DOE/EE-0113

ENERGY MATERIALS COORDINATING COMMITTEE (EMaCC)

Fiscal Year 1995

December 1996

Annual Technical Report

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

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Washington, DC 20585

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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 chairmen are:

Electrochemical Technologies - Richard Kelly, ER-132, (301) 903-6051
Metals and Intermetallics - David J. Beecy, FE-72, (301) 903-2787
Radioactive Waste Containers - Alan Berusch, RW-22, (202) 586-9362
Semiconductors - Jerry Smith, ER-132, (301) 903-4269
Structural Ceramics - Charles Sorrell, EE-232, (202) 586-1514
Superconductivity - James Daley, EE-142, (202) 586-1165

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

The EMaCC reports to the Director of the Office of Energy Research in his or her capacity as overseer of the technical programs of the Department. This annual technical report is mandated by the EMaCC terms of reference. This report summarizes EMaCC activities for FY 1995 and describes the materials research programs of various offices and divisions within the Department.

The Chairman of EMaCC for FY 1995 was Cynthia Carter. The compilation of this report was performed by Yok Chen, EMaCC Executive Secretary for FY 1996, with the assistance of FM Technologies, Inc.

Dr. Debbie Haught
Office of Transportation Technologies
Chairman of EMaCC, FY 1996

MEMBERSHIP LIST
DEPARTMENT OF ENERGY
ENERGY MATERIALS COORDINATING COMMITTEE

ORGANIZATION	REPRESENTATIVE	PHONE NO.
ENERGY EFFICIENCY AND RENEWABLE ENERGY		
Building Technology, State and Community Programs		
Building Systems	John Talbott, EE-41	202/586-9455
Industrial Technologies		
Industrial Energy Efficiency	Scott Richlen, EE-221	202/586-2078
Waste Materials Management	Kurt D. Sisson EE-222	202/586-6750
Materials Processing Division	Matthew McMonigle, EE-234	202/586-2082
Advanced Industrial Materials	Charles Sorrell, EE-232	202/586-1514
Separation Division	Brian Volintine, EE-233	202/586-1739
Transportation Technologies		
Advanced Transportation Materials	Sidney Diamond, EE-34	202/586-0832
	Jim Eberhardt, EE-34	202/586-1694
	Debbie Haught, EE-34	202/586-2211
Utility Technologies		
Wind/Hydro/Ocean Technologies	William Richards, EE-121	202/586-5410
Geothermal Technology	Raymond LaSala, EE-122	202/586-4198
Photovoltaic Technology	Richard King, EE-131	202/586-1693
Advanced Utility Concepts	James Daley, EE-142	202/586-1165
	Christine Platt, EE-142	202/586-8943
	Chris Kang, EE-142	202/586-4563

ORGANIZATION	REPRESENTATIVE	PHONE NO.
ENERGY RESEARCH		
Basic Energy Sciences		
Materials Sciences	Iran L. Thomas, ER-10	301/903-3081
	Robert J. Gottschall, ER-13	301/903-3427
Metallurgy and Ceramics	Alan Dragoo, ER-131	301/903-4895
	Yok Chen, ER-131	301/903-3428
	Helen Kerch, ER-131	301/903-3428
	John Mundy, ER-131	301/903-4271
Solid State Physics and Materials Chemistry	W. Oosterhuis, ER-132	301/903-3426
	Jerry Smith, ER-132	301/903-3426
	Richard Kelly, ER-132	301/903-3426
Chemical Sciences	Stephen A. Butter, ER-142	301/903-2367
Engineering and Geosciences	Oscar P. Manley, ER-15	301/903-5822
Advanced Energy Projects	Cynthia Carter, ER-16	301/903-5995
Safety and Health	Albert Evans, ER-13	301/903-3427
	Michael Teresinski, ER-13	301/903-5155
Laboratory Management		
Laboratory Technology Transfer	Ted Vojnovich, ER-80	202/586-2343
Fusion Energy		
Fusion Technologies	F. W. (Bill) Wiffen, ER-543	301/903-4963
ENVIRONMENTAL RESTORATION AND WASTE MANAGEMENT		
Waste Operations		
Waste Management Projects	Doug Tonkay, EM-30	301/903-7212
Science and Technology		
Research and Development	Stanley M. Wolf, EM-54	301/903-7962
NUCLEAR ENERGY, SCIENCE AND TECHNOLOGY		
Space and National Security Programs		
Defense Energy Projects	John W. Warren, NE-52	301/903-6491
Radioisotope Power Systems	William Barnett, NE-53	301/903-3097
Naval Reactors	David I. Curtis, NE-60	703/603-5565

ORGANIZATION	REPRESENTATIVE	PHONE NO.
Nuclear Safety Self-Assessment		
Nuclear Quality Assurance	John Dowicki, NE-84	301/903-7729
CIVILIAN RADIOACTIVE WASTE MANAGEMENT		
Analysis and Verification	Alan Berusch, RW-2	202/586-9362
DEFENSE PROGRAMS		
Research and Advanced Technology		
Research and Technology Development	Bharat Agrawal, DP-11	301/903-2057
Inertial Confinement Fusion	Carl B. Hilland, DP-28	301/903-3687
FOSSIL ENERGY		
Advanced Research	David J. Beecy, FE-72 James P. Carr, FE-72	301/903-2787 301/903-6519

ORGANIZATION OF THE REPORT

The FY 1995 budget summary table for DOE Materials Activities is presented on pages 6-8.

Following the budget summary table is a set of detailed program descriptions for the FY 1995 DOE Materials activities. These descriptions are presented according to the organizational structure of the Department. A mission statement, a budget summary table listing the project titles and FY 1995 funding, and detailed project summaries are presented for each Assistant Secretary office and the Office of Energy Research. The project summaries also provide DOE, laboratory, academic and industrial contacts for each project, as appropriate.

