material for Cryogenic and Ambient Applications - DOE Contact Jehanne Simon-Gillo (301) 903-1455; Ceradyne, Inc. Contact 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

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

PHASE I

Metallization of AlN through Reactive Wetting - DOE Contact Samuel Barish (301) 903-2917; Ceramic Composites, Inc. Contact Sharon S. Fehrenbacher (410)224-3710

The Development and Demonstration of Reliable Adherent Metalization of AlN - DOE Contact Samuel Barish (301) 903-2917; MER Corporation Contact Dr. R.O. Loutfy (520) 574-1980

Advanced Single Ion-Conducting Polymer Electrolytes for Lithium-Ion Batteries - DOE Contact Susan Rogers (202) 586-8997; Covalent Associates, Inc. Contact Dr. K.M. Abraham (781) 938-1140

New Lithium Salts for Safe Operation of High-Energy, High-Rate Lithium Ion Batteries - DOE Contact Susan Rogers (202) 586-8997; Electrophorics, Inc. Contact Dr. Larry J. Kepley (505) 720-1115

Novel Lithium-Ion Conducting Polymer Electrolyts for Lithium-Ion Batteries - DOE Contact Susan Rogers (202) 586-8997; Eltron Research, Inc. Contact Eileen Sammells (303) 530-0263

Low-Cost, Alkaline-Metal Salts for Rechargeable Lithium-Ion Batteries - DOE Contact Susan Rogers (202) 586-8997; Excellatron Solid State, LLC Contact Lonnie Johnson (770) 428-2201

Synthesis of New Solid Polymer Electrolytes - DOE Contact Susan Rogers (202) 586-8997; TPL, Inc. Contact H.M. Stoller (505) 342-4412

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

Membranes for Reverse Organic-Air Separations - DOE Contact Charlie Russomanno (202) 586-7543; Compact Membrane Systems, Inc. Contact Glenn Walker (937) 252-8969

Hydrogen Recovery Process Using New Membrane Materials - DOE Contact Charlie Russomanno (202) 586-7543; Membrane Technology and Research, Inc. Contact E.G. Weiss (650) 328-2228

A Novel, Inorganic, Surface-Diffusion Membrane for Hydrogen Separations - DOE Contact Charlie Russomanno (202) 586-7543; TDA Research, Inc. Contact John D. Wright (303) 940-2300

Nanopore-Silica Reactive Adsorbent - DOE Contact Charlie Russomanno (202) 586-7543; Industrial Science and Technology Network, Inc. Contact Dr. Arthur J. M. Yang (717) 843-0300

Molecular Imprinting of Enzymes with Hydrophobic Compounds to Improve Catalytic Activity in Nonaqueous Media - DOE Contact Amy Manheim (202) 586-1507; Albany Molecular Research Inc. Contact David P. Waldek (319) 626-5400

Small-Molecule Tumor-Targeting [99mTc] Agents for Breast Cancer Imaging - DOE Contact Prem Srivastava (301) 903-4071; Anasazi Biomedical Research, Inc. Contact Bernita L. Mach (336) 721-9071

New Boronated Amino Acids for Neutron Capture Therapy - DOE Contact Peter Kirchner (301) 903-9106; BioNeutrics, Inc. Contact Larry Tummel (865) 675-5627

Novel Membranes for Upgrading Natural Gas - DOE Contact Tony Zammerilli (304) 285-4641; Compact Membrane Systems, Inc. Contact Dr. Stuart Nemser (302) 999-7996

Nanostructured Thermal Barrier Coatings - DOE Contact Richard A. Johnson (304) 285-4564; Material Methods Contact Dr. Stephen M. Jaffe (949) 707-1829

Nanoengineered Intermetallics for Energy Systems - DOE Contact Richard Read (412) 386-5721; Powdermet, Inc. Contact Andrew Sherman (818) 768-640

Alternative Interconnect Materials for Improved Solid Oxide Fuel Cell Performance - DOE Contact Wayne Surdoval (412) 386-6002; Technology Management, Inc. Contact Michael A. Petrik (216) 586-5638

A Rapid-Oxidation Stabilization Technique for the Post-Processing of Carbon Foams and Carbon Materials - DOE Contact Richard Read (412) 386-5721; Wright Materials Research Company Contact Dr. Seng C. Tan (937) 642-0007

Low-Cost Arc Process to Produce Single-Walled Nano-Tubes Using Coal-Based Starting Materials - DOE Contact Neil Rossmeissl (202) 586-8668; Materials & Electrochemical Research (MER) Corp. Contact Dr. J.C. Withers (520) 574-1980

Novel Catalyst for Carbon Monoxide Removal from Fuel Cell Reformate - DOE Contact Ronald J. Fiskum (202) 586-9154; KSE, Inc. Contact Dr. James R. Kittrell (413) 549-5506

Development of Improved Oxygen-Reduction Catalysts Using Combinatorial Electrochemistry - DOE Contact Ronald J. Fiskum (202) 586-9154; The Electrosynthesis Company, Inc. Contact Hannah R. Weinberg (716) 684-0513

Phase-Corrective, Polymer-Coated, Lightweight Mirror - DOE Contact Eric Sander (202) 586-5852; Physical Optics Corporation Contact Gordon Drew (310) 320-3088

A Fast, High Light Output Scintillator for Gamma Ray and Neutron Detection - DOE Contact Jehanne Simon-Gillo (301) 903-1455; Radiation Monitoring Devices, Inc. Contact Dr. Gerald Entine (617) 926-1167

A New and Novel Method for Producing Niobium-Coated Copper Cavities - DOE Contact Jehanne Simon-Gillo (301) 903-1455; Tunnel Dust, Inc. Contact Dr. Viet Nguyen-Tuong (757) 890-0161

In-Situ Electron Beam Processing for Radio Frequency Cavities - DOE Contact Jerry Peters (301) 903-5228; FM Technologies, Inc. Contact Dr. Frederick M. Mako (703) 425-5111

An Innovative Fabrication Concept for Niobium-Tin Superconducting Wire - DOE Contact Jerry Peters (301) 903-5228; Alabama Cryogenic Engineering, Inc. Contact Dr. John B. Hendricks (256) 536-8629

High-Performance Niobium-Tin-Tantalum Superconductors Formed by Mechanical Alloying and Near-Net Shape Tube Filling - DOE Contact Jerry Peters (301) 903-5228; EURUS Technologies, Inc. Contact John Romans (850) 574-1800

Niobium Aluminum Precursor Surface Modification for Improved Multifilamentary Bonding - DOE Contact Jerry Peters (301) 903-5228; Supercon, Inc. Contact Elaine Tarkiainen (508) 842-0174

Ceramic Insulation for Heavy Ion Fusion and other High-Radiation Magnets - DOE Contact Warren Marton (301) 903-4958; Composite Technology Development, Inc. Contact Dr. Naseem A. Munshi (303) 664-0394

Development of High-Fiber-Volume, Radiation-Resistant, High-Pressure Laminate for Cryogenic Applications - DOE Contact Warren Marton (301) 903-4958; Cryogenic Materials, Inc. Contact Richard P. Reed (303) 494-1852

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

PHASE II (FIRST YEAR)

Thermally Stable Catalysts for Methane Combustion - DOE Contact Richard A. Johnson (304) 285-4564; TDA Research, Inc. Contact Michael E. Karpuk (303) 940-2301

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 Eileen E. Sammells (303) 440-8008

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 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 Timothy McKechnie (256) 851-7653

Hybrid 3-D SiC/C High Thermal Conductivity Composites - DOE Contact T. V. George (301) 903-4957; MER Corporation Contact R. O. Loutfy (520) 574-1980

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 Elaine Tarkiainen (508) 842-0174

Functionally Graded, Nanocrystalline, Multiphase, Boron-and-Carbon-Based Superhard Coatings - DOE Contact Yok Chen (301) 903-3428; Spire Corporation Contact 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 Francis F. Williams, Jr. (937) 426-6900

Meter Length YBCO Coated Conductor Development - DOE Contact Yok Chen (301) 903-3428; American Superconductor Corporation Contact Dr. Tom Rosa (508) 836-4200

Novel Catalyst for CH_4-CO Conversion - DOE Contact Amy Manheim (202) 586-1507; CeraMem Corporation Contact Dr. Robert L. Goldsmith (781) 899-4495

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

MATERIALS, PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

PHASE II (SECOND YEAR)

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

The Application of Plasma Assisted Chemical Vapor Deposition (PACVD) Coatings for Die Casting Dies - DOE Contact Ehr-Ping Huang Fu (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 Huang Fu (202) 586-1493; UES, Inc. Contact Francis F. Williams, Jr. (937) 426-6900

SMALL BUSINESS TECHNOLOGY TRANSFER RESEARCH PROGRAM

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

PHASE I

Low-Cost Silicon Carbide Ceramic Membranes - DOE Contact Charlie Russomanno (202) 586-7543; Custom Materials, Inc. Contact Dr. Dennis C. Nagle (410) 461-7759

Optimized Performance of Thin Film Polymer Light-Emitting Diodes Through Interface Layers - DOE Contact John Ryan (202) 586-9130; Luna Innovations Incorporated Contact Garnett S. Linkous (540) 953-4274

Development of High-Temperature Superconducting (HTS) Copper Current Leads with HTS Sections Operating in the Current-Sharing Mode - DOE Contact Jerry Peters (301) 903-5228; American Magnetics, Inc. Contact Roger M. Efferson (865) 482-1056

ZnO: Ga Single Crystal Scintillator - DOE Contact Michael P. Procario (301) 903-2890; Cermet, Inc. Contact Jeff Nause (404) 351-0005

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

PHASE II (FIRST YEAR)

Thin-Film Fiber Optic Sensors for Power Control and Fault Detection - DOE Contact Alec Bulawka (202) 586-5633; Airak Engineering, Inc. Contact Paul Grems Duncan (540) 864-6580

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

PHASE II (SECOND 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

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

PHASE I

The Use of Recycled Plastics as Alternative Soil Amendments in the Culture of Plants - DOE Contact Charlie Russomanno (202) 586-7543; AgBio Development, Inc. Contact Dr. Jan Meneley (303) 469-9221

Improved Ternary Substituted, Powder Processed, Melt Quenched, Niobium-Aluminum Strand for High-Field Dipole Applications - DOE Contact Jerry Peters (301) 903-5228; EURUS Technologies, Inc. Contact John Romans (850) 574-1800

Conceptual and Computational Design of Vanadium-Based Alloys for Fusion Reactor Structural Applications - DOE Contact Sam E. Berk (301) 903-4171; QuesTek Innovations, LLC Contact Raymond P. Genellie, Jr. (888) 783-7835

Advanced Materials and Processing Methods for Magnetohydrodynamic Mitigation Coatings - DOE Contact Sam E. Berk (301) 903-4171; Thor Technologies, Inc. Contact Dr. Stuart T. Schwab (505) 296-3615

Advanced Materials and Processing Methods for In-Situ Thermal Barrier Coating Repair - DOE Contact Richard A. Johnson (304) 285-4564; Thor Technologies, Inc. Contact Dr. Stuart T. Schwab (505) 296-3615

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

PHASE II (SECOND 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

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.

The Materials Science Program (MSP) is a key element of the longer-term OFES research activities aimed at providing the knowledge base for an attractive fusion energy source. The MSP focuses on research that addresses the effects on structural materials properties and performance from exposure to the neutronic, thermal, and chemical environments anticipated in the chambers of fusion experiments and energy systems.

The unique requirements on structural materials for fusion applications are the result of the intense neutron environment, dominated by the 14 MeV neutrons characteristic of the deuterium-tritium fusion reaction. For performance, structural materials in the fusion chamber 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).

Research on non-structural materials for fusion experiments and fusion energy systems is carried out in OFES programs for plasma-facing components, diagnostic and control systems, and breeding of tritium fuel.

These materials research programs are conducted with a high degree of international cooperation. Bilateral agreements with Japan and Russia enhance the ability of each party to mount fission reactor irradiation experiments. The Fusion Materials Implementing Agreement under the International Energy Agency serves as a useful venue for the exchange of information and the coordination of fusion materials programs in the US, Japan, Europe, Russia, and China.

239. **VANADIUM ALLOY AND INSULATING COATINGS RESEARCH**
$930,000
DOE Contact: S. Berk (301) 903-4171
ANL Contact: D. L. Smith (630) 252-4837

Most of the research is aimed at low activation structural materials for application in the chambers of fusion energy systems. Emphasis is on vanadium-base alloys and on their chemical corrosion/compatibility with other materials. The vanadium alloy research 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.

About one fourth of the research is aimed at coatings and coating technologies that can be used in elevated temperature flowing lithium coolant circuits. The work identifies promising candidate ceramics, develops the coating technology, and conducts the lithium exposure experiments to demonstrate stability and self-repair needed for fusion power system operation.

Keywords: Vanadium, Compatibility, Lithium, Irradiation Effects, Alloys, Coatings

240. **IRRADIATION EFFECTS MODELING**
$50,000
DOE Contact: S. Berk (301) 903-4171
LLNL Contact: T. Diaz de la Rubia (510) 422-6714

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

241. **FUSION MATERIALS RESEARCH**
$3,880,000
DOE Contact: S. Berk (301) 903-4171
ORNL Contacts: S. J. Zinkle (865) 576-7220

A broad range of research activities is conducted on structural materials and insulating ceramics for use in components of fusion energy systems. 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: for ferritic/martensitic steels, DBTT transition shifts and fracture toughness; for vanadium alloys, welding processes, effects of irradiation on fracture toughness, and compatibility in proposed coolant systems; for SiC/SiC composites, definition of the effects of irradiation on properties and structure and evaluation of advanced composite fibers and coatings. Insulating ceramic research is aimed at understanding 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. A modeling activity complements the experimental measurements.

Keywords: Ceramics, Steels, Vanadium, Silicon Carbide, Composites, Irradiation Effects, Electrical Properties

242. **FUSION STRUCTURAL MATERIALS RESEARCH**
$1,300,000
DOE Contact: S. Berk (301) 903-4171
PNNL Contacts: R. J. Kurtz (509) 373-7515

Research focuses on understanding of radiation effects that provides a basis for developing irradiation-insensitive materials. The objective is low activation materials for use as structures in the chambers of fusion energy 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 energy systems

Keywords: Steels, Vanadium, Silicon Carbide, Composites, Irradiation Effects, Modeling

243. **SIC/SIC COMPOSITE IRRADIATION EFFECTS RESEARCH**
$50,000
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

244. **FUSION MATERIALS FRACTURE AND DEFORMATION RESEARCH**
$140,000
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

245. **FUSION MATERIALS DAMAGE AND FUNDAMENTALS RESEARCH**
$250,000
DOE Contact: S. Berk (301) 903-4171
UCSB Contacts: G. R. Odette (805) 893-3525

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

246. **PLASMA FACING COMPONENTS MATERIALS RESEARCH**
$2,000,000
DOE Contact: S. Berk (301) 903-4171
SNL Contact: M. Ulrickson (505) 845-3020

Research activities include: improved techniques for joining beryllium or tungsten to copper alloys, 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 fluorine-lithium-beryllium (flibe) salts 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

OFFICE OF ENVIRONMENTAL MANAGEMENT

	FY 2000
OFFICE OF ENVIRONMENTAL MANAGEMENT - GRAND TOTAL	$3,260,572
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING	$3,260,572
The Influence of Radiation and Multivalent Cation Additions on Phase Separation and Crystallization of Glass	0
Atmospheric-Pressure Plasma Cleaning of Contaminated Surfaces	366,666
Irradiation Effects on Sorption and Mobilization of Radionuclides During Transport Through the Geosphere	200,000
Iron Phosphate Glasses: An Alternative for Vitrifying Certain Nuclear Wastes	173,333
Fundamental Thermodynamics of Actinide-Bearing Waste Forms	0
Optimization of Thermochemical, Kinetic, and Electrochemical Factors Governing Partitioning of Radionuclides During Melt Decontamination of Radioactively Contaminated Stainless Steel	0
Mechanism of Pitting Corrosion Prevention by Nitrite in Carbon Steel Exposed to Dilute Salt Solutions	0
Stability of High-Level Waste Forms	0
Radiation Effects in Nuclear Waste Materials	313,333
New Metal Niobate and Silicotitanate Ion Exchangers: Development and Characterization	300,000
Distribution & Solubility of Radionuclides & Neutron Absorbers in Waste Forms for Disposition of Plutonium Ash & Scraps, Excess Plutonium, and Miscellaneous Spent Nuclear Fuels	0
Modeling of Diffusion of Plutonium in Other Metals and of Gaseous Species in Plutonium-Based Systems	0
Corrosion of Spent Nuclear Fuel: The Long-Term Assessment	148,333
Direct Investigations of the Immobilization of Radionuclides in the Alteration Products of Spent Nuclear Fuel	342,000
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 Evolution 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
Ion-exchange Processes and Mechanisms in Glasses	0

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 of those awards were in scientific disciplines related to materials issues that have potential to solve Environmental Management challenges. The FY 2000 component of materials research is estimated to amount to $3,260,572. The entire EMSP portfolio can be viewed on the World Wide Web at http://emsp.em.doe.gov/portfolio.