FY 1995 BUDGET SUMMARY TABLE FOR DOE MATERIALS ACTIVITIES

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

	FY 1995
Office of Building Technology, State and Community Programs	$ 800,000
Office of Building Systems	800,000
Office of Industrial Technologies	$31,142,477
Office of Waste Reduction Technologies	825,000
Waste Material Management Division	825,000
Solar Materials Research	825,000
Office of Industrial Processes	30,317,477
Advanced Industrial Materials Program	8,932,000
Advanced Turbine Systems Program	11,000,000
Heat Exchanger Program	2,108,477
Continuous Fiber Ceramic Composites (CFCC) Program	8,277,000
Office of Transportation Technologies	$24,851,000
Office of Transportation Materials	12,646,000
Office of Propulsion Systems	12,205,000
Advanced Propulsion Division	7,595,000
Electric and Hybrid Propulsion Division	4,610,000
Office of Utility Technologies	$33,740,000
Office of Solar Energy Conversion	15,200,000
Photovoltaic Energy Technology Division	15,200,000
Office of Renewable Energy Conversion	540,000
Geothermal Division (GD)	540,000
Office of Energy Management	18,000,000
Advanced Utility Concepts Division	18,000,000
Superconductivity Systems Program	18,000,000

FY 1995 BUDGET SUMMARY TABLE FOR DOE MATERIALS ACTIVITIES (Continued)

	FY 1995
Office of Energy Research	$358,555,719
Office of Basic Energy Sciences	295,610,365
Division of Materials Sciences	275,708,000
Division of Chemical Sciences	5,800,000
Division of Engineering and Geosciences	6,559,365
Engineering Sciences Research	4,114,376
Geosciences Research	2,444,989
Division of Advanced Energy Projects	7,543,000
Office of Fusion Energy	22,870,000
Small Business Innovation Research Program	39,175,749
Small Business Technology Transfer Program	899,605
Office of Environmental Management	$ 30,489,600
Office of Waste Management	7,563,600
High Level Waste Division	7,563,600
Office of Science and Technology	22,926,000
Office of Nuclear Energy, Science and Technology	$ 48,165,000
Office of Engineering and Technology Development	2,165,000
Space and National Security Programs	2,165,000
Office of Naval Reactors	46,000,000*
Office of Civilian Radioactive Waste Management	$ 9,700,000
Office of Defense Programs	$ 90,355,000
The Weapons Research Development and Test Program	90,355,000
Sandia National Laboratories	42,452,000
Lawrence Livermore National Laboratory	20,876,000
Los Alamos National Laboratory	27,027,000

*This excludes $44 million for the cost of irradiation testing in the Advanced Test Reactor (ATR).

FY 1995 BUDGET SUMMARY TABLE FOR DOE MATERIALS ACTIVITIES (Continued)

	FY 1995
Office of Fossil Energy	$ 7,668,000
Office of Advanced Research	7,668,000
Fossil Energy AR&TD Materials Program	7,668,000
TOTAL	**$635,466,796**

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 1995
1. Office of Building Technology, State and Community Programs	$ 800,000
a. Office of Building Systems	800,000
2. Office of Industrial Technologies	$31,142,477
a. Office of Waste Reduction Technologies	825,000
(1) Waste Material Management Division	825,000
(a) Solar Materials Research	825,000
b. Office of Industrial Processes	30,317,477
(1) Advanced Industrial Materials Program	8,932,000
(2) Advanced Turbine Systems Program	11,000,000
(3) Heat Exchanger Program	2,108,477
(4) Continuous Fiber Ceramic Composites (CFCC) Program	8,277,000
3. Office of Transportation Technologies	$24,851,000
a. Office of Transportation Materials	12,646,000
b. Office of Propulsion Systems	12,205,000
(1) Advanced Propulsion Division	7,595,000
(2) Electric and Hybrid Propulsion Division	4,610,000
4. Office of Utility Technologies	$33,740,000
a. Office of Solar Energy Conversion	15,200,000
(1) Photovoltaic Energy Technology Division	15,200,000
b. Office of Renewable Energy Conversion	540,000
(1) Geothermal Division (GD)	540,000
c. Office of Energy Management	18,000,000
(1) Advanced Utility Concepts Division	18,000,000
(a) Superconductivity Systems Program	18,000,000

OFFICE OF BUILDING TECHNOLOGY, STATE AND COMMUNITY PROGRAMS

	FY 1995
Office of Building Technology, State and Community Programs - Grand Total	$800,000
Office of Building Systems	$800,000
Materials Properties, Behavior, Characterization or Testing	$800,000
Development of Non-CFC Foam Insulations	100,000
Evacuated Powder Panel Insulation	300,000
Gas-Filled Reflective Insulation Panel	50,000
Accelerated Lifetime Test Procedure Development	250,000
Standardized Procedures for Measuring Solar Reflectivity on Horizontal Surfaces	100,000

OFFICE OF BUILDING TECHNOLOGY, STATE AND COMMUNITY PROGRAMS

OFFICE OF BUILDING SYSTEMS

The goal of this Office is to provide a scientific and technical basis (including model standards) for reducing the use of energy in residential and commercial buildings by 35 percent by the year 2000 from that used in 1975, while maintaining existing levels of human comfort, health and safety. The Division's primary objectives are to support research that advances the scientific and technical options for increased energy efficiency in buildings, to promote the substitution of abundant fuels for scarce fuels in buildings, and to promulgate standards for increased efficiency of energy use. To accomplish a portion of this, the Building Materials program seeks to: (1) develop new and improve existing insulating materials; (2) develop and verify analytical models that are useful to building designers and researchers for predicting the thermal performance characteristics of materials; (3) develop methods for measuring the thermal performance characteristics; and (4) provide technical assistance and advice to industry and the public. The DOE contact is John Talbott, (202) 586-9455.

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

1. **DEVELOPMENT OF NON-CFC FOAM INSULATIONS**
   $100,000
   DOE Contact: John Talbott, (202) 586-9455
   ORNL Contact: Ken Wilkes, (615) 574-5931

This is the second year of a three-year extension of a joint project with the rigid foam industry for the development of alternative blowing agents to be used as drop-in replacements for the CFC blowing agents currently being used in the manufacture of foam insulation products. Prototype rigid foam boards blown with HCFC-141b and CFC-11 were sent to ORNL for testing and evaluation both in the laboratory and in outdoor test facilities. Tests are being conducted to determine mechanical and thermal properties and aging characteristics.

Keywords: CFC, Foam Insulation, Insulation Sheathing, Roofs

2. **EVACUATED POWDER PANEL INSULATION**
   $300,000
   DOE Contact: John Talbott, (202) 586-9455
   ORNL Contact: Ken Wilkes, (615) 574-5931

This project is for the development of an advanced technology super insulation concept. A layer of powder is sandwiched between two films and a soft vacuum is drawn on the powder filler. Current technology produces a R-40 per inch panel. More efficient powders and longer life encasing films are being developed.

Keywords: Insulation, Vacuum, Heat Transfer

3. **GAS-FILLED REFLECTIVE INSULATION PANEL**
   $50,000
   DOE Contact: John Talbott, (202) 586-9455
   LBL Contact: Dariush Aresteh, (415) 486-6844

This project is for the development of a super insulation concept that utilizes layers of reflective films enclosed in a flexible film panel which is filled with low conductivity gases. Mechanisms to provide greater structural rigidity are being investigated as are low permeability films and environmentally benign low conductivity gases.

Keywords: Insulation, Reflective Films, Low Conductivity Gases

4. **ACCELERATED LIFETIME TEST PROCEDURE DEVELOPMENT**
   $250,000
   DOE Contact: John Talbott, (202) 586-9455
   ORNL Contact: Ken Wilkes, (615) 574-5931

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

Keywords: Thermal Resistance, Test Procedures

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

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

Keywords: Solar, Reflectivity, Building Materials

OFFICE OF INDUSTRIAL TECHNOLOGIES

	FY 1995
Office of Industrial Technologies - Grand Total	$31,142,477
Office of Waste Reduction Technologies	$ 825,000
Waste Material Management Division	$ 825,000
Solar Materials Research	$ 825,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 825,000
Photocatalysts Based on Titanium Dioxide	300,000
Solar Materials Processing	525,000
Office of Industrial Processes	$30,317,477
Advanced Industrial Materials Program	$8,932,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$4,539,000
Synthesis and Design of $MoSi_2$ Intermetallic Materials	785,000
Development of Weldable, Corrosion Resistant Iron Aluminide Alloys	250,000
Composites and Coatings Through Reactive Metal Infiltration	478,000
Magnetic Field Processing of Inorganic Polymers	190,000
Development of New Composite Aerogel Materials	100,000
Microwave Processing of Continuous Ceramic Oxide Filaments	368,000
Conducting Polymers: Synthesis and Industrial Applications	316,000
Microwave Assisted Chemical Vapor Infiltration	210,000
Chemical Vapor Deposition Ceramic Synthesis	400,000
Gel Casting Technology	155,000
Uniform Droplet Spray Forming	470,000
Biomimetic Thin Film Synthesis	325,000
Chemical Recycling of Plastics	300,000
Composites and Blends from Biobased Materials	192,000
Materials Properties, Behavior, Characterization or Testing	$1,075,000
Characterization of Three-Way Automotive Catalysts	300,000
Composite Tubes - Materials for Recovery Boilers	775,000
Materials Structure and Composition	$1,518,000
Metallic and Intermetallic Bonded Ceramic Composites	330,000
Advanced Ordered Intermetallic Alloy Development	475,000
Rapid Solidification Processing of Metal Alloys	192,000
Processing of Polymers in a Magnetic Field	316,000
Microwave Joining of SiC	205,000

OFFICE OF INDUSTRIAL TECHNOLOGIES (Continued)

	FY 1995
Office of Industrial Processes (continued)	
Advanced Industrial Materials Program (continued)	
Device or Component Fabrication, Behavior or Testing	$ 1,800,000
Ni_3Al Technology Transfer - Steel Mill Rolls and Furnace Fixtures	1,050,000
Advanced Microwave Processing Concepts	250,000
Selective Inorganic Thin Films	400,000
Chemical Vapor Infiltration of TiB_2 Composites	100,000
Advanced Turbine Systems Program	$11,000,000
Device or Component Fabrication, Behavior or Testing	$11,000,000
Ceramic Components for Stationary Gas Turbines in Cogeneration Service	6,500,000
Long-Term Testing of Ceramic Components for Stationary Gas Turbines	500,000
ATS Materials Base Technology Support	4,000,000
Heat Exchanger Program	$ 2,108,477
Materials Properties, Behavior, Characterization or Testing	$ 617,000
Advanced Heat Exchanger Material Technology Development	617,000
Device or Component Fabrication, Behavior or Testing	$ 1,491,477
Ceramic Composite Heat Exchanger for the Chemical Industry	138,801
HiPHES System for Energy Production	316,676
HiPHES System for Ethylene Production	1,036,000
Continuous Fiber Ceramic Composites (CFCC) Program	$8,277,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$5,977,000
CFCC Program - Industry Tasks	5,977,000
Materials Properties, Behavior, Characterization or Testing	$2,300,000
Continuous Fiber Ceramic Composites (CFCC) Supporting Technologies	2,300,000

OFFICE OF INDUSTRIAL TECHNOLOGIES

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

OFFICE OF WASTE REDUCTION TECHNOLOGIES

WASTE MATERIAL MANAGEMENT DIVISION

SOLAR MATERIALS RESEARCH

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

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

6. **PHOTOCATALYSTS BASED ON TITANIUM DIOXIDE**
$300,000
DOE Contact: Frank Wilkins, (202) 586-1684
NREL Contact: Daniel M. Blake, (303) 275-3702

The objectives of this work are to develop materials that are more active photocatalysts for the oxidation of organic compounds in air or aqueous phases, determine the characteristics of titanium dioxide and modified forms that influence the activity, and test the catalysts in laboratory and pilot scale reaction systems. Potential catalysts are prepared inhouse, by NREL subcontractors, or obtained from commercial sources. The ultimate goal is to make photocatalytic oxidation processes for removal of hazardous organic compounds from contaminated air and water a cost-effective treatment option for environmental remediation and process emission control.