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

247. **THE INFLUENCE OF RADIATION AND MULTIVALENT CATION ADDITIONS ON PHASE SEPARATION AND CRYSTALLIZATION OF GLASS**
$0[1]
DOE Contact: Justine Alchowiak (202) 586-4629
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

[1] Prior Year Funding

248. **ATMOSPHERIC-PRESSURE PLASMA CLEANING OF CONTAMINATED SURFACES**
$366,666
DOE Contact: Justine Alchowiak (202) 586-4629
University of California at Los Angeles Contact:
Robert F. Hicks (310) 206-6865
LANL Contact: Hans Herrmann (505) 665-6157

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. Recent improvements in the source design have made it compact, rugged, reliable and easily configured to treat objects of different sizes and shapes. The objectives of this research program are to fully characterize the discharge physics and chemistry, to engineer the exhaust containment system, and to test the plasma device on contaminated structures within the Department of Energy complex.

Keywords: Plasma Etching, Plutonium

249. **IRRADIATION EFFECTS ON SORPTION AND MOBILIZATION OF RADIONUCLIDES DURING TRANSPORT THROUGH THE GEOSPHERE**
$200,000
DOE Contact: Justine Alchowiak (202) 586-4629
University of Michigan Contacts: Lu-Min Wang (313) 647-8530

Site restoration activities at DOE facilities and the permanent disposal of nuclear waste inevitably involve understanding the behavior of materials in a radiation field. Radionuclide decay and associated radiation effects lead to physical and chemical changes in important properties (e.g., sorption and cation exchange capacity). During the past three years, radiation effects in selected near-field materials have been evaluated in accelerated laboratory experiments utilizing energetic electrons and ions and *in situ* transmission electron microscopy (TEM). Zeolites and layered silicates were found to be highly susceptible to irradiation-induced solid-state amorphization. The critical doses for complete amorphization of these phases are as low as <0.1 displacement per atom (dpa) or 108 GY in ionization energy deposition (i.e., the dose for a zeolite with 10 wt.% loading of ^{137}Cs in 400 years). Even partial amorphization will cause a dramatic reduction (up to 95%) in ion-exchange and sorption/desorption capacities for radionuclides, such as Cs and Sr. Because the near-field or chemical processing materials, e.g., zeolites or crystalline silicotitanate (CST), will receive a substantial radiation dose after they have incorporated radionuclides, the results suggest that radiation may, in some cases, retard the release of sorbed or ion-exchanged radionuclides. These results have a direct bearing on repository performance assessments (e.g., the extent to which zeolites can retard the release of radionuclides) and on the technologies used to process high-level liquid waste (e.g., separation of 137Cs from HLW using CST at the Savannah River Site).

Radionuclides to be studied include Cs, Sr, U, and Se, which are important because: 1)they represent a range of sorptive behavior that should bracket the behavior of most other radionuclides (except ^{99}Tc) and 2) they are considered to make important contributions to total radiation exposures, as illustrated in the recent Total Systems Performance Assessment-Viability Assessment of the proposed repository at Yucca Mountain. Selected clay and zeolite samples will be irradiated with high energy electrons, high energy ions and neutrons to simulate the radiation effects from a variety of radioactive decay processes at a much accelerated rate using a unique combination of irradiation facilities available at the University of Michigan (the Ford Nuclear Reactor and the Michigan Ion Beam Laboratory). Ion exchange/sorption experiments will be conducted on samples irradiated to various doses to determine the impact of the radiation effects on the sorption capacity and retention of radionuclides. Novel ion implantation and surface analysis techniques, e.g., atomic force microscopy and Z-contrast high resolution scanning transmission electron microscopy (STEM), will be used to identify atomic-scale effects of radiation damage associated with single or small clusters of radionuclides sorbed onto mineral surfaces.

Keywords: Radiation Effects, Near-field, Geologic Repository

250. **IRON PHOSPHATE GLASSES: AN ALTERNATIVE FOR VITRIFYING CERTAIN NUCLEAR WASTES**
$173,333
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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 pre-treatment processes, as well as the larger waste volumes resulting from dilution, will add billions of dollars to the DOE's cost of cleaning up the former nuclear weapons production facilities. Such additional costs may be avoided by developing a small number of alternative waste glasses which are suitable for vitrifying those specific waste feeds that are incompatible with borosilicate glasses.

A low cost and technically effective 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. However, the scientific and technical knowledge base that is needed to vitrify nuclear waste in iron phosphate glasses on a production scale is currently lacking. In addition, the high priority wastes that are likely to cause problems in borosilicate melts need to be identified and property data need to be acquired for iron phosphate wasteforms made from these wastes. This research is addressing these needs, 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 glasses can be used to vitrify those nuclear wastes which are poorly suited for borosilicate glasses.

Keywords: Iron Phosphate Glasses, Vitrification, Nuclear Waste

251. **FUNDAMENTAL THERMODYNAMICS OF ACTINIDE-BEARING MINERAL WASTE FORMS**
$0[1]
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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

252. **OPTIMIZATION OF THERMOCHEMICAL, KINETIC, AND ELECTROCHEMICAL FACTORS GOVERNING PARTITIONING OF RADIONUCLIDES DURING MELT DECONTAMINATION OF RADIOACTIVELY CONTAMINATED STAINLESS STEEL**
$0[1]
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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

[1] Prior Year Funding

253. **MECHANISM OF PITTING CORROSION PREVENTION BY NITRITE IN CARBON STEEL EXPOSED TO DILUTE SALT SOLUTIONS**
$0[1]
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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

[1] Prior Year Funding

254. **STABILITY OF HIGH-LEVEL WASTE FORMS**
$0[1]
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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 over-estimated 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

255. **RADIATION EFFECTS IN NUCLEAR WASTE MATERIALS**
$313,333
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The objective of this project is to develop a fundamental understanding of radiation effects in glass and ceramics, as well as the influence of radiation effects on aqueous dissolution kinetics. This study will provide the underpinning science to develop improved glass and ceramic waste forms for the immobilization and disposition of high-level tank waste, excess plutonium, plutonium residues and scrap, surplus weapons plutonium, other actinides, and other nuclear waste streams. Furthermore, this study will develop predictive models for the performance of nuclear waste forms and stabilized nuclear materials. The research focuses on the effects of alpha and beta decay on defect production, defect interactions, diffusion, solid-state phase transformations, and gas accumulation, and dissolution kinetics. Plutonium incorporation, gamma irradiation, ion-beam irradiation, and electron beam irradiation are used to simulate the effects of alpha decay and beta decay on relevant glasses and ceramics in experimental studies. Computer simulation methods are used to provide an atomic-level interpretation of experimental data, calculate important fundamental parameters, and provide multi-scale computational capabilities over different length (atomic to macroscopic) and time (picoseconds to millenia) scales.

Keywords: Glass, Ceramics, Radiation Effects

256. **NEW METAL NIOBATE AND SILICOTITANATE ION EXCHANGERS: DEVELOPMENT AND CHARACTERIZATION**
$300,000
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Previous research by this group provided preliminary data of a novel class of niobate-based molecular sieves (Na/Nb/M/O, M=transition metals) that show exceptionally high selectivity for divalent cations under extreme conditions (acid solutions, competing cations) and novel silicotitanate phases that are also selective for divalent cations. Furthermore, these materials are easily converted by a high-temperature *in situ* heat treatment into a refractory ceramic waste form with low cation leachability. The new niobate-based waste form is a perovskite phase, which is also a major component of Synroc, a titanate ceramic waste form used for sequestration of high-level wastes (HLW) from reprocessed, spent nuclear fuel. These new niobate ion exchangers also showed orders of magnitude better selectivity for Sr^{2+} under acid conditions than any other material.

The goal of this project is to provide DOE with alternative materials that can exceed the performance of monosodium titanate (MST) for strontium and actinide removal at the Savannah River Site (SRS), remove strontium from acidic waste at Idaho National Engineering and Environmental Laboratory (INEEL), and sequester divalent cations from contaminated groundwater and soil plume. The research team will focus on three tasks that will provide both the basic research necessary for the development of highly selective ion exchange materials and also materials for short-term deployment within the DOE complex: (1) structure/property relationships of a novel class of niobate based molecular sieves (Na/Nb/M/O, M=transition metals), which show exceptionally high selectivity for divalent cations under extreme conditions (acid solutions, competing cations); (2) the role of ion exchanger structure change (both niobates and silicotitanates) on the exchange capacity (for elements such as strontium and actinide-surrogates), which result from exposure to DOE complex waste simulants; (3) thermodynamic stability of metal niobates and silicotitanate ion exchangers.

Keywords: Niobate, Silicotitanate, Ion Exchanger

257. **DISTRIBUTION & SOLUBILITY OF RADIONUCLIDES & NEUTRON ABSORBERS IN WASTE FORMS FOR DISPOSITION OF PLUTONIUM ASH & SCRAPS, EXCESS PLUTONIUM, AND MISCELLANEOUS SPENT NUCLEAR FUELS**
$0[1]
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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

[1] Prior Year Funding

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

258. MODELING OF DIFFUSION OF PLUTONIUM IN OTHER METALS AND OF GASEOUS SPECIES IN PLUTONIUM-BASED SYSTEMS
$0[1]
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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

259. CORROSION OF SPENT NUCLEAR FUEL: THE LONG-TERM ASSESSMENT
$148,333
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Spent nuclear fuel accounts for over 95% of the total radioactivity in the radioactive wastes in the United States that require disposal, disposition, or remediation. 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 kinetics for this transformation are rapid, essentially instantaneous on geologic time scales. Under reducing conditions, UO_2 is stable, but may alter to U^{4+} compounds such as coffinite, $USiO_4$, depending on groundwater compositions. Under both oxidizing and reducing conditions, the formation of new uranium phases may lead to the release or retardation of trace elements, such as the fission product elements and actinides in spent nuclear fuel. Over the long term, and depending on the extent to which the secondary uranium phases can incorporate fission products and actinides, these alteration phases become the near-field source term.

Fortunately, previous experimental studies and field studies have established that natural uranite and its alteration products are good "natural analogues" for studying the corrosion of UO_2 in spent nuclear fuel. This research program is addressing the following issues:

[1] Prior Year Funding

- What are the long-term corrosion products of natural UO_{2+x}, uranite, under oxidizing and reducing conditions?

- What is the paragenesis or the reaction path of the phases that form during alteration? How is the sequence formation related to the structure of these uranium phases and reacting groundwater composition?

- What is the trace element content in the corrosion products as compared to the original UO_{2+x}? Do the trace element contents substantiate models developed to predict radionuclide incorporation into the secondary phases?

- Are the corrosion products accurately predicted from geochemical codes (e.g., EQ3/6) that are used in performance assessments?

- How persistent over time are the metastable phase assemblages that form? Will these phases serve as effective barriers to radionuclide release?

Experimental results and theoretical models for the corrosion of spent nuclear fuel under oxidizing and reducing conditions will be tested by comparison to results from studies of samples from the Oklo natural fission reactors.

Keywords: Uranium Oxides, Mineralogy, Corrosion, Phase Stability

260. **DIRECT INVESTIGATIONS OF THE IMMOBILIZATION OF RADIONUCLIDES IN THE ALTERATION PRODUCTS OF SPENT NUCLEAR FUEL**
$342,000
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This project emphasizes the synthesis of uranium phases and uranium phases doped with certain radionuclides in order to examine radionuclide incorporation in uranyl compounds. The identities of alteration phases important for spent-fuel corrosion will be gleaned from the results of long-term experiments on the corrosion of spent UO_2 fuel and unirradiated UO_2, as well as more recent studies of U-metal fuel corrosion, that are currently underway at ANL. The focus will be on synthesizing actinide compounds similar to those that have been identified as corrosion products of spent uranium-based fuels. The goals of the experiments are to synthesize and characterize actinide and fission-product host phases formed on U-based waste forms under oxidizing conditions, such as expected at the candidate geological repository at Yucca Mountain. Target phases for synthesis include those identified in current corrosion experiments with U-based fuels being conducted at Argonne. Those experiments demonstrate that many radionuclides are retained in U-bearing alteration products. Synthesis and characterization of U(VI) phases doped with specific radionuclides helps clarify the mechanisms of radionuclide incorporation into uranyl-based compounds. Where possible, stable-isotope equivalents of radionuclides are used during synthesis; however, pure Np and Pu analogues of selected uranium compounds will also be synthesized. In addition, U compounds doped with low levels of selected radionuclides will be characterized in order to understand mechanisms of trace-element substitution.

Methods used to characterize solid phases include X-ray powder diffraction and transmission electron microscopy. Selected samples are also analyzed by single-crystal X-ray structure analyses and X-ray absorption spectroscopy, where possible.

Keywords: Uranium Oxides, Mineralogy, Phase Stability, Corrosion, Radionuclides

261. **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

262. **MECHANISMS OF RADIONUCLIDE-HYDROXYCARBOXYLIC ACID INTERACTIONS FOR DECONTAMINATION OF METALLIC SURFACES**
$383,333
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State University of New York at Stony Brook
Contact: Gary P. Halada (516) 632-8526

This project addresses key fundamental issues involved in the use of simple and safe methods for the removal of radioactive contaminants from slightly contaminated steel and other surfaces at the DOE sites so that the metals can be reused. The objectives are to (1) determine the nature of the association of radionuclides U, Pu, Co and Sr with stainless steel, and (2) selectively remove the radionuclides using hydroxycarboxylic acids (citric acid and its analogs). The basic mechanisms involving coordination, complexation, dissolution and removal will be elucidated in a systematic manner.

This is a collaborative research project between Brookhaven National Laboratory (BNL) and the State University of New York at Stony Brook (SUNY-SB). This project is divided into three phases. In Phase I the basic mechanism of interaction of actinides with metal oxides on metallic surfaces will be investigated. Phase II will determine the interaction of hydroxycarboxylic acids citric, malic and tartaric acids with the actinide contaminated metallic surfaces. Phase III involves investigation of interaction of hydroxycarboxylic acid with actual contaminated samples from DOE sites and interpretation of results based on knowledge gained from Phases I and II. The nature of radionuclide association with representative metal oxides typically formed on metallic surfaces which have undergone oxidation characteristic of long term environmental exposure will be investigated. The rate and extent of incorporation of radionuclide into amorphous and crystalline forms of iron oxides (goethite, hematite, magnetite and lepidocrocite), and metallic coupons will be determined. Exposure of metallic coupons to radionuclides during and following accelerated aqueous corrosion will utilize standard electrochemical cells and equipment. Advanced spectroscopic techniques (XPS, XANES, EXAFS, EDX, SIMS, FTIR and LD-ITMS at PNNL) will be used to characterize the (1) nature of the radionuclide association with the metal oxides and contaminated surfaces, and (2) radionuclide-citrate complexes and mixed-metal (actinide-metal-citrate) complexes that have been removed from contaminated surfaces. In addition, the photochemical and biochemical degradation of the resulting actinide-organic complexes will be examined, with application to recovery of radionuclides in a concentrated form and reduction of secondary waste generation.