Keywords: Photocatalyst, Titanium Dioxide, Oxidation, Remediation

7. **SOLAR MATERIALS PROCESSING**
$525,000
DOE Contact: Frank Wilkins, (202) 586-1684
NREL Contact: Allan Lewandowski, (303) 384-7470

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

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

OFFICE OF INDUSTRIAL PROCESSES

ADVANCED INDUSTRIAL MATERIALS PROGRAM

New or improved materials can save significant energy and improve productivity by enabling systems to operate at higher temperatures, last longer, and reduce capital costs. The emphasis of the Advanced Industrial Materials program is on industrial needs identified for the seven OIT industries of the Future. Efforts in 1995 were focused on forging partnerships between industry and the National

Laboratories for commercialization of new materials and processes. The program manager is Charles A. Sorrell, (202) 586-1514.

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

8. **SYNTHESIS AND DESIGN OF $MoSi_2$ INTERMETALLIC MATERIALS**
   $785,000
   DOE Contact: Charles A. Sorrell, (202) 586-1514
   Los Alamos National Laboratory Contacts:
   J. J. Petrovic, (505) 667-0125 and Richard Castro, (505) 667-5191

The objective of this project is to develop $MoSi_2$-based composites that will combine good room temperature fracture toughness with excellent oxidation resistance and high-temperature strength for industrial applications. Processing methods such as spray forming and electrophoretic deposition are being investigated also. Focus has been on development and characterization of $MoSi_2$-SiC, $MoSi_2$-Si_3N_4 and $MoSi_2$-Al_2O_3 composites; as well as on plasma sprayed $MoSi_2$ materials and microlaminate composites. Current emphasis is on the fabrication of prototype $MoSi_2$ industrial components (e.g., fuel burners, gas injection tubes, furnace heating elements, and metal processing equipment) and, in particular, $MoSi_2$ components for fiber glass processing. The project has a number of research collaborations in place with industrial partners.

Keywords: Composites, Intermetallics, Molydisilicides

9. **DEVELOPMENT OF WELDABLE, CORROSION RESISTANT IRON ALUMINIDE ALLOYS**
   $250,000
   DOE Contact: Charles A. Sorrell, (202) 586-1514
   ORNL Contact: P. J. Maziasz, (615) 574-5082

Iron-aluminides show excellent corrosion/oxidation resistance to at least 1100°C. Alloying has been shown to considerably improve room-temperature ductility and high-temperature tensile and creep strength relative to binary alloy systems. The objectives of this project are to complete alloy development efforts to maximize weldability and properties improvements in FeAl alloys for structural applications, and to develop the potential for weldable FeAl alloys for use in weld-overlay cladding applications. The initial alloy development phase to improve the weldability and mechanical properties of these alloys was completed in FY 1994. The optimum FeAl base alloy for weldability, fabricability and mechanical properties was found to be an Fe-36Al-0.2Mo-0.05Zr-0.13C (at%) alloy; an FeAl alloy with significantly better weldability and high temperature strength. Improved resistance to hydrogen effects at room-temperature is obtained with a boron micro-alloyed modification of the base alloy. In FY 1995 this project entered the fabrication technology phase, to produce components for industry testing. Two parallel paths are being pursued. One is to develop coatings and cladding of FeAl on conventional structural steels and alloys being used in industrial applications today. These should enable immediate testing of FeAl for its oxidation/corrosion/wear resistance in demanding industrial environments of interest. The other is to fabricate monolithic FeAl components and hardware for industrial testing.

Keywords: Iron Aluminides, Coatings, Claddings, Thermophysical Properties

10. **COMPOSITES AND COATINGS THROUGH REACTIVE METAL INFILTRATION**
    $478,000
    DOE Contact: Charles A. Sorrell, (202) 586-1514
    Sandia National Laboratories Contact:
    R. E. Loehman, (505) 844-2222

Ceramic-metal composites have advantages as engineering materials because of their high stiffness-to-weight ratios, good fracture toughness, and because their electrical and thermal properties can be varied through control of their composition and microstructure. However, broader commercial application of these materials requires improvements in synthesis and processing so that high-performance parts can be produced more economically. 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. Efforts have focused on determining the kinetics of infiltration of Al into dense mullite as well as identifying other metal-ceramic systems for potential reactive metal infiltration processing. Measured properties of composites have shown significantly improved toughness with little loss in stiffness compared with the ceramic preform.

Keywords: Metal Matrix Composites, Reactive Metal Infiltration, Ceramics

11. **MAGNETIC FIELD PROCESSING OF INORGANIC POLYMERS**
    $190,000
    DOE Contact: Charles A. Sorrell, (202) 586-1514
    Idaho National Engineering Laboratory Contact:
    D. C. Kunerth, (208) 526-0103

The application of magnetic fields during processing has been shown to modify the physical and chemical properties of inorganic polymers. The objective of this project is to develop the technical basis for improving the physical properties of inorganic polymers using electromagnetic fields. Current efforts focus on developing a basic understanding of magnetic field processing of polyphosphazene materials to be utilized as chemical separation membranes. The physical and chemical properties of the polyphosphazene polymers have been modified using magnetic fields. Results show that membrane morphologies and transport properties change with the application of magnetic fields; providing a small amount of molecular texturing. In addition, processing techniques as simple as DC magnetic fields developed by permanent magnets or microwave fields can be used.

Keywords: Polymers, Magnetic Field Processing

12. **DEVELOPMENT OF NEW COMPOSITE AEROGEL MATERIALS**
    $100,000
    DOE Contact: Charles A. Sorrell, (202) 586-1514
    Lawrence Berkeley Laboratory Contact:
    A. Hunt, (415) 486-5370

Aerogel materials are porous, low density, nanostructured solids with many unique properties including very low thermal conductivity, transparency, high surface area, and low sound velocity. The objective of this project is to develop new aerogel-based composites materials through sol-gel chemistry, supercritical drying, and chemical vapor infiltration. An infrared opacified silica aerogel was produced using chemical vapor infiltration methods that displayed improved thermal and physical properties. This provides higher temperature and stronger aerogel thermal insulation. The process was generalized to produce a wide variety of new composite materials. Some of these composites displayed unusual characteristics (e.g., photo-luminescence in silicon silica composites) due to quantum confinement effects.

Keywords: Thermal Insulation, Sol-Gel, Aerogels

13. **MICROWAVE PROCESSING OF CONTINUOUS CERAMIC OXIDE FILAMENTS**
    $368,000
    DOE Contact: Charles A. Sorrell, (202) 586-1514
    Los Alamos National Laboratory Contacts:
    G. J. Vogt, (505) 665-4988 and J. D. Katz, (505) 665-1424

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

Keywords: Microwave Processing, Filaments

14. **CONDUCTING POLYMERS: SYNTHESIS AND INDUSTRIAL APPLICATIONS**
    $316,000
    DOE Contact: Charles A. Sorrell, (202) 586-1514
    Los Alamos National Laboratory Contact:
    S. Gottesfeld, (505) 667-0853

The process of separating pure components out of a mixture of gases is of great industrial importance. Current gas separation technologies have major shortcomings, including poor energy efficiency and the generation of secondary pollution. The objective of this project is to develop superior membranes for gas separation using doped polyaniline polymers.Because these materials are electrical conductors, membrane properties can be changed following synthesis, and even during use, to control the process flow. A key portion of this project is fabrication of integrally skinned, asymmetric membranes of polyaniline using highly refined solution chemistry. The resultant membranes, consisting of a dense very thin "skin" (1 mm thick, or less) on top of a porous (e.g., 40 mm thick) base layer, should enable a dramatic increase in gas permeability while maintaining the high selectivity by the dense "skin."

Keywords: Electrically Conducting Polymers, Gas Separation, Capacitors

15. **MICROWAVE ASSISTED CHEMICAL VAPOR INFILTRATION**
    $210,000
    DOE Contact: Charles A. Sorrell, (202) 586-1514
    Los Alamos National Laboratory:
    D. J. Devlin, (505) 667-9914

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

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

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

Comprehensive models, including detailed gas-phase and surface chemistry coupled with reactor fluid mechanics, are required to optimize and scale-up chemical vapor deposition (CVD) processes. The objective of this project is to use the unique diagnostic and modeling capabilities at the Sandia National Laboratory - Livermore to understand and develop new techniques for chemical vapor deposition (CVD). A research reactor, originally constructed with DOE-OIT funding, is being used to determine identities and amounts of gaseous phase species present during CVD. Research efforts are focused on development of CVD processes for oxide fiber-preforms and plate glass surfaces for the improvement of properties.

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

17. **GEL CASTING TECHNOLOGY**
    $155,000
    DOE Contact: Charles A. Sorrell, (202) 586-1514
    ORNL Contact: M. A. Janney, (615) 576-5183

The sol-gel process is being adapted to production of aluminum oxide tubes for use in high-intensity industrial lighting. The sol-gel process will produce identical materials at lower temperatures and in far less time than do conventional methods which involve prolonged high temperature sintering with sintering aids. The process also allows for fabrication of large and complex shapes. Tubes which meet lighting specifications for crystallinity and transparency have been fabricated in a variety of sizes and shapes at Oak Ridge National Laboratory.

Keywords: Sol-Gel, Aluminum Oxide, Lighting Tubes

18. **UNIFORM DROPLET SPRAY FORMING**
    $470,000
    DOE: Contact: Charles A. Sorrell, (202) 586-1514
    ORNL Contact: Vinod Sikka, (615) 574-5123

A method for producing very uniform, spherical droplets of molten metal, with controllable diameters between micron and millimeter size was developed by faculty at the Massachusetts Institute of Technology and Tufts University and applied to low melting point metals. The purpose of this project is to adapt the process to higher melting materials, e.g., intermetallic alloys, stainless, steel, superalloys; to provide superior metal powders for the powder metallurgy industry and to develop methods for spray coating or casting of high temperature materials, such as aluminide intermetallics. Participants in the research include Massachusetts Institute of Technology, Tufts University and powder metal companies. The process has been scaled up for production of droplets of high melting alloys. Spray forming of metallic systems is being investigated. Production of new alloys and laminar materials will be explored in the future.

Keywords: Spray Forming, Spray Casting

19. **BIOMIMETIC THIN FILM SYNTHESIS**
    $325,000
    DOE Contact: Charles A. Sorrell, (202) 586-1514
    Pacific Northwest National Laboratory Contact:
    G. L. Graff, (509) 375-6786

The objective of this project is to adapt the features of mineralization processes used by bioorganisms to the development of materials with improved properties over conventionally processed materials and demonstrate industrial relevance of biomimetics thin film processing for industrial coatings. Calcium phosphate films have been deposited on Ti metal bone implants coated with self-assembled monolayers. Use of solution techniques to develop oriented, fully dense films of magnetite has been successful. Solution complexation methods have been used to grow thick tin oxide coatings on plastics under mild pH conditions. Impermeable high density polyethylene (HDPE)/Al/HDPE sandwich composite has been produced using cup drawing techniques. Future efforts will explore the potential for biomimetic processingin biomedical applications and in high-value-added products or industries such as microelectronics where the patterning advantage of biomimetics can be exploited.

Keywords: Biomimetic, Organic Interfaces, Ceramic Coatings

20. **CHEMICAL RECYCLING OF PLASTICS**
$300,000
DOE Contact: Charles A Sorrell, (202) 586-1514
National Renewable Energy Laboratory Contact:
R. J. Evans, (303) 231-1384

The goal of this project is to identify conditions for the production of high-value chemicals from mixtures of waste plastics by the use of selective pyrolysis. Sorting the feed and purifying the products are minimized by controlling reaction conditions so that target products can be collected in high yields. Control is achieved by taking advantage of differences in reaction rates, catalysis, and co-reactants. Target waste streams are post-consumer wastes that can range from commodity plastics to high-value engineering blends. Efforts are focused on increasing the yield and purity of the monomer, caprolactam, from nylon 6 carpet. In other applications, the conversion of poly(ethylene terephthalate) (PET) to its monomer, dimethyl terephthalate has expanded from mixed plastic bottle wastes to polyester fiber textile blends. Also, the intelligent chemical processing system has demonstrated quantitative and qualitative ability to analyze carpet mixtures.