Keywords: Radionuclides, Decontamination, Actinides, Corrosion

263. **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

264. **MECHANISMS AND KINETICS OF ORGANIC AGING IN HIGH-LEVEL NUCLEAR WASTES**
$300,000
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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

265. **MODELING OF SPINEL SETTLING IN WASTE GLASS MELTER**
$291,667
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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

266. **ION-EXCHANGE PROCESSES AND MECHANISMS IN GLASSES**
$0[1]
DOE Contact: Justine Alchowiak (202) 586-4629
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

[1] Prior Year Funding

OFFICE OF NUCLEAR ENERGY, SCIENCE AND TECHNOLOGY

	FY 2000
OFFICE OF NUCLEAR ENERGY, SCIENCE AND TECHNOLOGY - GRAND TOTAL	$13,915,323
OFFICE OF SPACE AND DEFENSE POWER SYSTEMS	$2,871,000
SPACE AND NATIONAL SECURITY PROGRAMS	$2,871,000
MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING	$2,263,000
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	1,445,000
Carbon-bonded Carbon Fiber Insulation Production, Maintenance, Manufacturing Process Development, and Product Characterization	318,000
Manufacturing of Robust Ceramic/metal Joints for Alkali Metal Thermal to Electric Converters (AMTEC)	100,000
New Methods for Joining Beta"-alumina to Niobium 1% zirconium for Alkali Metal Thermal to Electric Converters (AMTEC)	100,000
AMTEC Electrode and Beta"-alumina Solid Electrolyte Development	300,000
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING	$608,000
Development and Production of Materials for Amtec Cells	608,000
OFFICE OF TECHNOLOGY AND INTERNATIONAL COOPERATION	$11,044,323
NUCLEAR ENERGY PLANT OPTIMIZATION	$3,985,011
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING	$3,985,011
Steam Generator NDE Test Mockup Facility	400,000
Advanced Eddy-current Inspection System for Detection and Characterization of Defects in Steam Generator Tubes	232,000
Overcoming Solubility Limitations to Zinc Addition in PWRs	170,000
Develop Empirical Data to Characterize Aging Degradation of Polymers Used in Electrical Cable	578,390
Develop Condition Monitoring (Cm) Techniques for Electrical Cable	605,420
Mechanical Behavior of Irradiated Structural Stainless Steels	400,000
Fatigue	599,380
Assessment of Aging Effects on Components and Structures from Nuclear Power Plants	349,850
Irradiation Induced Swelling and Stress Relaxation of PWR Reactor Core Internal Components	449,971
Impact of Nickel Oxide Solubility on Axial Offset Anomaly in PWRs	200,000

OFFICE OF NUCLEAR ENERGY, SCIENCE AND TECHNOLOGY (continued)

	FY 2000
OFFICE OF TECHNOLOGY AND INTERNATIONAL COOPERATION (CONTINUED)	
NUCLEAR ENERGY RESEARCH INITIATIVE	$7,059,312
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING	$3,046,953
Application of Innovative Experimental and Numerical Techniques for the Assessment of Reactor Pressure Vessel Structural Integrity	200,000
Innovative Chemithermal Techniques for Verifying Hydrocarbon Integrity in Nuclear Safety Materials	356,860
Continuous-wave Radar to Detect Defects Within Heat Exchanger and Steam Generator Tubes	327,975
Fundamental Mechanisms of Corrosion of Advanced Zirconium Based Alloys at High Burn-up	713,425
Monitoring the Durability Performance of Concrete in Nuclear Waste Containment	150,210
Deterministic Prediction of Corrosion Damage in High Level Nuclear Waste	216,696
Effects of Water Radiolysis in Water Cooled Nuclear Reactors	429,604
Mapping Flow Localization Processes in Deformation of Irradiated Reactor Structural Alloys	214,000
A Novel Approach to Materials Development for Advanced Reactor Systems	148,124
An Investigation of the Mechanism of IGA/SCC of Alloy 600 in Corrosion Accelerating Heated Crevice Environments	290,059
MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING	$4,012,359
Novel Concepts for Damage-resistant Alloy in next Generation Nuclear Power Systems	530,000
Advanced Ceramic Composites for High-temperature Fission Reactors	250,000
Development of Improved Burnable Poisons for Commercial Nuclear Power Reactors	389,000
Fuel for a Once-through Cycle (Th, U) O_2 in a Metal Matrix	360,008
Advanced Proliferation Resistant, Lower Cost, Uranium-thorium Dioxide Fuels for Light Water Reactors	1,161,848
Development of a Stabilized Light Water Reactor (LWR) Fuel Matrix for Extended Burnup	357,056
Continuous Fiber Ceramic Composite Cladding for Commercial Water Reactor Fuel	156,221
An Innovative Ceramic Corrosion Protection System for Zircaloy Cladding	198,226
A Single Material Approach to Reducing Nuclear Waste Volume	210,000
Developing Improved Reactor Structural Materials Using Proton Irradiation a Rapid Analysis Tool	400,000

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 2000, essentially all materials programs were aimed at: (1) certification of new low thorium-iridium alloy blanks, (2) maintenance of iridium alloy and carbon bonded carbon fiber (CBCF) insulation radioisotope heat source material and components manufacturing capability, and (3) 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

267. 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

$1,445,000
DOE Contact: L. Herrera (301) 903-8218
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 2000 all approvals were obtained for the production of flight quality clad vent sets at the Oak Ridge National Laboratory. The capability was established for producing integral (Galileo Type) weld shields. Vent notches were widened and integral weld shields were installed in 66 shield cups returned to Oak Ridge from the Los Alamos National Laboratory. Integral weld shields were also installed in shield cup assemblies from qualification production. Blanks of a new low-thorium alloy of iridium were used to successfully form both vent cups and shield cups. This new low-thorium iridium alloy blanks were produced using the arc melting, extrusion, and rolling process normally employed for DOP-26.

Keywords: Consumable Arc Melt, Extrusion, Noble Metal, Rolling, Forming

268. CARBON-BONDED CARBON FIBER INSULATION PRODUCTION, MAINTENANCE, MANUFACTURING PROCESS DEVELOPMENT, AND PRODUCT CHARACTERIZATION

$318,000
DOE Contact: L. Herrera (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-RTGs 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. In FY 2000, a careful inventory was made of all materials required for the production of CBCF insulator sets, and a new storage facility was prepared. An additional nine CBCF insulator sets were produced and all inspection results required for certification of CBCF sets produced in FY1999 and FY2000 were obtained.

Keywords: Insulators/Thermal, High Temperature Service, Fibers

269. **MANUFACTURING OF ROBUST CERAMIC/ METAL JOINTS FOR ALKALI METAL THERMAL TO ELECTRIC CONVERTERS (AMTEC)**
$100,000
DOE Contact: L. Herrera (301) 403-8218
Triton Systems, Inc. Contact: F. Kuchinski (978) 250-4200

The feasibility of using advanced joining methods of beta to other components in the tube/plenum assembly to permit the use of higher temperature stable joining materials without adversely affecting the beta alumina solid electrolyte during processing. Thermal cycling, helium leak testing, and thermal/sodium compatibility testing proposed to demonstrate the approach.

Keywords: Joining Methods, AMTEC

270. **NEW METHODS FOR JOINING BETA"-ALUMINA TO NIOBIUM 1% ZIRCONIUM FOR ALKALI METAL THERMAL TO ELECTRIC CONVERTERS (AMTEC)**
$100,000
DOE Contact: L. Herrera (301) 903-8218
AMPS Contact: T. Hunt (734) 677-4260

Several new concepts for high temperature mechanical ceramic to refractory metal sealants are being proposed for initial experimental evaluation. The candidate seals will be operated in Alkali Metal Thermal to Electric Converter (AMTEC) cells and cell performance measured.

Keywords: Mechanical Joining, AMTEC

271. **AMTEC ELECTRODE AND BETA"-ALUMINA SOLID ELECTROLYTE DEVELOPMENT**
$300,000
DOE Contact: L. Herrera (301) 903-8218
Texas A&M University Contact: M. Schuller (409) 845-8767

The development of improved performance electrode materials, principally iridium and mixed conductor electrode materials, was continued for potentially improved performance AMTEC cells.

Keywords: Electrode Materials, AMTEC

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

272. **DEVELOPMENT AND PRODUCTION OF MATERIALS FOR AMTEC CELLS**
$608,000
DOE Contact: L. Herrera (301) 903-8218
ORNL Contact: J. King (923) 574-4807

Arc melted molybdenum-41% rhenium was produced for potential use as the primary structural material for AMTEC cells. Enough of this material was produced to provide adequate material for evaluations. Studies indicated that this alloy had a much lower oxidation rate than Nb-1Zr which had previously been projected for use. In addition to a lower oxidation rate, the oxidation that did occur in the MoRe alloy had no effect on the mechanical properties. Various aspects of fabricability such as machinability and weldability were demonstrated. A report on the production and properties of the arc melted MoRe was prepared and distributed to assist in AMTEC cell design.

Keywords: Molybdenum, Rhenium, Arc Melt, AMTEC

OFFICE OF TECHNOLOGY AND INTERNATIONAL COOPERATION

NUCLEAR ENERGY PLANT OPTIMIZATION

Nuclear Energy Plant Optimization projects are designed to address issues associated with aging management and plant performance optimization of light water reactors. The projects address both non-destructive testing, and the mechanical properties of structural components and cabling.

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

273. **STEAM GENERATOR NDE TEST MOCKUP FACILITY**
$400,000
DOE Contact: T. R. Allen (301) 903-1647
EPRI Contact: J. Benson (650) 855 2146
ANL Contact: D. Kupperman (630) 252-5108

To provide suitable test specimens and databases of NDE and characterization results that can be used to develop improved NDE techniques and signal analysis methods for the detection and characterization of SCC in steam generator tubing and provide the capability to assess and demonstrate the effectiveness of such methods.

Keywords: Stress Corrosion Cracking, Non-Destructive Examination, Steam Generator

274. **ADVANCED EDDY-CURRENT INSPECTION SYSTEM FOR DETECTION AND CHARACTERIZATION OF DEFECTS IN STEAM GENERATOR TUBES**
$232,000
DOE Contact: T. R. Allen (301) 903-1647
EPRI Contact: J. Benson (650) 855-2146
ANL Contacts: T. Wei (630) 252-4688

Develop an advanced eddy-current inspection technique and data analysis methodology for more reliable detection and accurate sizing of defects in steam generator tubes, including repaired tubes.

Keywords: Stress Corrosion Cracking, Non-Destructive Examination, Steam Generator

275. **OVERCOMING SOLUBILITY LIMITATIONS TO ZINC ADDITION IN PWRS**
$170,000
DOE Contact: T. R. Allen (301) 903-1647
ORNL Contacts: J. Michael Simonson (865) 574-4962

Through a series of tests, determine the solution thermodynamics of the Zn/ZnO system at high temperature in order to allow PWRs to safely inject as close as possible to the maximum Zinc concentration without ZnO precipitation on the core.

Keywords: Corrosion, Thermodynamics

276. **DEVELOP EMPIRICAL DATA TO CHARACTERIZE AGING DEGRADATION OF POLYMERS USED IN ELECTRICAL CABLE**
$578,390
DOE Contact: T. R. Allen (301) 903-1647
EPRI Contact: G. Toman (704) 547-6073
SNL Contact: K. Gillen (505) 844-7494

Develop empirical data to characterize the aging behavior of polymer materials in electrical cable insulation and jackets for the following environments; typical power plant conditions, R&D laboratory experimental conditions, and environmental qualification tests.

Keywords: Polymers, Aging, Irradiation, Electrical Insulation

277. **DEVELOP CONDITION MONITORING (CM) TECHNIQUES FOR ELECTRICAL CABLE**
$605,420
DOE Contact: T. R. Allen (301) 903-1647
EPRI Contact: G. Toman (704) 547-6073
SNL Contact: K. Gillen (505) 844-7494

Develop nondestructive or essentially-nondestructive, science-based, CM techniques for electrical cable insulation and jacket materials that are capable of characterizing the current condition of either a local section or an entire cable run using parameters (e.g., density) correlated to aging models or other well-defined criteria. Confirmation of ability of identification of damaged insulation via electrical testing in an ionizable gas environment and extension ionized gas testing to locate and characterize damage sites will also be included. Development of a distributed temperature and radiation monitoring system based on fiber optic transmission characteristics will also be evaluated.

Keywords: Aging, Irradiation, Electrical Insulation, Fiber Optics

278. **MECHANICAL BEHAVIOR OF IRRADIATED STRUCTURAL STAINLESS STEELS**
$400,000
DOE Contact: T. R. Allen (301) 903-1647
EPRI Contact: H. T. Tang (650) 855-2012
ANL Contacts: D. L. Porter (208) 533-7659

Determine the mechanical behavior of irradiated structural stainless steels under conditions of interest to LWRs and to develop constitutive models describing the behavior that can be used to develop tools to predict component life, assess the results of NDE examinations and guide the timing of corrective actions.

Keywords: Austenitic Stainless Steel, Irradiation, Mechanical Properties, Modeling, Stress Corrosion Cracking

279. **FATIGUE**
$599,380
DOE Contact: T. R. Allen (301) 903-1647
EPRI Contacts: J. Carey (650) 855-2105, S. Rosinski (704) 547-6123 and B. Carter (704) 547-6019

Provide cost effective methods of evaluating the cyclic life of nuclear components, including the effects of reactor coolant environment, based on the safety margins of the ASME Code, and to provide utilities with appropriate "tools" to manage fatigue effects.

Keywords: Fatigue, ASME Code, Environmental Fatigue

280. **ASSESSMENT OF AGING EFFECTS ON COMPONENTS AND STRUCTURES FROM NUCLEAR POWER PLANTS**
$349,850
DOE Contact: T. R. Allen (301) 903-1647
EPRI Contacts: J. Carey (650) 855-2105
and S. Rosinski (704) 547-6123
ORNL Contact: T. M. Rosseel (865) 574-5380
PNNL Contact: S. K. Sundaram (509) 373-6665

Obtain materials and components that have been in service in operating reactors to be used for comparison with laboratory aged materials to validate models for aging effects and nondestructive examination methods. Provide information on the significance of aging effects and the effectiveness of plant programs for managing aging effects.

Keywords: Aging, Non-Destructive Examinations, Modeling

281. **IRRADIATION INDUCED SWELLING AND STRESS RELAXATION OF PWR REACTOR CORE INTERNAL COMPONENTS**
$449,971
DOE Contact: T. R. Allen (301) 903-1647
EPRI Contact: H. T. Tang (650) 855-2012

Characterize irradiation induced void swelling and stress relaxation related degradation that could occur in operating reactors, and calibrate and extend the breeder reactor based swelling model for PWR applications.

Keywords: Irradiation-Induced Swelling, Stress Relaxation

282. **IMPACT OF NICKEL OXIDE SOLUBILITY ON AXIAL OFFSET ANOMALY IN PWRs**
$200,000
DOE Contact: B. P. Singh (301) 903-3741
EPRI Contact: Paul Frattini (650) 855 2027
ORNL Contact: J. M. Simonson (865) 574-4962

To rapidly develop the database on Nickel solubility from NiO up to clad temperatures. These data are essential to understanding and managing corrosion product transport and deposition in the potential Axial Offset Anomaly (AOA) core. Ultimately, solubility screening tools should be coupled to core design thermal hydraulic and neutronic codes to produce high duty cores with reduced AOA risk.

Keywords: Solubility, Corrosion

NUCLEAR ENERGY RESEARCH INITIATIVE

Nuclear Energy Research Initiative projects are designed to address materials issues associated with advanced nuclear reactors. The projects address the development and characterization of fuel, structural materials and waste forms.

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

283. **APPLICATION OF INNOVATIVE EXPERIMENTAL AND NUMERICAL TECHNIQUES FOR THE ASSESSMENT OF REACTOR PRESSURE VESSEL STRUCTURAL INTEGRITY**
$200,000
DOE Contact: T. P. Miller (301) 903-4517
SNL Contact: T. Y. Chu (505) 845-3217

The lower head of the reactor pressure vessel (RPV) can be subjected to significant thermal and pressure loads in the event of a core meltdown accident. The mechanical behavior of the reactor vessel lower head is of importance both in severe accident assessment and the assessment of accident mitigation strategies. For severe accident assessment the failure of the lower head defines the initial conditions for all ex-vessel events, and in accident mitigation the knowledge of mechanical behavior of the reactor vessel defines the possible operational envelope for accident mitigation. The need for validated models of the lower head in accident scenarios is accomplished by well-controlled, well-characterized large-scale experiments simulating realistic thermal/mechanical loads to the reactor pressure vessel.