Keywords: Plastics Recycling, Pyrolysis, Waste Streams

21. **COMPOSITES AND BLENDS FROM BIOBASED MATERIALS**
$192,000
DOE Contact: Charles A Sorrell, (202) 586-1514
National Renewable Energy Laboratory Contacts:
S. S. Kelley and S. S. Shojaie, (303) 384-6123

The program is focused on the development of composites and blends from biobased materials for use as membranes, high-value plastics, and lightweight composites. Biobased materials include novel cellulose derivatives, wood modified with synthetic monomers, and wood fiber/synthetic plastic composites. Research efforts have focused on two areas: (1) composites and blends from cellulose derivatives, and (2) wood reinforced with synthetic monomers. The program is designed to evaluate the thermal, mechanical, and permeselective properties of these materials and relate their performance to the chemical structure and morphology of the composites or blends. Current efforts are focused on utilizing cellulose esters to prepare novel composites and blends. These materials have improved permeselective and/or compaction properties relative to unmodified cellulose esters.

Keywords: Biobased Materials, Composites, Thermomechanical Testing

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

22. **CHARACTERIZATION OF THREE-WAY AUTOMOTIVE CATALYSTS**
$300,000
DOE Contact: Charles A Sorrell, (202) 586-1514
ORNL Contact: E. A Kenik, (615) 574-5066
General Motors-AC Rochester Division Contact:
W. LaBarge, (313) 257-0875

Platinum-rhodium based three-way-catalysts (TWC) currently meet the required emissions standards; however, higher than optimum Pt-Rh loadings are often required to meet lifetime requirements. Understanding the changes of the TWC conversion efficiency with aging is a critical need in improving the catalysts. The objective of this project is to critically evaluate catalytic materials in as-produced and aged conditions and correlate materials and systems development to improve catalyst performance and lifetime while decreasing emissions. Current efforts focus on characterizing the microstructural and chemical state of both noble metals and substrates in as-produced catalyst materials with a wide range of spectroscopy and analysis techniques.

Keywords: Automotive Catalysts, Surface Analytical Analysis, Light and Electron Optical Analysis

23. **COMPOSITE TUBES - MATERIALS FOR RECOVERY BOILERS**
$775,000
DOE Contact: Charles A Sorrell, (202) 586-1514
ORNL Contact: James R. Kaiser, (615) 574-4453

The purpose of this project is to determine the cause of failure of composite tubes used in Kraft Black Liquor recovery boilers during pulp and paper making, and to develop new materials to eliminate failures. The project consists of three efforts: (1) to obtain operating data and failure analyses from pulp and paper companies, boiler manufacturers and composite tube manufacturers, (2) determination of residual stresses in new and used composite tubes and microstructural characteristics of tubes as related to stresses and failure mechanisms, and (3) development of new materials and/or fabrication methods for improvements in boiler efficiency, service life, and safety. Participants include Oak Ridge National

Laboratory, Institute of Paper Science and Technology, and 11 industrial collaborators.

Keywords: Recovery Boilers, Composite Tubes, Paper

MATERIALS STRUCTURE AND COMPOSITION

24. **METALLIC AND INTERMETALLIC BONDED CERAMIC COMPOSITES**
    $330,000
    DOE Contact: Charles A Sorrell, (202) 586-1514
    ORNL Contacts: T. N. Tiegs and K B. Alexander, (615) 574-0631
    Lawrence Berkeley Laboratory Contact: R. O. Ritchie, (415) 642-0417

To improve the reliability of ceramic components, new approaches to increasing the fracture toughness of ceramics over an extended temperature range are needed. One method is the incorporation of ductile phases into ceramic matrix alloys for local plastic deformation during crack bridging processes. This deformation acts to dissipate the strain energy introduced by the applied stress, thus increasing the fracture toughness of the composite. This objective of this program is to develop ceramic composites with high fracture toughness for intermediate temperature use in wear, tribological and engine applications. Results have shown that nickel aluminide additions have been shown to be an effective toughening agent in ceramic matrices if the microstructural distribution is carefully controlled. The microstructural features yielding optimal toughening have been identified and composites have been fabricated with properties comparable to, or better than, commercial ceramic composites at a lower raw material cost.

Keywords: Ceramics, Composites, Nickel Aluminide

25. **ADVANCED ORDERED INTERMETALLIC ALLOY DEVELOPMENT**
    $475,000
    DOE Contact: Charles A Sorrell, (202) 586-1514
    ORNL Contact: C. T. Liu, (615) 574-4459

Many ordered intermetallics possess unique properties and have the potential to be developed as new materials for energy related applications. The objective of this project is to develop low-density, high-strength ordered intermetallic alloys for high-temperature structural use in advanced heat engines, energy conversion systems, and other industrial systems. Current efforts are focused on: (1) increasing the tensile ductility of NiAl and improving impact resistance of these alloys by control of microstructure and alloy composition, (2) increasing the tensile ductility and fracture resistance of TiAl-base alloys by control of grain size and lamellar structure, and (3) characterizing the oxidation and corrosion resistance of intermetallic alloys for industrial applications.