This project consists of both experimental and analytical efforts in investigating the structural integrity of reactor pressure vessels. Experiments simulating the thermal/ mechanical loads to a reactor pressure vessel generate data that can be implemented into a finite element code, such as the commercially available code ABAQUS, to assess the ability of the code to capture the response of the pressure vessel to severe accident conditions. In addition, the pressure vessel material (SA533B1 steel) used in these experiments is prototypic of reactor PWR vessel material and is well characterized by material property testing as part of this program.

The NERI/NRC/OECD sponsored program consists of eight international partners: Belgium, Czech Republic, Finland, France, Germany, Spain and Sweden and the U.S. U.S. support is provided by the NRC and the Department of Energy NERI program. This experimental/ analytical program builds on the accomplishments of a previous NRC sponsored Lower Head Failure (LHF) program (NUREG/ CR-5582). The current program is referred to as the OECD Lower Head Failure (OLHF) program to distinguish it from the previous program and to recognize the international participation of the OECD.

Keywords: Ferritic Steel, Mechanical Behavior, Reactor Pressure Vessel

284. **INNOVATIVE CHEMITHERMAL TECHNIQUES FOR VERIFYING HYDROCARBON INTEGRITY IN NUCLEAR SAFETY MATERIALS**
$356,860
DOE Contact: T. P. Miller (301) 903-4517
Pacific-Sierra Research Corporation
Contact: L. R. Mason (703) 807-5668

This research and development program is designed to explore new methods of assessing current condition and predicting remaining life of critical hydrocarbon materials in nuclear power plant environments. Of these materials, "1E" safety cable insulation is the primary focus. Additionally, o-ring, seal, and lubricant products designed for nuclear applications round out the materials studied. This 3-phase applied research program is providing industry with new innovative methods and reference data to conduct pragmatic material condition-monitoring programs for a wide range of polymer-based products. Key research objectives (products) include a material-condition-monitoring database, optimization and standardization of various testing procedures, implementation of proven engineering development methodologies, and inter-technology correlation analyses. Milestones are defined by a 5-task work-breakdown schedule. Task 1 encompasses front-end R&D program activities and planning of additional tasks. Task 2 concerns identification of subject cable materials, their acquisition, accelerated aging, testing by a suite of chemithermal methods, and results reporting.

Keywords: Polymers, Aging

285. **CONTINUOUS-WAVE RADAR TO DETECT DEFECTS WITHIN HEAT EXCHANGER AND STEAM GENERATOR TUBES**
$327,975
DOE Contact: T. P. Miller (301) 903-4517
SNL Contact: Thurlow W. H. Caffey
(505) 844-4217

The overall objective of this three-year program is to design, fabricate, and demonstrate a complete defect-detection system using an in-tube radar (ITR) within a variety of steam-generator tubing typically found in nuclear-electric power plants. The ITR is fundamentally different from the eddy-current methods now in use because it is based on backscatter from a defect rather than the disturbance of current flow in the tube wall. An electric field, parallel to the axis of the tube, is transmitted into the tube wall, reflected from a defect, and returned to an internal receiver all operating in the near field. The fundamental premise is that the change in axial electric field caused by the defect will be distinguishable from the null field present in the absence of defects.

This first year's work had the following research objectives:

Defect Modeling: Three-dimensional (3D) electromagnetic codes in cylindrical coordinates, including the transmitter, were needed to determine the backscatter from defects of different geometries, orientations, and wall locations.

Alignment Sensitivity: Preliminary modeling showed that there would be no transmission from the transmitter to the receiver if both were located exactly on the centerline of the tube. However, further modeling was needed to show that slight departures from the ideal coaxial geometry, consistent with mechanical tolerances, would still allow acceptable performance.

Prototype Design: Mechanical packaging, centering provisions, fiber-optic links, on-board power, antennas, amplifiers, and translation system designs had to begin both to provide some parameters needed for the above modeling codes, and to ensure timely completion of the project.

Keywords: Non-Destructive Testing, Cracking

286. FUNDAMENTAL MECHANISMS OF CORROSION OF ADVANCED ZIRCONIUM BASED ALLOYS AT HIGH BURN-UP
$713,425
DOE Contact: T. P. Miller (301) 903-4517
Westinghouse Electric Company Contact:
R. G. Lott (412) 256-1061

The corrosion behavior of nuclear fuel cladding is a key factor limiting the performance of nuclear fuel elements. Improved cladding alloys, which resist corrosion and radiation damage, will facilitate higher burnup core designs. The objective of this project is to understand the mechanisms by which alloy composition, heat treatment and microstructure affect corrosion rate. This knowledge will be used to predict the behavior of existing alloys outside the current experience base (for example, at high burnup) and predict the effects of changes in operating conditions on zirconium alloy behavior.

Zirconium alloys corrode by the formation of a highly adherent protective oxide layer. The working hypothesis of this project is that alloy composition, microstructure and heat treatment affect corrosion rates through their effect on the protective oxide structure and ion transport properties. Therefore, particular emphasis has been placed on detailed characterizations of the oxides formed on a series of experimental alloys. The goal of this project is to identify these differences and understand how they affect corrosion behavior. To do this, several microstructural examination techniques including transmission electron microscopy (TEM), electrochemical impedance spectroscopy (EIS) and a selection of fluorescence and diffraction techniques using synchrotron radiation at the Advanced Photon Source (APS) are being employed.

Detailed characterizations of oxides are only useful if the observations can be linked to the corrosion behavior of the alloy. That link requires a model of the corrosion mechanism. The modeling effort is designed to organize the data from the characterization studies in a self-consistent manner and link those observations to the corrosion behavior. The ultimate objective of this project is to link the characterization and theoretical modeling efforts to yield improved alloy specifications.

Keywords: Zirconium, Corrosion, Synchrotron Radiation, TEM, Electrochemical Impedance Spectroscopy

287. MONITORING THE DURABILITY PERFORMANCE OF CONCRETE IN NUCLEAR WASTE CONTAINMENT
$150,210
DOE Contact: T. P. Miller (301) 903-4517
Massachusetts Institute of Technology
Contact: F. Ulm (617) 253-3544

Concrete is commonly employed in radioactive waste disposal as an effective construction material for containment barriers, liners, and encasement of containers. The objective of this research is to develop the scientific knowledge and the appropriate engineering tools required to evaluate and quantify the durability performance of nuclear waste concrete containment subjected to the pessimistic chemical degradation scenario of calcium leaching. Monitoring the durability performance means here the quantitative assessment, in time and space, of the integrity of the containment during the entire storage period and requires the consideration of the multiple couplings between diffusion-dissolution of calcium and deformation and cracking.

With regard to the time-scale, the durability design of waste containers needs to consider some reference scenario of chemical degradation, in particular the pessimistic one of calcium leaching by pure water. This design scenario refers to the risk of water intrusion in the storage system. For the reference scenario at hand, it is generally assumed that concrete is subject to leaching by permanently renewed deionized water acting as a solvent. The calcium ion concentration in the interstitial pore solution leads to dissolution of the calcium bound in the skeleton of Portlandite Crystals, $Ca(OH)_2$, and calcium-silica-hydrates (C-S-H), with sharp dissolution fronts. This calcium leaching leads to a degradation of the mechanical properties of concrete (material strength, Young's modulus). Cracks increase the diffusivity of the calcium ions through the structure, and can lead to an acceleration of the chemical degradation, and hence to an acceleration of the overall structural aging kinetics. This process can lead to a closed loop of accelerated structural degradation.

Keywords: Nuclear Waste, Concrete, Mechanical Properties, Leaching

288. **DETERMINISTIC PREDICTION OF CORROSION DAMAGE IN HIGH LEVEL NUCLEAR WASTE**
$216,696
DOE Contact: T. P. Miller (301) 903-4517
SRI International Contact: G. Engelhardt
(650) 859-3671

This research involves developing deterministic models and associated computer codes for predicting the evolution of corrosion damage to high level nuclear waste (HLNW) containers. Safe disposal of our nation's HLNW represents one of the greatest technical challenges of the twentieth and twenty-first centuries. The principal challenge is to ensure isolation of the waste from the biosphere for periods up to 10,000 years under conditions that can only now be estimated. The lack of existing databases for the corrosion of candidate alloys over times that represent even a small fraction of the intended service life means that we cannot rely on empirical methods to provide the design, materials selection, and reliability assessment information that is required to assure the public that the technology chosen for the disposal of HLNW is effective and safe. Instead, only strategies based on the employment of deterministic models can be used, because the natural laws (laws of conservation) that are the foundation of these models constrain the solutions to physical reality and are invariant with time.

Existing deterministic models of general and localized corrosion allow us to predict the accumulation of corrosion damage in many systems. However, these models must be customized for predicting damage in HLNW canisters in a tuff repository. Thus, the influence of radiolysis on the corrosion potential and hence on the corrosion rate, for example, must be included in the models. Particular attention must be given to repassivation phenomena, because they eventually determine the extent of damage. Attempts to quantitatively describe localized corrosion damage without proper consideration of repassivation phenomena greatly underestimate the service lives of containers. It is also important to customize the models to the conditions to which the containers are expected to be exposed over the their design lives.

The principal objectives of this project are to:

- Develop deterministic models and associated computer codes for predicting the evolution of corrosion damage (i.e., "integrate' damage) to HLNW containers in the Yucca Mountain repository. Corrosion processes that will be considered include general corrosion (oxidation), pitting corrosion, crevice corrosion, and stress corrosion cracking.

- Develop deterministic methods for extrapolating corrosion rate data obtained under "accelerate" laboratory conditions to the field.

- Use the models to predict the fates of containers after exposure in the repository under various conditions (e.g., humid air, contact with dripping water, repository inundation).

It is evident that the first objective is the basis of the project, and that other objectives can be achieved only if deterministic models for predicting corrosion damage to HLNW containers are developed.

Keywords: Nuclear Waste, Corrosion

289. **EFFECTS OF WATER RADIOLYSIS IN WATER COOLED NUCLEAR REACTORS**
$429,604
DOE Contact: T. P. Miller (301) 903-4517
University of Notre Dame Contact: S. M. Pimblott
(219) 631-7151

The goal of this research program is to develop a model that describes the chemical effects of radiation on aqueous systems and on aqueous/solid interfaces at temperatures associated with nuclear power plants and the Advanced Light Water Reactor (ALWR). The program has four thrusts:

Radiation Chemistry Modeling - An experiment-and-calculation based model will be developed to predict yields of the oxidizing and reducing radicals and the molecular species H_2 and H_2O_2 in aqueous systems like those associated with the ALWR chemistry.

High Temperature and High LET Effects - Experiments will measure the effect of dose on yields of O_2 and H_2O_2 produced in radiolysis with g-rays electrons and with H^+, He^{2+} and O^{8+} (C^{6+}) ions.

Interfacial Effects of Radiation - Experiments will gather information about radiation effects at aqueous/oxide interfaces of importance in fields such as reactor pipe corrosion and in storage of spent nuclear fuel.

Low Energy Electrons at Zirconia and Iron Oxide Surfaces and Interfaces - UHV experiments performed at Pacific Northwest National Laboratory with low energy electrons and photons will be used to simulate the damage caused at interfaces caused by the cascade of reactive secondary electrons produced by high-energy radiation.

Keywords: Corrosion, Zirconia, Radiolysis, Radiation

290. **MAPPING FLOW LOCALIZATION PROCESSES IN DEFORMATION OF IRRADIATED REACTOR STRUCTURAL ALLOYS**
$214,000
DOE Contact: T. P. Miller (301) 903-4517
ORNL Contact: K. Farrell (865) 574-5059

The materials from which nuclear power reactors are constructed, namely ferritic steels for pressure vessels, austenitic stainless steel for core internals and piping, and zirconium alloys for fuel cladding and tubing, are normally quite ductile and workable. They are ductile because they undergo plastic flow, or deformation, by the generation and movement of dislocations on slip planes within the atomic lattice of the metal. Many intersecting slip planes are operative. The dislocations can move from one slip plane to another and they become entangled into a three-dimensional network of dislocation cells. This ability to develop a network of dislocation cells ensures that the material work hardens and deforms in a homogenous manner. That ability is lost when the materials are exposed to the action of penetrating neutrons in the reactor. The neutrons create disturbed regions in the regular arrangement of atoms in the atomic lattice. These disturbed regions, or radiation damage clusters, impede the slip dislocations and inhibit the formation of dislocation cells. Instead, the deformation becomes localized in narrow bands or channels, and sometimes in twin bands. This intensification of strain and stress by dislocation channel deformation (DCD) changes the mechanical properties of the material and causes embrittlement. The degree of embrittlement is related to the nature and the details of the dominant deformation mode, which are functions of the radiation exposure and of the mechanical test conditions.

Most mechanical property data for use in design data banks is derived from tensile tests. Radiation damage raises the tensile yield strength and UTS, induces yield point drops in materials that do not normally show sharp yield points, reduces the work hardening rate and the elongation, and causes premature plastic instability and failure. All of these changes are now known or suspected to involve DCD but only a few quantitative correlations have been made. If such correlations are made in detail they can allow preparation of deformation mode maps in which the regions and boundaries of the deformation modes are plotted in terms of plastic strain and neutron fluence. Mechanical properties representing the different deformation modes can be overlaid on the maps, and the maps become pictorial repositories of knowledge relevant to the irradiation behavior of the materials. These maps will not only simplify, condense, verify and specify essential properties and applications limits for crucial reactor components, but they will add immeasurably to our understanding of the interplay between radiation damage microstructures, deformation modes and mechanical properties responses. They should bring cohesion and assurance into the processes of selection, assessment, and application of reactor materials. Presently, deformation mode maps for irradiated materials exist only for nickel and gold. The goal of this project is to determine deformation mode maps for A533B ferritic steel, 316 stainless steel, and Zircaloy-4 alloy.

Keywords: Mechanical Properties, Stainless Steel, Zircaloy, Radiation

291. **A NOVEL APPROACH TO MATERIALS DEVELOPMENT FOR ADVANCED REACTOR SYSTEMS**
$148,124
DOE Contact: T. P. Miller (301) 903-4517
University of Michigan Contact: G. S. Was (734) 763-4675

Component degradation by irradiation is a primary concern in current reactor systems as well as advanced designs and concepts where the demand for higher efficiency and performance will be considerably greater. In advanced reactor systems, core components will be expected to operate under increasingly hostile (temperature, pressure, radiation flux, dose, etc.) conditions. The current strategy for assessing radiation effects for the development of new materials is impractical in that the costs and time required to conduct reactor irradiations are becoming increasingly prohibitive, and the facilities for conducting these irradiations are becoming increasingly scarce. The next generation reactor designs will require more extreme conditions (temperature, flux, fluence), yet the capability for conducting irradiations for materials development and assessment in the next 20 years is significantly weaker than over the past 20 years. Short of building new test reactors, what is needed now are advanced tools and capabilities for studying radiation damage in materials that can keep pace with design development requirements. The most successful of these irradiation tools has been high-energy (several MeV) proton irradiation. Proton irradiation to several tens of displacements per atom (dpa) can be conducted in a short amount of time (weeks), with relatively inexpensive accelerators, and result in negligible residual radioactivity. All of these factors combine to provide a radiation damage assessment tool that reduces the time and cost to develop and assess reactor materials by factors of 10 to 100. What remains to be accomplished is the application of this tool to specific materials problems and the extension of the technique to a wider range of problems in preparation for advanced reactor materials development and assessment.

The objective of this project is to identify the material changes due to irradiation that affect stress corrosion cracking (IASCC) of stainless steels, embrittlement of pressure vessel steels and corrosion and mechanical properties of Zircaloy fuel cladding. Until such changes are identified, no further progress can be made on identifying the mechanisms and solving the problems. An understanding of the mechanisms will allow for the development of mitigation strategies for existing core components and also the development of radiation-resistant alloys or microstructures that are essential for the success of advanced reactor designs.

Keywords: Stress Corrosion Cracking, Proton Irradiation, Zircaloy, TEM

292. **AN INVESTIGATION OF THE MECHANISM OF IGA/SCC OF ALLOY 600 IN CORROSION ACCELERATING HEATED CREVICE ENVIRONMENTS**
$290,059
DOE Contact: T. P. Miller (301) 903-4517
Rockwell Science Center, LLC Contact:
J. Lumsden, III (805) 373-4136

The concentrated solutions and deposits in tube/tube support plate crevices of nuclear steam generators have been correlated with several forms of corrosion on the outer secondary side of Alloy 600 steam generator tubes including intergranular attack/stress corrosion cracking (IGA/SCC), pitting, and wastage. Crevice chemistries in an operating steam generator cannot be measured directly because of their inaccessibility. In practice, computer codes, which are based upon hypothesized chemical reactions and thermal hydraulic mechanisms, are used to predict crevice chemistry. The objective of the Rockwell program is to provide an experimental base to benchmark crevice chemistry models, to benchmark crevice chemistry control measures designed to mitigate IGA/SCC, and to model IGA/SCC crack propagation processes. The important variables will be identified, including the relationship between bulk water chemistry and corrosion accelerating chemistries in a crevice. One important result will be the identification of water chemistry control measures needed to mitigate secondary side IGA/SCC in steam generator tubes. A second result will be a system, operating as a side-arm boiler, which can be used to monitor nuclear steam generator crevice chemistries and crevice chemistry conditions causing IGA/SCC.

Keywords: Stress Corrosion Cracking, Nickel-Base Alloys, Corrosion, Steam Generator

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

293. **NOVEL CONCEPTS FOR DAMAGE-RESISTANT ALLOY IN NEXT GENERATION NUCLEAR POWER SYSTEMS**
$530,000
DOE Contact: T. P. Miller (301) 903-4517
PNNL Contact: S. M. Bruemmer (509) 376-0636

The objective of the research is to develop the scientific basis for a new class of radiation-resistant materials to meet the needs for higher performance and extended life in next generation power reactors. New structural materials are being designed to delay or eliminate the detrimental radiation-induced changes that occur in austenitic alloys, i.e., a significant increase in strength and loss in ductility (<10 displacements per atom (dpa)), environment-induced cracking (<10 dpa), swelling (<50 dpa), and embrittlement (<100 dpa). Non-traditional approaches are employed to ameliorate the root causes of materials degradation in current light water reactor (LWR) systems. Changes in materials design are based on mechanistic understanding of radiation damage processes and environmental degradation and the extensive experience of the principal investigators with core component response.

Keywords: Alloy Development, Ion Irradiation, Nuclear Reactor Materials

294. **ADVANCED CERAMIC COMPOSITES FOR HIGH-TEMPERATURE FISSION REACTORS**
$250,000
DOE Contact: T. P. Miller (301) 903-4517
PNNL Contact: R. H. Jones (509) 376-4276

This research seeks to develop the understanding needed to produce radiation-resistant SiC/SiC composites for advanced fission reactor applications. Structural and thermal performance of SiC/SiC composites in a neutron radiation field depends primarily on the radiation-induced defects and internal stresses resulting from this displacement damage. The researchers are working to develop comprehensive models of the thermal conductivity, fiber/matrix interface stress and mechanical properties of SiC/SiC composites as a function of neutron fluence, temperature, and composite microstructure. This model will be used to identify optimized composite structures that result in the maximum thermal conductivity and mechanical properties in a fission neutron field.

Keywords: SiC, Ceramic Composites, Nuclear Reactor Materials, Mechanical Properties

295. **DEVELOPMENT OF IMPROVED BURNABLE POISONS FOR COMMERCIAL NUCLEAR POWER REACTORS**
$389,000
DOE Contact: T. P. Miller (301) 903-4517
ORNL Contact: M. L. Grossbeck (865) 574-5065

Burnable poisons are used in nuclear reactors to aid in reactivity control and to reduce power peaking. The materials used at the present time suffer from two common disadvantages. The first is that the elements currently used, such as gadolinium and boron result in a small residual negative reactivity. Ideally, the burnable poison should be entirely depleted by the time the fuel is depleted. In fact, some burnable poison or isotopes that result from neutron absorption in the burnable poison remain at the time of fuel depletion and serve to limit the amount of fuel that can be used. The second is that boron transmutes to helium, which creates undesirable internal fuel pin pressures. Elimination or reduction of these two effects will lead to higher fuel burnup and longer core life resulting in lower cost of operation.

For many absorbing elements, such as gadolinium, it is isotopes other than the primary absorber that lead to residual reactivity. A goal of this research is to investigate the possibility of separating isotopes to isolate the absorbing isotope of interest, thus reducing or eliminating the residual reactivity. Absorbing elements such as samarium, gadolinium, dysprosium, and other identified candidates are being considered. State of the art two-dimensional computer codes will be used to determine the effects of the new burnable poisons, in both homogeneous and self-shielded configurations, on reactivity and core safety parameters. The second phase of the project will investigate isotope separation by the plasma separation process, and test separations will be attempted. In the final phase of the project, product forms determined from phase one will be fabricated using techniques of ceramic processing.

Keywords: Burnable Poisons, Nuclear Reactor Fuel

296. **FUEL FOR A ONCE-THROUGH CYCLE (TH, U) O_2 IN A METAL MATRIX**
$360,008
DOE Contact: T. P. Miller (301) 903-4517
ANL Contact: S. M. McDeavitt (630) 252-4308

Metal-matrix cermet nuclear fuels have potential for use in a once through, high-burnup, proliferation resistant fuel cycle. This project combines the advantages to be gained from cermet fuel with the resources extension potential of the thorium oxide fuel cycle and the inherent proliferation resistance of mixed oxide ceramics. These advantages fit well with the DOE's focus on the development of Generation IV nuclear power systems and proliferation resistant fuel cycles. The goal of this project is to demonstrate the feasibility of a metal-matrix fuel comprising $(Th,U)O_2$ microspheres in a zirconium matrix that can achieve high-burnup and be directly disposed as nuclear waste.

Keywords: Nuclear Reactor Fuel, Cermet, Thorium Oxide

297. **ADVANCED PROLIFERATION RESISTANT, LOWER COST, URANIUM-THORIUM DIOXIDE FUELS FOR LIGHT WATER REACTORS**
$1,161,848
DOE Contact: T. P. Miller (301) 903-4517
INEEL Contact: P. E. MacDonald (208) 525-9634

The overall object of this project is to evaluate the efficacy of high burnup mixed thorium-uranium dioxide (ThO_2-UO_2) fuels for light water reactors (LWRs). A mixed thoria-urania fuel that can be operated to a relatively high burnup level in current and future LWRs may have the potential to: (1) improve fuel cycle economics (allow higher sustainable plant capacity factors); (2) improve fuel performance; (3) increase proliferation resistance; and (4) be a more stable and insoluble waste product than UO_2.

One of the important goals of this project is to study fuels that would be assembly-for-assembly compatible with the fuel in current LWRs. This implies that both utilities and vendors would find this fuel acceptable for manufacturing and use in current LWRs, if the economics prove to be desirable.

Keywords: Thorium-Uranium Dioxide, Nuclear Fuel

298. **DEVELOPMENT OF A STABILIZED LIGHT WATER REACTOR (LWR) FUEL MATRIX FOR EXTENDED BURNUP**
$357,056
DOE Contact: T. P. Miller (301) 903-4517
PNNL Contact: B. D. Hanson (509) 376-3760

The main objective of this project is to develop an advanced fuel matrix based on the currently licensed UO_2 structure capable of achieving extended burnup while improving safety margins and reliability for present operations. Burnup is currently limited by the fission gas release and associated increase in fuel rod internal pressure, fuel swelling, and by cladding degradation. Once fuels exceed a threshold burnup, a "rim" or high burnup structure (HBS) forms. The HBS is characterized by the development of a subgrain microstructure having high porosity and low thermal conductivity. It is believed that the lower thermal conductivity results in larger temperature gradients and contributes to subsequent fission gas release. Fuel designs that decrease the centerline temperature while limiting the HBS restructuring, thereby decreasing the fission gas release should be able to achieve higher burnup and even allow higher operating power for increased efficiency.

Research at Pacific Northwest National Laboratory (PNNL) has demonstrated that the soluble fission products and actinides present in the matrix of irradiated (spent) fuels stabilized the fuel matrix with respect to oxidation to U_3O_8. The higher the soluble dopant concentration, the more resistant the fuel has been to undergoing the restructuring of the matrix from the cubic phase of UO_2 to the orthorhombic U_3O_8 phase. In this project, the attempt is to utilize the changes in fuel chemistry that result from doping the fuel to design a fuel that minimized HBS formation. The use of dopants that can act as getters of free oxygen and fission products to minimize fuel-side corrosion of the cladding is also being studied.

In addition to the use of dopants, project researchers are studying techniques such as the use of large grain sizes and radial variations in enrichment to minimize HBS formation and fission gas release. In this project, a combination of modeling and experimental studies is being used to determine the optimum design.

Keywords: Uranium Oxide, Nuclear Fuel, Phase Stability

299. **CONTINUOUS FIBER CERAMIC COMPOSITE CLADDING FOR COMMERCIAL WATER REACTOR FUEL**
$156,221
DOE Contact: T. P. Miller (301) 903-4517
Gamma Engineering Corporation Contact: H. Feinroth (301) 840-8415

The objective of this project is to study the use of advanced ceramic materials as cladding for water reactor fuel elements, and to determine, via engineering type tests, the feasibility of substituting such advanced ceramic materials for the Zircaloy cladding now in use. The ceramic materials to be developed and tested in this research program are known as oxide-based continuous fiber ceramic composites (CFCC's).

Oxide-based CFCC's have three main characteristics that recommend them for water reactor nuclear fuel cladding application. First, because CFCC's consist of very strong, micron sized fibers in a dense ceramic matrix, they do not behave in a brittle manner. Instead they have a failure mode that is non-catastrophic and similar to metals. Second, CFCC's retain their strength to much higher temperatures (e.g. >2000°F) as compared to metals such as zircaloy, which lose much of their strength above 1000°F. And third, oxide-based CFCC's (as opposed to carbide and nitride based CFCC's) remain chemically passive in high temperature steam. Thus, they do not react violently with water during a hypothetical Loss of Coolant Accident (LOCA), they do not produce heat during such an accident, and they do not produce hydrogen gas. Such characteristics, if applied to cladding in commercial water reactors, would lead to significant reductions in the consequences of low probability core overheating accidents, such as LOCA's. This could lead to improved and simplified reactor plant designs, simplified regulatory criteria, and improved public acceptance of nuclear power resulting from real reduction in residual risk.

This project seeks to address the feasibility of using CFCC's as reliable fuel cladding. Its aim is to determine the feasibility of providing an improved water reactor fuel element which is significantly more resistant to damage during a LOCA accident than is the current water reactor fuel element. Specifically, the goals for the project are to (1) evaluate and select two or three specific oxide based CFCC materials which have the potential to meet LWR fuel cladding requirements (2) fabricate LWR fuel clad test specimens from such materials using advanced CFCC fabrication techniques (3) conduct in-pile corrosion tests on these specimens, along with standard zircaloy specimens, and (4) expose such specimens to simulated LOCA test conditions to confirm their superior performance during LOCA accident conditions.

Keywords: Continuous Fiber Ceramic Composites, Nuclear Fuel, Corrosion

300. **AN INNOVATIVE CERAMIC CORROSION PROTECTION SYSTEM FOR ZIRCALOY CLADDING**
$198,226
DOE Contact: T. P. Miller (301) 903-4517
University of Florida Contact: R. H. Baney (352) 392-5167

The operational lifetime of current Light Water Reactor (LWR) fuel is limited by thermal, chemical, and mechanical constraints associated with the fuel rods being used to generate nuclear heat. A primary limiting factor of this fuel is the waterside corrosion of the zirconium based alloy cladding surrounding the uranium pellet. This research project intends to develop thin ceramic films with adhesive properties to the metal cladding in order to eliminate the oxidation and hydriding of Zircaloy cladding. The corrosion protection system will allow fuel to operate safely at significantly higher burnups resulting in major benefits to plant safety and plant economics.

A major technical challenge for coating a metal with a ceramic protection system is to develop a cohesive bond between the two materials. The differences between the thermal expansion of the ceramic coating and the thermal expanding metal can, if not properly addressed, interfere with the ceramic's ability to maintain a bond and thus maintain a protective layer.

Keywords: Zircaloy, Ceramic Coating, Corrosion, Nuclear Fuel

301. **A SINGLE MATERIAL APPROACH TO REDUCING NUCLEAR WASTE VOLUME**
$210,000
DOE Contact: T. P. Miller (301) 903-4517
ANL Contact: J. V. Beitz (630) 252-7393

This project is developing an innovative single material, minimum volume approach for the selective sorption of metal ion radionuclides from aqueous waste solutions and creation of a final nuclear waste form that is suitable for long term storage or geological burial. The project is based on a chemically functionalized porous silica that is termed Diphosil. Diphosil was created as an ion exchange medium that selectively and nearly irreversibly sorbs highly charged metal ions, such as actinides, from appreciably acidic aqueous solutions. The chelating power of Diphosil is due to diphosphonic acid groups that are anchored to its silica surface via organic spacer groups. Approximately 90% of the weight of dry Diphosil is silica (SiO_2).

Underlying this project is the hypothesis that heating metal ion-loaded Diphosil in air will oxidize its organic content to water vapor and carbon dioxide and its phosphonic acid groups to phosphoric acid that would react with the sorbed metal ions to give metal phosphates. Based on literature reports of the properties of porous silica, it was further hypothesized that additional heating would either volatilize any excess phosphoric acid or cause it to react with the silica to form silicon phosphates. At still higher temperature, pore collapse should occur thereby microencapsulating and chemically fixing the sorbed metal ions in phosphate-rich metal phases in vitreous silica. Vitreous silica is one of the most radiation resistant glasses known.

Keywords: Nuclear Waste, Silica, Ion Exchange

302. **DEVELOPING IMPROVED REACTOR STRUCTURAL MATERIALS USING PROTON IRRADIATION A RAPID ANALYSIS TOOL**
$400,000
DOE Contact: T. P. Miller (301) 903-4517
ANL Contact: T. R. Allen (208) 533-7760

The purpose of this program is to design advanced reactor materials with improved resistance to void swelling and irradiation assisted stress corrosion cracking (IASCC) using three principal methods: bulk composition engineering, grain boundary composition engineering, and grain boundary structural engineering. The focus of the first year was bulk compositional engineering in which five different alloying additions were made to a base Fe-18Cr-8Ni-1.25Mn alloy whose bulk composition corresponds to 304 stainless steel. This alloy was chosen as the reference alloy for the program because 304 stainless steel is known to be susceptible to both swelling and IASCC. In addition to the studies on bulk composition engineering, work commenced on the grain boundary structural engineering. Thermomechanical treatments were developed for the Fe-18Cr-8Ni-1.25Mn alloy that increased the fraction of coincidence site lattice (CSL) boundaries.

Each of the bulk composition alloying additions was chosen for a specific purpose. Fe-18Cr-40Ni-1.25Mn was chosen because higher bulk nickel concentration is known to reduce swelling, but its affect on IASCC is unknown. Fe-18Cr-8Ni-1.25Mn+Zr was chosen because Zr is an oversized element that might trap point defects and prevent swelling and grain boundary segregation. Fe-16Cr-13Ni-1.25Mn, Fe-16Cr-13Ni-1.25Mn+Mo, and Fe-16Cr-13Ni-1.25Mn+Mo+P were chosen to determine why 316 stainless steel is more resistant to swelling and IASCC than 304 stainless steel.

Keywords: Proton Irradiation, Swelling, Environmental Cracking, Alloy Development

NATIONAL NUCLEAR SECURITY ADMINISTRATION

	FY 2000
NATIONAL NUCLEAR SECURITY ADMINISTRATION - GRAND TOTAL	**$116,511,000**
OFFICE OF NAVAL REACTORS	**$74,500,000[1]**
OFFICE OF DEFENSE PROGRAMS	**$42,011,000**
THE WEAPONS RESEARCH, DEVELOPMENT AND TEST PROGRAM	**$42,011,000**
SANDIA NATIONAL LABORATORIES	**$15,432,000**
MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING	**$8,094,000**
Scientifically Tailored Materials	2,180,000
Materials Processing	2,585,000
Atomic-scale Studies of Surface Defect Chemistry	476,000
Exploiting Lens Technology Through Novel Materials	526,000
Functional Materials for Microsystems: Smart Self-assembled Photochromic Films	293,000
Self-healing Molecular Assemblies for Control of Friction and Adhesion in MEMS	365,000
Self-assembled Templates for Fabricating Novel Nano-arrays and Controlling Materials Growth	324,000
Next-generation Output-based Process Control	245,000
Functional Materials for Electrochemomechanical Actuation of Micro-valves and Micro-pumps	192,000
Switchable Hydrophobic-Hydrophilic Surfaces	335,000
Nanostructured Materials Integrated in Microfabricated Optical Devices	302,000
All-ceramic Thin Film Battery	271,000
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING	**$5,959,000**
Aging and Reliability	2,100,000
Precipitate Strengthening by Nanoparticles in Ni: NiO and Al_2O_3 Precipitates	300,000
Identification of Diffusing Species During Copper Corrosion	400,000
Stress Relaxation to Form Amorphous Diamond MEMS	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
Molecular Characterization of Energetic Material Initiation	44,000
Innovative Experimental and Computational Diagnostics for Monitoring Corrosion in Weapons Environments	218,000
Linking Atomistic Computations with Phase Field Modeling	229,000
A Combinatorial Microlab Investigation of Critical Copper-corrosion Mechanisms	489,000
Microscale Shock Wave Physics Using Photonic Driver Techniques	288,000
Wetting and Spreading Dynamics of Solder and Braze Alloys	486,000

[1]This excludes $49.9 million for the cost of irradiation testing in the Advanced Test Reactor (ATR).