Keywords: Intermetallics, Ordered Alloys, Shape Memory Alloys

26. **RAPID SOLIDIFICATION PROCESSING OF METAL ALLOYS**
    $192,000
    DOE Contact: Charles A Sorrell, (202) 586-1514
    Idaho National Engineering Laboratory Contact: J. E. Flinn, (208) 526-8127

The industrial sector requires metallic alloys whose properties, performance, and reliability extend beyond those obtained from current processing practices. These needs can be fulfilled by metallic alloys that have fine and stable (to high temperatures) microstructures. Rapid solidification processing (RSP) by design can fulfill these need through control of alloy chemistry and powder processing parameters. Significant improvements have been observed for RSP 304 SS, A286, and 718 alloys compared to their ingot metallurgy counterparts. A nickel-base alloy has been designed for the RSP approach using the knowledge from the research findings and input from the industrial sector. In addition, four Cooperative Research and Development Agreements (CRADAs) have been signed to compare the microstructure, properties and performance limits of selected alloys/materials currently being used with those obtained by RSP. These materials are for high temperature electrical, corrosion and wear, and photovoltaic applications.

Keywords: Rapid Solidification, Alloys, High Temperature Microstructure

27. **PROCESSING OF POLYMERS IN A MAGNETIC FIELD**
    $316,000
    DOE Contact: Charles A Sorrell, (202) 586-1514
    Los Alamos National Laboratory Contacts: Elliot P. Douglas, 505 665-4828

The purpose of this project is to demonstrate the utility of magnetic fields to beneficially modify or control the physical, optical and electrical properties of materials through the application of magnetic fields during polymerization processing and solidification. Researchers at Los Alamos National Laboratory, in collaboration with an industrial partner, have demonstrated that using high (10-20 Tesla) magnetic fields to orient liquid crystal polymers during processing can lead to substantial improvements in mechanical properties. Working at the National High Magnetic Field Laboratory, liquid crystal polymers were processed using a specially designed high temperature probe built for the 20 Tesla superconducting magnet. The probe insulates the liquid helium bath of the superconducting magnet from the high temperatures used in the processing, and results in a thermal gradient of more than 400°C over a distance of approximately 2.5 cm. The tensile modulus, in the magnetic field alignment direction, of a polymer processed in a 15 Tesla magnetic field was double that of the same material processed with no magnetic field present. Current work is focusing on understanding the mechanisms of the orientation process and the relationship among field strength, time in the field, and properties.

Keywords: Organic Polymers, Magnetic Processing, Mechanical Properties

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

The objective of this project is to develop and optimize a joining method that can be applied to large scale fabrication of components such as radiant burner tubes and high temperature, high pressure heat exchangers. Microwave joining of both reaction bonded silicon carbide and sintered silicon carbide has been demonstrated for tubes up to 5 cm in diameter. Joints are leak tight at service temperature, and have adequate mechanical strength for desired applications. Work is continuing to scale-up tube joining further (up to 11.4 cm diameter) and to develop a joining method using preceramic polymers. Collaborative work with an industrial partner has been initiated to demonstrate scale-up of the joining technique on a radiant burner tube assembly application in the steel industry.

Keywords: Microwave Processing, Microwave Joining, SiC

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

29. **Ni_3Al TECHNOLOGY TRANSFER - STEEL MILL ROLLS AND FURNACE FIXTURES**
$1,050,000
DOE Contact: Charles A. Sorrell, (202) 586-1514
ORNL Contacts: M. L. Santella, (615) 574-4805 and V. K. Sikka, (615) 574-5112

The objective of this project is to apply the excellent oxidation and carburization resistance and higher strength of nickel aluminides to Industries of the Future related manufacturing applications. Progress in bringing technologies to development and commercialization in FY 1995 included: (1) Development of a new process known as *Exo-Melt* for the commercial melting of nickel aluminide alloys (winner of an R&D 100 Award in 1995); (2) In-service testing of nickel aluminide rolls for steel mill reheat furnaces for over a year. Alloy and welding methods were developed by Oak Ridge National Laboratory; alloys were produced by Metallamics, Inc., rolls were cast by Sandusky International, and rolls continue to be tested by Bethlehem Steel; (3) Long-term, in-service testing of nickel aluminide tray and fixtures for industrial carburizing furnaces. Alloy and casting methods were developed by Oak Ridge National Laboratory, casting was done by Alloy Engineering and Casting Co., and testing is being performed by General Motors Saginaw Division.

Keywords: Nickel Aluminides, Processing, Melting, In-Service Testing

30. **ADVANCED MICROWAVE PROCESSING CONCEPTS**
$250,000
DOE Contact: Charles A. Sorrell, (202) 586-1514
ORNL Contacts: R. J. Lauf and H. D. Kimrey, (615) 574-5176

The purpose of this project is to explore the feasibility of several advanced microwave processing concepts to develop new energy-efficient materials and processes as well as to reduce consumption of strategic metals. A variable frequency microwave furnace was developed by Oak Ridge National Laboratory and commercialized by Lambda Technologies. Current emphasis is on determining the curing behavior of thermosetting resins and polymer-matrix composites under microwave heating conditions. The cure time, physical properties, and uniformity of neat resins and prepreg layups as a function of microwave heating conditions such as average frequency, bandwidth, and power are being investigated.

Keywords: Microwave Processing, Polymers, Composites, Variable Frequency

31. **SELECTIVE INORGANIC THIN FILMS**
$400,000
DOE Contact: Charles A. Sorrell, (202) 586-1514
Sandia National Laboratories Contact: Mark Phillips, (505) 844-8969

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

Keywords: Coatings, Sol-Gel Processing

32. **CHEMICAL VAPOR INFILTRATION OF TiB_2 COMPOSITES**
$100,000
DOE Contact: Charles A. Sorrell, (202) 586-1514
Oak Ridge National Laboratory Contact: T. Besmann, (615) 574-6852

This program is designed to develop a Hall-Heroult aluminum smelting cathode with substantially improved properties. The carbon cathodes in current use require significant anode-to-cathode spacing in order to prevent shorting, causing significant electrode inefficiencies. A fiber reinforced-TiB_2 matrix composite would have the requisite wettability, strength, strain-to-failure, cost, and lifetime to solve this problem. The approach is to fabricate a cathode material through chemical vapor infiltration (CVI). Large-scale specimens (8 in^2 plates) for testing by the Alcoa Technical Center in bench-scale Hall-Heroult cells were prepared, at substantially reduced processing times, utilizing a forced chemical vapor infiltration (FCVI) system with a modified reactant feed system.