NATIONAL NUCLEAR SECURITY ADMINISTRATION (Continued)

	FY 2000
OFFICE OF DEFENSE PROGRAMS (CONTINUED)	
THE WEAPONS RESEARCH, DEVELOPMENT AND TEST PROGRAM (CONTINUED)	
SANDIA NATIONAL LABORATORIES (CONTINUED)	
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING (CONTINUED)	
Improved Materials Aging Diagnostics and Mechanisms Through 2d Hyperspectral Imaging Methods and Algorithms	260,000
Making the Connection Between Microstructure and Mechanics	245,000
DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING	$249,000
Non-volatile Protonic Memory	249,000
INSTRUMENTATION AND FACILITIES	$1,130,000
Advanced Analytical Techniques	1,130,000
LOS ALAMOS NATIONAL LABORATORY	$19,951,000
Enhanced Surveillance Campaign	19,951,000
LAWRENCE LIVERMORE NATIONAL LABORATORY	$6,628,000
MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING	$2,940,000
Engineered Nanostructure Laminates	1,500,000
Energetic Materials Strategic Chemistry	350,000
Cheetah Thermochemical Code	190,000
Explosives Development	900,000
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING	$688,000
Interfaces, Adhesion, and Bonding	288,000
Laser Damage: Modeling and Characterization	400,000

NATIONAL NUCLEAR SECURITY ADMINISTRATION (Continued)

	FY 2000
OFFICE OF DEFENSE PROGRAMS (CONTINUED)	
THE WEAPONS RESEARCH, DEVELOPMENT AND TEST PROGRAM (CONTINUED)	
LAWRENCE LIVERMORE NATIONAL LABORATORY (CONTINUED)	
INSTRUMENTATION AND FACILITIES	$3,000,000
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	1,000,000
Beryllium Ablator Coatings for NIF Targets	600,000

NATIONAL NUCLEAR SECURITY ADMINISTRATION

The mission of the National Nuclear Security Administration is:

- To enhance United States national security through the military application of nuclear energy.
- To maintain and enhance the safety, reliability and performance of the U.S. nuclear weapons stockpile, including the ability to design, produce and test, in order to meet national security requirements.
- To provide the U.S. Navy with safe, militarily effective nuclear propulsion plants and to ensure the safe and reliable operation of those plants.
- To provide international nuclear safety and nonproliferation.
- To reduce global danger from weapons of mass destruction.
- To support U.S. leadership in science and technology.

OFFICE OF NAVAL REACTORS

The Deputy Administrator for Naval Reactors within the National Nuclear Security Administration is responsible for conducting requirements under Section 309(a) of the Department of Energy Organization Act which assigns civilian power reactor programs and all DOE naval nuclear propulsion functions. Executive Order 12344, as set forth in Public Law 106-65, stipulates responsibilities and authority of the Naval Nuclear Propulsion Program, of which the Deputy Administrator for Naval Reactors is a part.

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 $124.4 million in FY2000. Approximately $49.9 million represents the cost for irradiation testing in the Advanced Test Reactor. The Naval Reactors contact is David I. Curtis, (202) 264-8124.

OFFICE OF DEFENSE PROGRAMS

The Deputy Administrator for Defense Programs within the National Nuclear Security Administration is responsible for carrying out national security objectives established by the President for nuclear weapons and assisting in reducing the global nuclear danger by planning for, maintaining and enhancing the safety, reliability and performance of the U.S. stockpile of nuclear weapons and associated materials, capabilities and technologies in a safe, environmentally sound, and cost-effective manner.

The Deputy Administrator for Defense Programs also directs all defense weapons programs and projects at the Los Alamos National Laboratory, Los Alamos, New Mexico; Sandia National Laboratories, Albuquerque, New Mexico and Livermore, California; Lawrence Livermore National Laboratory, Livermore, California; the Kansas City Plant, Kansas City, Missouri; the Pantex Plant, Amarillo, Texas; Y-12 Plant at Oak Ridge, Tennessee; the tritium operations facilities at Savannah River, Aiken, South Carolina, and the Nevada Test Site, Nevada.

THE WEAPONS RESEARCH, DEVELOPMENT AND TEST PROGRAM

SANDIA NATIONAL LABORATORIES

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

303. **SCIENTIFICALLY TAILORED MATERIALS**
$2,180,000
DOE Contact: Bharat Agrawal (301) 903-2057
SNL Contact: Ken Wilson (925) 294-2497

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 polymeric materials and materials for microsystems.

Keywords: New Materials, Materials by Design, Polymeric Materials, Materials for Microsystems

304. **MATERIALS PROCESSING**
$2,585,000
DOE Contact: Bharat Agrawal (301) 903-2057
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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 the theme areas of Joining/ Solidification Science and Advanced/Innovative Processes.

Keywords: Processing, Fabrication, Joining, Solidification, Advanced Materials Processing

305. **ATOMIC-SCALE STUDIES OF SURFACE DEFECT CHEMISTRY**
$476,000
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

306. **EXPLOITING LENS TECHNOLOGY THROUGH NOVEL MATERIALS**
$526,000
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

307. **FUNCTIONAL MATERIALS FOR MICROSYSTEMS: SMART SELF-ASSEMBLED PHOTOCHROMIC FILMS**
$293,000
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

308. SELF-HEALING MOLECULAR ASSEMBLIES FOR CONTROL OF FRICTION AND ADHESION IN MEMS
$365,000
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

309. SELF-ASSEMBLED TEMPLATES FOR FABRICATING NOVEL NANO-ARRAYS AND CONTROLLING MATERIALS GROWTH
$324,000
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

310. NEXT-GENERATION OUTPUT-BASED PROCESS CONTROL
$245,000
DOE Contact: Gerald Green (202) 586-8377
SNL Contact: Duane Dimos (505) 844-6385

The goal of process-based quality is to accept WR product without inspection. For simple processes, traditional feedback control of process input variables might achieve this goal. However, input-based control systems are a major source of DP production problems for complex processes, because it is impractical, if not impossible, to control all of the factors that affect process output. We are utilizing recent advances in sensor technology, process modeling, intelligent data analysis, and computing power to develop a broadly applicable next-generation control technology that monitors and controls process output rather than input.

Keywords: Process Control, Sensors, Process Modeling, Intelligent Data Analysis

311. FUNCTIONAL MATERIALS FOR ELECTROCHEMOMECHANICAL ACTUATION OF MICRO-VALVES AND MICRO-PUMPS
$192,000
DOE Contact: Gerald Green (202) 586-8377
SNL Contact: Jill Hruby (925) 294-2596

It is generally recognized that integrated microsystems for DP applications, chemical sensing, and medical devices will not be possible without development of fast and efficient microactuators that can be used as valves and pumps. Conventionally actuated devices can affect the operating characteristics of microsystems and cannot be miniaturized without significant loss in performance. We propose to take advantage of ElectroChemoMechanical (ECM) functions of conductive polymers to be used as the work-producing unit in microactuators. The focus of the work is threefold. First, molecular structure and composition of conductive polymer gels will be tailored to maximize physical/mechanical response to electrochemical stimulation. Secondly, computational modeling, a key component of this proposal, will complement the formulation development. Lastly, polymer actuator geometry and microelectrodes will be designed, build and tested to optimize microscale performance.

Keywords: Microsystems, Sensors, Microactuators, Conducting Polymers

312. **SWITCHABLE HYDROPHOBIC-HYDROPHILIC SURFACES**
$335,000
DOE Contact: Gerald Green (202) 586-8377
SNL Contact: Terry Michalske (505) 844-5829

The ability to perform chemical and biological analyses on a microchip requires understanding how to transport, separate, and detect species in nanoliter quantities of liquid confined in channels having dimensions of microns. At such small length scales, surface effects play a dominant role. If smart coatings could be developed whose surface properties and chemical interactions could be switched in a controlled fashion, it might be possible to create complete analytical systems within a simple architecture of interconnected channels. It has been shown that fluids can be pumped and mixed in microchannels by manipulating whether the channel surfaces repel or attract water. Switching of interfacial energies could also be used to control selective adsorption for advanced separations and sensor devices. The objective of this proposal is to investigate mechanisms for switching the interfacial energies of organic coatings using phase transitions induced via on-chip stimuli.

Keywords: Microsystems, Chemical Analysis, Biological Analysis, Organic Materials

313. **NANOSTRUCTURED MATERIALS INTEGRATED IN MICROFABRICATED OPTICAL DEVICES**
$302,000
DOE Contact: Gerald Green (202) 586-8377
SNL Contact: Terry Michalske (505) 844-5829

We combine the emerging strength of nanocomposite materials at Sandia with the recognized expertise and processing capabilities involving microfabricated optical device structures for the development of microsensor arrays and unique tunable micro-optical devices. The project involves the design, development, and characterization of molecular (nanoscale) to micron scale structures to achieve desired material and device function. At the core of the material is a liquid crystalline (LC) lipid bilayer that mimics the properties of a biological cell membrane. The bilayer is functionalized with molecular receptors, for specific recognition of chemical and biological species, and optical reporters that signal the occurrence of the recognition event. These molecular and supramolecular structures will be supported on a structurally oriented, mesoporous, inorganic matrix. Together, the materials form a unique nanocomposite with molecularly dynamic organic components for rapid optical response to specific analytes coupled to a robust inorganic scaffold with highly defined and tunable surface area and pore volume.

Keywords: Microsensor Arrays, Microsystems, Nanocomposites

314. **ALL-CERAMIC THIN FILM BATTERY**
$271,000
DOE Contact: Gerald Green (202) 586-8377
SNL Contact: William F. Hammetter (505) 272-7603

Power sources that generate the necessary power and energy to operate microsystems without substantially increasing the size of the device are required to achieve autonomy. Thin film batteries are an attractive power source for these applications; however, currently they are inadequate to operate the microsystems effectively. We propose to develop a rechargeable thin film All-Ceramic Lithium-Ion Battery (ACB) using solution route deposition methods. The ACB will have higher power output, longer run times, and a greatly simplified production scheme in comparison to existing technology.

Keywords: Batteries, Microsystems, Thin Films, Lithium Ion Battery

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

315. **AGING AND RELIABILITY**
$2,100,000
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 thermomechanical degradation of solder joints and develop a methodology for measuring polymer degradation near room temperature.

Keywords: Aging, Reliability

316. **PRECIPITATE STRENGTHENING BY NANOPARTICLES IN Ni: NiO AND Al_2O_3 PRECIPITATES**
$300,000
DOE Contact: Bharat Agrawal (301) 903-2057
SNL Contact: J. Charles Barbour (505) 844-5517

In order to provide higher levels of mechanical work in small micro-electromechanical systems (MEMS), the yield strength of the component materials should be increased beyond the limits for conventional bulk materials. Several ways to meet this challenge are to invent new materials or to strengthen a given materials system. This work examines the underlying physics of these strengthening mechanisms. Ion implantation was utilized in this study because this technique has been shown to allow controlled modification of near-surface composition and microstructure leading to strengthening and reduced friction and wear. A scientific objective is to understand and quantify the relationship of mechanical properties to implantation-modified microstructure. Ion implantation of O and Al were used to form nanometer-size precipitates of NiO or Al_2O_3 in the near-surface of Ni. The yield strengths of the treated layers were determined by nanoindentation testing in conjunction with finite-element modeling. The strengths range up to ~5 GPa, substantially above values for hard bearing steels. These results agree quantitatively with predictions of dispersion-hardening theory based on the precipitate microstructures observed by transmission electron microscopy. Such surface hardening by ion implantation may be beneficial for Ni components in micro-electromechanical systems; their tribological properties will be investigated in the near future. Further, the agreement between conventional, particle-strengthening theory and the experimental results was found to be good agreement in absolute magnitude and in the variation among microstructures. Thus, it appears that the continuum analysis of hard-particle dispersion strengthening remains applicable for particle sizes and separations approaching 1 nm.

Keywords: Microsystems, Strengthening, Nanoparticle Dispersions

317. **IDENTIFICATION OF DIFFUSING SPECIES DURING COPPER CORROSION**
$400,000
DOE Contact: Bharat Agrawal (301) 903-2057
SNL Contact: J. Charles Barbour (505) 844-5517

The highest number of materials-related significant findings for the weapons stockpile are associated with corrosion of electronic components. Moreover, sulfidation of copper and copper alloys has proven to be one of the more important corrosion issues to arise repeatedly. Therefore, we have begun work to understand the corrosion mechanisms for copper and its alloys. Specifically, we seek to understand the copper sulfidation mechanisms in order to create a predictive model of electronic component life in the stockpile. As a first goal, the predominant diffusing species was identified for the sulfidation of copper exposed to both humid and dry atmospheres containing ~150 ppb H_2S as the sulfidizing component of the environment. These corrosion studies were done at room temperature. Marker experiments showed that for both dry and humid environments the copper was the fastest moving species in the system. The solid-state supply of copper through the growing sulfide layer was actually faster than the supply of sulfidizing species from the gas phase. Further, the growth kinetics showed that at low humidities the sulfidation continued linearly (consistent with a surface chemical reaction limited mechanism) to quite thick layers, greater than 1 micrometer in thickness. The growth kinetics at high humidity changed from linear to parabolic (consistent with a change to a solid-state diffusion limited mechanism) for a sulfide thickness of approximately 150-300 nm, and this change would actually limit the overall thickness of sulfide formed over long periods of time.

Keywords: Corrosion, Aging, Reliability

318. **STRESS RELAXATION TO FORM AMORPHOUS DIAMOND MEMS**
$300,000
DOE Contact: Bharat Agrawal (301) 903-2057
SNL Contact: J. 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 coefficients, and have extremely low wear rates, thus earning the name of amorphous diamond, a-D. One major limitation of these films is that very large compressive stresses (10 GPa) are generated during growth. 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 has emerged from this work and lead to the fabrication of microelectromechanical (MEMS) devices. Further, the ability to create multi-level a-D MEMS devices was demonstrated. Several new applications of a-D in the areas of MEMS were identified this year, including a-D membrane-based adaptive optic devices, MEMS microswitches, hybrid a-D/poly-Si MEMS structures, and a-D bioMEMS structures. These developments hinged on improving the deep etch process for fabricating a-D membranes, identifying new materials and processes to enable multi-level MEMS structures, and improving our understanding of structural relaxation in a-D that occurs with annealing. The basic materials research for some of these developments was performed using our fabricated MEMS structures, which is an effective demonstration of the utility of MEMS structures for enabling materials property measurements when no other direct measurement is possible. The MEMS-based measurements reveal that a-D is exceptionally stiff (with an elastic modulus exceeding 700 GPa, about 4.5 times that of Si) and strong (with a fracture strength of about 8 GPa, about 2 to 3 times that of Si) and there may be anisotropic ordering of the 3-fold and 4-fold carbon components in the film. Designs for advanced MEMS structures were also developed, including captured hubs which would permit the creation of rotating gear structures.

Keywords: Amorphous-Diamond, Stress, MEMS

319. **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. We have expanded our materials studies to include organic and inorganic/organic hybrid systems for specific NW applications. These materials offer greater photosensitivity, optical tuning and adjustable temperature response. Optical tuning in this context means being able to move the absorption regime of the materials into the visible region and so as to enable system designs which use rad-hard semiconductor light sources (e.g., VCSELs) to write channels 'on the fly'. For application as weak-links in NW systems, one needs a well-controlled temperature response and our research is aimed at materials having this capability as well. Our research has made progress in all of the above areas. 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

320. **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. Present emphasis is on shock-induced depoling of normally poled PZT 95/5 and a variant PSZT (also used in power supplies). Twenty-two experiments were conducted under a variety of shock-loading conditions. One-dimensional experiments examined how dielectric properties change under shock compression, differences in depoling characteristics in PZT 95/5 materials fabricated by a new "chem prep" process, and how cold temperatures (-60 C) affect depoling kinetics. Multi-dimensional experiments have examined depoling kinetics under the more complex shock loading conditions that occur in power supplies. The substantial database now available is being used to assess and improve our capabilities for numerically simulating the operation of pulsed power devices.

Keywords: Ferroelectrics, Shock Physics, Power Supplies

321. **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 $(Pb,Ba)(Zr,Ti,Bi)O_3$, or PBZT-Bi, which is used in explosively-driven pulsed power sources. The lattice disorder due to the substitution of Ba and Bi at the A and B sites, respectively, of the perovskite (ABO_3) produces dielectric properties qualitatively different from those of PZTs and other normal ferroelectrics. PBZT is a member of a class of materials referred to as relaxor ferroelectrics or relaxors. Recent studies have addressed related perovskite mixed-oxide relaxor ferroelectrics with B-site substitution, $Pb(Zn_{1/3}Nb_{2/3})O_3$-$xPbTiO_3$. In particular, PZN-9.5% PT is a composition near a morphotropic phase boundary separating tetragonal and rhombohedral structures at ambient temperature. This leads to a highly polarizable (soft) lattice and, thus, large electromechanical (piezoelectric) coupling and dielectric constant with applications in actuators and multilayer capacitors. The effects of temperature, hydrostatic pressure, frequency and biasing dc electric field have been measured for a single crystal of PZN-9.5% PT. These data provide a detailed view of the dynamics and energetics of the relaxation response of the polarization and the underlying physics that governs the exceptional dielectric properties in this material. One important result is a pressure-induced crossover from normal ferroelectric to relaxor ferroelectric behavior in PZN-PT that reflects a general feature of compositionally disordered soft mode ferroelectrics.

Keywords: Ferroelectrics, Performance Modeling, PBZT-Bi

322. **MOLECULAR CHARACTERIZATION OF ENERGETIC MATERIAL INITIATION**
$44,000
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

323. **INNOVATIVE EXPERIMENTAL AND COMPUTATIONAL DIAGNOSTICS FOR MONITORING CORROSION IN WEAPONS ENVIRONMENTS**
$218,000
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

324. **LINKING ATOMISTIC COMPUTATIONS WITH PHASE FIELD MODELING**
$229,000
DOE Contact: Gerald Green (202) 586-8377
SNL Contact: Stephen M. Foiles (505) 844-7064

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

325. **A COMBINATORIAL MICROLAB INVESTIGATION OF CRITICAL COPPER-CORROSION MECHANISMS**
$489,000
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 pH2O and pH2S, 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

326. **MICROSCALE SHOCK WAVE PHYSICS USING PHOTONIC DRIVER TECHNIQUES**
$288,000
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

327. WETTING AND SPREADING DYNAMICS OF SOLDER AND BRAZE ALLOYS
$486,000
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

328. IMPROVED MATERIALS AGING DIAGNOSTICS AND MECHANISMS THROUGH 2D HYPERSPECTRAL IMAGING METHODS AND ALGORITHMS
$260,000
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

329. MAKING THE CONNECTION BETWEEN MICROSTRUCTURE AND MECHANICS
$245,000
DOE Contact: Gerald Green (202) 586-8377
SNL Contact: Julia M. Phillips (505) 844-1071

The purpose of microstructural control is to optimize materials properties. To that end, we have developed sophisticated and successful computational models of both microstructural evolution and mechanical response. However there is currently no way to couple these models to quantitatively predict the properties of a given microstructure. The problem arises because continous response models, such as finite element, finite volume, or materials point methods, do not incorporate a real length scale. In this project, we are taking a tiered risk approach to incorporate microstructure and its resultant length scales in mechanical response simulations. The successful coupled model will predict both properties as a function of microstructure and microstructural development as a function of processing conditions.

Keywords: Microstructure, Mechanical Properties, Computational Materials Science

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

330. **NON-VOLATILE PROTONIC MEMORY**
$249,000
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

331. **ADVANCED ANALYTICAL TECHNIQUES**
$1,130,000
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

332. **ENHANCED SURVEILLANCE CAMPAIGN**
$19,951,000
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

The Stockpile Surveillance Program provides protection to the U.S. nuclear weapons stockpile by an intensive program that assures it is free of defects that may affect performance, safety, or reliability. It consists of two elements, the Stockpile Evaluation Program and the Enhanced Surveillance Campaign. The Stockpile Evaluation Program provides the examinations and assessments of WR stockpile weapons and components. The Enhanced Surveillance Program provides means to strengthen the Stockpile Evaluation Program to meet the challenges of an aging stockpile in an era of no nuclear testing as well as providing lifetime assessments and predictions for SLEP planning.

The Enhanced Surveillance Campaign will protect the health of the stockpile by providing advance warning of manufacturing and aging defects to allow refurbishment before performance is impaired. The Campaign will provide diagnostics for screening of weapons systems to identify units that must be refurbished as well as for early detection of defects. It will also predict material and component aging rates as a basis for annual certification, refurbishment scope and timing, and nuclear weapon complex planning. Results of the work will include improvements to the basic Surveillance Program. Since nuclear weapons will be retained in the stockpile for lifetimes beyond our experience, the Department of Energy (DOE) needs a firm basis on which to determine when stockpile systems must be refurbished or reconditioned. If new refurbishment capability is needed, the DOE needs to know: (1) when these capabilities must be operational and what the required capacity should be; (2) if the capacity for existing facilities is adequate and when potential refurbishment for the various stockpile systems must be scheduled; (3) a basis from which to characterize the functional reliability of aged components, as part of the annual assessment process

The work in the ES Campaign began in late FY97 and will be completed at the end of FY06. The principal milestones and deliverables (Level 1) for this campaign are: (1) performance predictions for highest risk non-nuclear components in FY03; (2) provide key diagnostics to surveillance program in FY01 through FY05; (3) provide a recommendation based on available data regarding the need for and capacity of a pit manufacturing facility in FY04; (4) determine aging behavior of materials used in microsystems in FY04; (5) provide basis for certification of aged components in FY06; (6) provide validated lifetime assessments for SLEP decision in FY06.

Our work is divided into six major technical elements (MTE): pits, CSAs/Cases, high explosives (HE), systems, non-nuclear components (NNC), and non-nuclear materials (NNM). The pit, CSA/Cases, and high explosives MTEs are each divided into two projects; lifetime assessments and diagnostics. The Systems MTE is divided into three projects; flight instrumentation, assessments/methodologies, and surveillance modernization. The Non-nuclear components MTE is divided into two projects; stockpile components and microsystems. The Non-nuclear materials MTE is divided into two projects; material lifetimes and advanced analytic techniques.

Complete details for the Enhanced Surveillance Campaign can be found in the ESC Program plan and the ESC Implementation plan updated on a yearly basis.

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

333. **ENGINEERED NANOSTRUCTURE LAMINATES**
$1,500,000
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 500 mm 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% of theory. Also, new mechanisms for mechanically strengthening materials are accessible with nanostructure laminates.

Applications now under development include: EUV, soft X-ray and X-ray optics for spectroscopy and imaging; high performance capacitors for energy storage; capacitor structures for industrial applications; high performance tribological coatings; high strength materials; integrated circuit interconnects; machine tool coatings; projection X-ray lithography optics.

Keywords: Thin Films, Multilayer Technology, Passive Electronic Devices, EUV, SXR and XR Optics, Optic Systems

334. **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

335. **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

336. **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

337. **INTERFACES, ADHESION, AND BONDING**
$288,000
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. Work includes both pure materials and materials doped with impurities. 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, Segregation

338. **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

339. **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

340. **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

341. **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

342. **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

343. **POLYIMIDE COATING TECHNOLOGY FOR ICF TARGETS**
$1,000,000
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 deposition based polyimide coating technology to produce a smooth 150 to 200 μm polyimide ablator coating on a 2mm diameter capsule target for the National Ignition Facility (NIF). The approach involves first vapor depositing monomeric species to form a polyamic acid coating on a spherical hollow mandrel. The surfaces of these coated mandrels are then smoothed by exposure to dimethyl sulfoxide vapor while being levitated on a nitrogen gas flow. The smoothed shells are then heated *in situ* to imidize the coatings. The focus of the past year has been improvement of the capsule surface finish.

Keywords: Polymers, Laser Fusion Targets, Polyimide, Ablator

344. **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 200 μm 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 by reducing grain size. Coating through apertures to reduce self-shadowing was studied, but the emphasis over the last year has been on studying ion bombardment during deposition. The effects of varying both the ion energy and the current density have been investigated.

Keywords: Beryllium, Laser Fusion Targets, Ablator, Sputter Deposition

OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT

	FY 2000
OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT - GRAND TOTAL	$29,121,295
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING	
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

345. **WASTE PACKAGES**
$29,121,295
DOE Contact: Paige Russell, (702) 794-1315
M&O Contacts: Larry Trautner, (702) 295-4414 and Robert Andrews, (702) 295-5549

The development of the nation's high-level waste repository has been delegated to DOE's Yucca Mountain Site Characterization 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. The current design was selected in 1999. Progress on the waste package and the supporting materials studies has been documented in various reports.

The waste package design effort includes the development of waste packages to accommodate uncanistered commercial spent nuclear fuel (SNF),canistered SNF, canistered defense high-level waste, Navy fuel, and other DOE-owned spent nuclear fuel. The analytical process that is underway to support these designs included thermal, structural, and neutronic analyses. Also included are materials selection and engineering development. The current design consists of a corrosion-resistant outer barrier of alloy 22 and a stainless steel inner shell, which provides structural support. The alloy 22 outer barrier has a thickness of 20 mm and the stainless steel inner shell is 50 mm thick. Titanium is still used 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 22 (UNS# N06022), titanium grade 7, and 316L stainless steel. 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 FY 1997. 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 FOSSIL ENERGY

	FY 2000
OFFICE OF FOSSIL ENERGY - GRAND TOTAL	$10,751,000
OFFICE OF ADVANCED RESEARCH	$10,751,000
FOSSIL ENERGY ADVANCED RESEARCH MATERIALS PROGRAM	$6,751,000
MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING	$2,021,000
Fabrication Technologies for Fuel Cell Applications	64,000
Intermetallic Reinforced Cr Alloys	145,000
Corrosion Protection of Ultrahigh Temperature Metallic Alloys	197,000
Mo-Si Alloy Development	119,000
Development of Modified Austenitic Alloys	199,000
Development of Recuperator Materials	85,000
Crada with INCO on High Creep Strength Alloys	50,000
Influence of Processing on Microstructure and Properties of Aluminides	170,000
Extended-Lifetime Metallic Coatings for High-Temperature Environmental Protection	211,000
Fabrication of Fiber-Reinforced Composites by Chemical Vapor Infiltration and Deposition	65,000
Development of Oxidation/ Corrosion-Resistant Composite Materials and Interfaces	219,000
Modeling for CVD of Solid Oxide Electrolyte	54,000
Development of a Commercial Process for the Production of Silicon Carbide Fibrils	80,000
Development of Hot Pressing as a Low-Cost Processing Technique for Fuel Cell Fabrication	82,000
Development of Novel Activated Carbon Composites	237,000
Carbon Fiber Composite Molecular Sieves Technology Transfer	44,000
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING	$1,022,000
Oxide Dispersion Strengthened (ODS) Alloys	235,000
Investigation of the Weldability of Polycrystalline Iron Aluminides	70,000
Friction Welding of ODS Alloys	15,000
Evaluation of the Intrinsic and Extrinsic Fracture Behavior of Iron Aluminides	30,000
Investigation of Iron Aluminide Weld Overlays	45,000
In-Plant Corrosion Probe Tests of Advanced Austenitic Alloys	80,000
Corrosion and Mechanical Properties of Alloys in FBC and Mixed-Gas Environments	175,000
Reduction of Defect Content in ODS Alloys	57,000
Support Services for Ceramic Fiber-Ceramic Matrix Composites	58,000
Reliable Ceramic Coatings for High-Temperature Environmental Resistance in Fossil Environments	82,000
Development of Nondestructive Evaluation Methods for Structural Ceramics	175,000

OFFICE OF FOSSIL ENERGY (continued)

	FY 2001
OFFICE OF ADVANCED RESEARCH (CONTINUED)	
FOSSIL ENERGY ADVANCED RESEARCH MATERIALS PROGRAM (CONTINUED)	
DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING	$3,708,000
Materials and Components in Fossil Energy Applications Newsletter	60,000[1]
Development of Ceramic Membranes for Hydrogen Separation	350,000
Proton Exchange Membranes for Hydrogen Separation	356,000
Solid State Electrolyte Systems for Fuel Cells and Gas Separation	730,000
Improved Fuel Cell Materials and Economical Fabrication	50,000
Efficient SOFC Electrolyte Fabrication	197,000
Bismuth Oxide Solid Electrolyte Oxygen Separation Membranes	257,000
Metallic Filters for Hot-Gas Cleaning	150,000
Refractory Materials Issues in Gasifiers	100,000
Pd-Ag Membranes for Hydrogen Separation	100,000
High-temperature Materials Testing in Coal Combustion Environments	500,000
Molecular Sieves for Hydrogen Separation	150,000
Systems Analysis of Processes Involving Hydrogen Separation Membrane	50,000
Oxide-dispersion-strengthened Fe_3Al-based Alloy Tubes	50,000
Development of ODS Alloy for Heat Exchanger Tubing	173,000
Fatigue and Fracture Behavior of Cr-X Alloys	29,000
Management of the Fossil Energy Advanced Research Materials Program	400,000
Gordon Research Conference Support	6,000
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, 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 ADVANCED RESEARCH MATERIALS PROGRAM

Fossil Energy materials-related research is conducted under the Advanced Research Materials Program. The goal of the Fossil Energy Advanced Research 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 heat exchanger applications; new corrosion- and erosion-resistant alloys with unique mechanical properties for advanced fossil energy systems; functional materials such as metal and ceramic hot-gas filters, gas separation materials based on ceramic membranes (porous and ion transport), fuel cells, and activated carbon materials; and corrosion research to understand the behavior of materials in coal-processing environments. In cooperation with DOE-ORO, Oak Ridge National Laboratory has the responsibility of the technical management and implementation of all activities on the DOE Fossil Energy Advanced Research Materials Program. DOE-FE administration of the Program is through the National Energy Technology Laboratory and the Advanced Research Product Team.

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

346. **FABRICATION TECHNOLOGIES FOR FUEL CELL APPLICATIONS**
$64,000
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Oak Ridge National Laboratory Contact: M. L. Santella (865) 574-4805

This task involves developing the materials, processes, and procedures that will be required to design and fabricate fuel cells. It directly addresses issues related to developing an economically viable Solid Oxide Fuel Cell (SOFC) system with acceptable lifetime and cost. The primary focus will be on developing and implementing joining technologies for producing the various metal-metal, ceramic-ceramic, and metal-ceramic connections required for producing cell stacks, containments, and other related structures. An immediate objective is to evaluate the use of iron aluminide alloys (Fe_3Al) for containment structures for high-temperature, solid oxide fuel cells.

Keywords: Alloys, Fuel Cells

347. **INTERMETALLIC REINFORCED Cr ALLOYS**
$145,000
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M. H. Rawlins (865) 576-4507
Oak Ridge National Laboratory Contacts:
M. P. Brady (865) 574-5153

The objective of this task is to develop high-strength, oxidation- and corrosion-resistant Cr alloys for use as hot components in advanced fossil energy conversion and combustion systems to help meet the 65% 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. These alloys are also potentially enabling in aggressive, high-temperature molten salt and slag environments, such as those encountered in gasification systems, for use in process monitoring (e.g. thermowells) and as structural components or protective coatings. The development effort will be devoted to in-situ composite alloys based on a Cr solid solution matrix reinforced with the Cr_2X (X = Nb, Ta, ...) Laves phase.

Keywords: Alloys, Chromium-Niobium, Corrosion, Intermetallic Compounds

348. **CORROSION PROTECTION OF ULTRAHIGH TEMPERATURE METALLIC ALLOYS**
$197,000
DOE Contacts: F. M. Glaser (301) 903-2784,
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M. H. Rawlins (865) 576-4507
Oak Ridge National Laboratory Contact:
P. F. Tortorelli (865) 574-5119

The objective of this task is to develop high-strength, oxidation- and corrosion-resistant Cr alloys for use as hot components in advanced fossil energy conversion and combustion systems to help meet the 65% 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. These alloys are also potentially enabling in aggressive, high-temperature molten salt and slag environments, such as those encountered in gasification systems, for use in process monitoring (e.g., thermowells) and as structural components or protective coatings. The development effort will be devoted to in-situ composite alloys based on a Cr solid solution matrix reinforced with the Cr_2X (X = Nb, Ta, ...) Laves phase.

Keywords: Coatings, Corrosion

349. **Mo-Si ALLOY DEVELOPMENT**
$119,000
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Oak Ridge National Laboratory Contact:
J. H. Schneibel (865) 574-4644
Ames Laboratory Contact: M. J. Kramer
(515) 294-0276

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

350. **DEVELOPMENT OF MODIFIED AUSTENITIC ALLOYS**
$199,000
DOE Contacts: F. M. Glaser (301) 903-2784,
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Oak Ridge National Laboratory Contact:
R. W. Swindeman (865) 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

351. **DEVELOPMENT OF RECUPERATOR MATERIALS**
$85,000
DOE Contacts: F. M. Glaser (301) 903-2784, V. U. S. Rao (412) 386-4743 and M. H. Rawlins (865) 576-4507
Oak Ridge National Laboratory Contact: R. W. Swindeman (865) 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

352. **CRADA WITH INCO ON HIGH CREEP STRENGTH ALLOYS**
$50,000
DOE Contacts: F. M. Glaser (301) 903-2784, V. U. S. Rao (412) 386-4743 and M. H. Rawlins (865) 576-4507
Oak Ridge National Laboratory Contact: P. J. Maziasz (865) 574-5082

This activity was a collaborative work with INCO Alloys to develop an improved version of Alloy 803 .

Keywords: Alloys

353. **INFLUENCE OF PROCESSING ON MICROSTRUCTURE AND PROPERTIES OF ALUMINIDES**
$170,000
DOE Contacts: F. M. Glaser (301) 903-2784, V. U. S. Rao (412) 386-4743 and M. H. Rawlins (865) 576-4507
Oak Ridge National Laboratory Contact: I. G. Wright (865) 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

354. **EXTENDED-LIFETIME METALLIC COATINGS FOR HIGH-TEMPERATURE ENVIRONMENTAL PROTECTION**
$211,000
DOE Contacts: F. M. Glaser (301) 903-2784, V. U. S. Rao (412) 386-4743 and M. H. Rawlins (865) 576-4507
Oak Ridge National Laboratory Contact: P. F. Tortorelli (865) 574-5119

The purpose of this task is to examine important composition and microstructure issues associated with the development of extended-lifetime corrosion-resistant metallic coatings for high-temperature applications associated with the key technologies of the Office of Fossil Energy's Vision 21 concept. Two linked technical objectives support this purpose. They are (1) for a given fossil environment, establishment of the coating composition and microstructure necessary for long-term high-temperature corrosion protection and (2) determination of the relationships among composition, microstructure, and a coating method.

Keywords: Coatings, Corrosion

355. **FABRICATION OF FIBER-REINFORCED COMPOSITES BY CHEMICAL VAPOR INFILTRATION AND DEPOSITION**
$65,000
DOE Contacts: F. M. Glaser (301) 903-2784, V. U. S. Rao (412) 386-4743 and M. H. Rawlins (865) 576-4507
Oak Ridge National Laboratory Contact: T. M. Besmann (865) 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

356. **DEVELOPMENT OF OXIDATION/ CORROSION-RESISTANT COMPOSITE MATERIALS AND INTERFACES**
$219,000
DOE Contacts: F. M. Glaser (301) 903-2784, V. U. S. Rao (412) 386-4743 and M. H. Rawlins (865) 576-4507
Oak Ridge National Laboratory Contact: R. A. Lowden (865) 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

357. **MODELING FOR CVD OF SOLID OXIDE ELECTROLYTE**
$54,000
DOE Contacts: F. M. Glaser (301) 903-2784, V. U. S. Rao (412) 386-4743 and M. H. Rawlins (865) 576-4507
Oak Ridge National Laboratory Contact: D. P. Stinton (865) 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.

This project shall investigate the application of stagnation point flow to the deposition of yttrium-stabilized zirconia (YSZ) solid electrolyte films, including an experimental effort at ORNL and a modeling effort at the University of Louisville.

Keywords: Ceramics, Composites, Modeling, Fuel Cells

358. **DEVELOPMENT OF A COMMERCIAL PROCESS FOR THE PRODUCTION OF SILICON CARBIDE FIBRILS**
$80,000
DOE Contacts: F. M. Glaser (301) 903-2784,
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M. H. Rawlins (865) 576-4507
Oak Ridge National Laboratory Contact:
D. P. Stinton (865) 574-4556
ReMaxCo Technologies, Inc. Contact:
R. D. Nixdorf (865) 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

359. **DEVELOPMENT OF HOT PRESSING AS A LOW-COST PROCESSING TECHNIQUE FOR FUEL CELL FABRICATION**
$82,000
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D. P. Stinton (865) 574-4556
Boston University Contact: Vinod Sarin
(617) 353-6451

This project focuses on the development of a hot-pressing technique for fabricating the air electrode (cathode) structure, with the objective to obtain an electronically-conducting porous structure with high gas permeability and a high electronic/ionic/gas contact area. Such a structure will provide low gas-phase mass transfer resistance and low electrode-polarization resistance.

Keywords: Fuel Cells

360. **DEVELOPMENT OF NOVEL ACTIVATED CARBON COMPOSITES**
$237,000
DOE Contacts: F. M. Glaser (301) 903-2784,
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M. H. Rawlins (865) 576-4507
Oak Ridge National Laboratory Contact:
T. D. Burchell (865) 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

361. **CARBON FIBER COMPOSITE MOLECULAR SIEVES TECHNOLOGY TRANSFER**
$44,000
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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

362. **OXIDE DISPERSION STRENGTHENED (ODS) ALLOYS**
$235,000
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M. H. Rawlins (865) 576-4507
Oak Ridge National Laboratory Contact:
I. G. Wright (865) 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

363. **INVESTIGATION OF THE WELDABILITY OF POLYCRYSTALLINE IRON ALUMINIDES**
$70,000
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Oak Ridge National Laboratory Contact:
R. W. Swindeman (865) 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

364. **FRICTION WELDING OF ODS ALLOYS**
$15,000
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Oak Ridge National Laboratory Contact:
I. G. Wright (865) 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

365. **EVALUATION OF THE INTRINSIC AND EXTRINSIC FRACTURE BEHAVIOR OF IRON ALUMINIDES**
$30,000
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I. G. Wright (865) 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

366. **INVESTIGATION OF IRON ALUMINIDE WELD OVERLAYS**
$45,000
DOE Contacts: F. M. Glaser (301) 903-2784,
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M. H. Rawlins (865) 576-4507
Oak Ridge National Laboratory Contact:
R. W. Swindeman (865) 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

367. **IN-PLANT CORROSION PROBE TESTS OF ADVANCED AUSTENITIC ALLOYS**
$80,000
DOE Contacts: F. M. Glaser (301) 903-2784,
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M. H. Rawlins (865) 576-4507
Oak Ridge National Laboratory Contact:
R. W. Swindeman (865) 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

368. **CORROSION AND MECHANICAL PROPERTIES OF ALLOYS IN FBC AND MIXED-GAS ENVIRONMENTS**
$175,000
DOE Contacts: F. M. Glaser (301) 903-2784,
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I. G. Wright (865) 574-4451
Argonne National Laboratory Contact:
K. Natesan (630) 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

369. **REDUCTION OF DEFECT CONTENT IN ODS ALLOYS**
$57,000
DOE Contacts: F. M. Glaser (301) 903-2784, V. U. S. Rao (412) 386-4743 and M. H. Rawlins (865) 576-4507
Oak Ridge National Laboratory Contact: I. G. Wright (865) 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

370. **SUPPORT SERVICES FOR CERAMIC FIBER-CERAMIC MATRIX COMPOSITES**
$58,000
DOE Contacts: F. M. Glaser (301) 903-2784, V. U. S. Rao (412) 386-4743 and M. H. Rawlins (865) 576-4507
Oak Ridge National Laboratory Contact: D. P. Stinton (865) 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 Advanced Research 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

371. **RELIABLE CERAMIC COATINGS FOR HIGH-TEMPERATURE ENVIRONMENTAL RESISTANCE IN FOSSIL ENVIRONMENTS**
$82,000
DOE Contacts: F. M. Glaser (301) 903-2784, V. U. S. Rao (412) 386-4743 and M. H. Rawlins (865) 576-4507
Oak Ridge National Laboratory Contact: P. F. Tortorelli (865) 574-5119

The purpose of this work is to support the development of advanced ceramic-based materials for applications in fossil environments by examining critical phenomena related to high-temperature environmental resistance of ceramic coatings used to provide protection under the aggressive conditions commonly found in advanced coal-fired plants. In support of this purpose, technical objectives focus not only on chemical compatibility of standard and developmental ceramic coatings in a variety of environments, but also on their mechanical reliability.

Keywords: Coatings, Corrosion

372. **DEVELOPMENT OF NONDESTRUCTIVE EVALUATION METHODS FOR STRUCTURAL CERAMICS**
$175,000
DOE Contacts: F. M. Glaser (301) 903-2784, V. U. S. Rao (412) 386-4743 and M. H. Rawlins (865) 576-4507
Oak Ridge National Laboratory Contact: D. P. Stinton (865) 574-4556
Argonne National Laboratory Contacts: W. A. Ellingson (630) 252-5068

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: Non-Destructive Evaluation, Ceramics, Flaws, Fracture

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

373. ***MATERIALS AND COMPONENTS IN FOSSIL ENERGY APPLICATIONS* NEWSLETTER**
$60,000[1]
DOE Contacts: F. M. Glaser
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(412) 386-4743 and M. H. Rawlins
(865) 576-4507
Oak Ridge National Laboratory Contact:
I. G. Wright (865) 574-4451

The purpose of this task is to publish a bimonthly, joint DOE-EPRI newsletter to address current developments in materials and components in fossil energy applications.

Keywords: Materials, Components

374. **DEVELOPMENT OF CERAMIC MEMBRANES FOR HYDROGEN SEPARATION**
$350,000
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M. H. Rawlins (865) 576-4507
Oak Ridge National Laboratory Contact:
R. R. Judkins (865) 574-4572
East Tennessee Technology Park Contact:
D. E. Fain (865) 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

375. **PROTON EXCHANGE MEMBRANES FOR HYDROGEN SEPARATION**
$356,000
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(412) 386-4743 and M. H. Rawlins
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Oak Ridge National Laboratory Contact:
T. R. Armstrong (865) 574-7996
Eltron Research, Inc. Contact: Shane Roark
(303) 530-0263

The objectives of this program are to develop: (1) novel designs for compact hydrogen separation membranes, (2) model the designs to determine manufacturing feasibility, (3) fabricate 1 or 2 novel membranes for testing, (4) develop reliability models for asymmetric membranes, (5) evaluate constrained sintering of asymmetric membranes (6) characterize materials developed by Eltron using state-of-the-art X-ray diffraction and neutron scattering analysis and (7) develop a database of materials properties of all current and past protonic conductors.

Keywords: Membranes, Separation

376. **SOLID STATE ELECTROLYTE SYSTEMS FOR FUEL CELLS AND GAS SEPARATION**
$730,000
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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

[1]Matching funding provided by EPRI.

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

377. **IMPROVED FUEL CELL MATERIALS AND ECONOMICAL FABRICATION**
$50,000
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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

378. **EFFICIENT SOFC ELECTROLYTE FABRICATION**
$197,000
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The purpose of this task is to develop an atmospheric pressure chemical vapor deposition (APCVD) process for fabricating yttria-stabilized zirconia (YSZ) electrolytes for a solid oxide fuel cell (SOFC). The process utilizes halide-based precursors flowing over a heated substrate in an atmospheric pressure reactor. The elimination of the typical requirement of a low pressure reactor will substantially reduce fabrication costs. Development of the process is needed because the higher pressures generally cause poor coatings to be deposited and significant homogeneous nucleation that results in the formation of powder.

Keywords: Coatings, Fuel Cells

379. **BISMUTH OXIDE SOLID ELECTROLYTE OXYGEN SEPARATION MEMBRANES**
$257,000
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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

380. **METALLIC FILTERS FOR HOT-GAS CLEANING**
$150,000
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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

381. **REFRACTORY MATERIALS ISSUES IN GASIFIERS**
$100,000
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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

382. **Pd-Ag MEMBRANES FOR HYDROGEN SEPARATION**
$100,000
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The Palladium Membrane Reactor (PMR) 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

383. **HIGH-TEMPERATURE MATERIALS TESTING IN COAL COMBUSTION ENVIRONMENTS**
$500,000
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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 1700-2600°F, 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 1800-2000°F at other locations to compare results with those from the EERC tests.

Keywords: Testing

384. **MOLECULAR SIEVES FOR HYDROGEN SEPARATION**
$150,000
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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

385. **SYSTEMS ANALYSIS OF PROCESSES INVOLVING HYDROGEN SEPARATION MEMBRANE**
$50,000
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The purpose of this project is to analyze conceptual systems and cost analyses for a coal processing plant to produce hydrogen using the membranes developed in the Program while recovering carbon dioxide (CO_2) for offsite processing or sequestration in a Vision 21 context.

Keywords: Membranes, Vision 21

386. **OXIDE-DISPERSION-STRENGTHENED Fe_3Al-BASED ALLOY TUBES**
$50,000
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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-Al base alloys and the Ni-base superalloys currently in service.

The development of suitable ODS Fe_3Al 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

387. **DEVELOPMENT OF ODS ALLOY FOR HEAT EXCHANGER TUBING**
$173,000
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Mark Harper (304) 526-5057

This work is intended to generate information and understanding for incorporation into a database being generated by the team assembled by Special Metals Corporation to allow oxide dispersion-strengthened (ODS) alloys to be used in the design, construction, and operation of heat exchangers in the very high-temperature environments of interest in Vision 21 power plant modules. This effort has three main objectives: firstly, to characterize the effectiveness of modified processing routes aimed at optimizing the mechanical properties of the ODS-FeCrAl alloy INCO® MA956 for application as tubing. Property measurements from this activity will form part of the data package required for submission of a case for obtaining ASME Boiler and Pressure Vessel Code qualification for this alloy. Secondly, to evaluate the available techniques for joining ODS alloys, to provide a sound basis for fabrication options. The third objective is to develop a basis for service lifetime prediction based on the high-temperature oxidation behavior of this alloy.

Keywords: Alloys, Tubing

388. **FATIGUE AND FRACTURE BEHAVIOR OF Cr-X ALLOYS**
$29,000
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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

389. **MANAGEMENT OF THE FOSSIL ENERGY ADVANCED RESEARCH MATERIALS PROGRAM**
$400,000
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The goal of the Fossil Energy Advanced Research 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 heat exchanger applications; new corrosion- and erosion-resistant alloys with unique mechanical properties for advanced fossil energy systems; functional materials such as metal and ceramic hot-gas filters, gas separation materials based on ceramic membranes (porous and ion transport), fuel cells, and activated carbon materials; and corrosion research to understand the behavior of materials in coal-processing environments. In cooperation with DOE-ORO, Oak Ridge National Laboratory (ORNL) has the responsibility of the technical management and implementation of all activities on the DOE Fossil Energy Advanced Research Materials Program. DOE-FE administration of the Program is through the National Energy Technology Laboratory and the Advanced Research Product Team.

Keywords: Management, Materials Program

390. **GORDON RESEARCH CONFERENCE SUPPORT**
$6,000
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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

391. **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

392. **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: Aluminides, Coatings, Foil-Lamination Process

393. **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

394. **ADVANCED REFRACTORY RESEARCH**
$600,000
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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

395. **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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