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

ADVANCED TURBINE SYSTEMS PROGRAM

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

33. **CERAMIC COMPONENTS FOR STATIONARY GAS TURBINES IN COGENERATION SERVICE**
$6,500,000
DOE Contact: S. Blazewicz, (202) 586-4679
Solar Contact: M. Van Roode, (619) 544-5549

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

Keywords: Structural Ceramics, Cogeneration, Gas Turbines

34. **LONG-TERM TESTING OF CERAMIC COMPONENTS FOR STATIONARY GAS TURBINES**
$500,000
DOE Contact: S. Blazewicz, (202) 586-4679
ORNL Contact: M. Ferber, (615) 576-0818

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

Keywords: Structural Ceramics, Cogeneration, Gas Turbines

35. **ATS MATERIALS BASE TECHNOLOGY SUPPORT**
$4,000,000
DOE Contact: S. Blazewicz, (202) 586-4679
ORNL Contact: M. Karnitz, (615) 576-5150

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

Keywords: Gas Turbines, Castings, Thermal Barrier Coatings

HEAT EXCHANGER PROGRAM

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

36. **ADVANCED HEAT EXCHANGER MATERIAL TECHNOLOGY DEVELOPMENT**
$617,000
DOE Contact: G. Varga, (202) 586-0082
ORNL Contact: M. Karnitz, (423) 574-5150

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

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

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

37. **CERAMIC COMPOSITE HEAT EXCHANGER FOR THE CHEMICAL INDUSTRY**
$138,801
DOE Contact: G. Varga, (202) 586-0082
Babcock & Wilcox Contact: D. Hindman, (804) 522-5825

The performance evaluation of an advanced ceramic composite heat exchanger in the high temperature, corrosive environment of a hazardous waste incinerator has been completed. Evaluation of the materials involved has been completed and a final report is in preparation.

Keywords: Ceramic Composites, Structure

38. **HiPHES SYSTEM FOR ENERGY PRODUCTION**
$316,676
DOE Contact: G. Varga, (202) 586-0082
Solar Turbines Contact: B. Harkins, (619) 544-5398

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

Keywords: Ceramic Composites, Heat Exchangers

39. **HiPHES SYSTEM FOR ETHYLENE PRODUCTION**
$1,036,000
DOE Contact: G. Varga, (202) 586-0082
Stone & Webster Engineering Corp. Contact: J. Gondolfe, (713) 368-4379

This project has been reoriented. The new target is a steam cracker for ethylene production, a more attainable goal with a more wide-spread applicability than the steam reformer planned previously. Research on critical material needs continues taking full advantage of previous data which will apply to the new goal.

Keywords: Composites, Heat Exchangers

CONTINUOUS FIBER CERAMIC COMPOSITES (CFCC) PROGRAM

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

40. **CFCC PROGRAM - INDUSTRY TASKS**
    $5,977,000
    DOE Contact: M. Smith, (202) 586-3646

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

Keywords: Ceramic Composites, Continuous Fiber

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

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

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

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

OFFICE OF TRANSPORTATION TECHNOLOGIES

	FY 1995
Office of Transportation Technologies - Grand Total	$24,851,000
Office of Transportation Materials	$12,646,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 5,282,000
Powder Characterization (WBS No. 1118)	110,000
Microwave Sintering (WBS No. 1124)	400,000
Cost-Effective Silicon Nitride Powder (WBS No. 1125)	0
Cost-Effective Sintering of Silicon Nitride Ceramics (WBS No. 1127)	121,000
Advanced Processing (WBS No. 1141)	0
Improved Processing (WBS No. 1142)	650,000
Processing of Silicon Based Ceramics (WBS No. 1225)	267,000
In Situ Toughened Silicon Nitride (WBS No. 1226)	353,000
In Situ Toughened Silicon Nitride (WBS No. 1231)	350,000
Low Thermal Expansion Ceramics (WBS No. 1243)	100,000
NZP Components (WBS No. 1245)	0
Low Cost Aluminum Titanate/NZP Ceramics (WBS No. 1246)	0
Advanced Manufacturing (WBS No. 1520)	397,000
Advanced Ceramic Manufacturing (WBS No. 1521)	991,000
Advanced Ceramic Manufacturing (WBS No. 1522)	1,543,000
Materials Properties, Behavior, Characterization or Testing	$ 3,873,000
Development of Standard Test Methods for Evaluating the Wear Performance of Ceramics (WBS No. 2222)	30,000
Advanced Statistics Calculations (WBS No. 2313)	0
Microstructural Analysis (WBS No. 3111)	50,000
Microstructural Characterization of Silicon Carbide and Silicon Nitride Ceramics for Advanced Heat Engines (WBS No. 3114)	200,000
Project Data Base (WBS No. 3117)	240,000
Fracture Behavior of Toughened Ceramics (WBS No. 3213)	290,000
Cyclic Fatigue of Toughened Ceramics (WBS No. 3214)	220,000
Tensile Stress Rupture Development (WBS No. 3215)	300,000
Life Prediction Verification (WBS No. 3216)	200,000
Toughened Ceramics Life Prediction (WBS No. 3217)	200,000
Life Prediction Methodology (WBS No. 3222)	0
Life Prediction Methodology (WBS No. 3223)	600,000
Environmental Effects in Toughened Ceramics (WBS No. 3314)	383,000
High Temperature Tensile Testing (WBS No. 3412)	500,000
Standard Tensile Test Development (WBS No. 3413)	125,000
Non-Destructive Evaluation (WBS No. 3511)	335,000
Computed Tomography (WBS No. 3515)	120,000
Nuclear Magnetic Resonance (NMR) Imaging (WBS No. 3516)	80,000
Technology Transfer and Management Coordination	$ 950,0000
Management and Coordination (WBS No. 111)	700,000
International Exchange Agreement (IEA) (WBS No. 4115)	0
Standard Reference Materials (WBS No. 4116)	150,000
Mechanical Property Standardization (WBS No. 4121)	100,000

OFFICE OF TRANSPORTATION TECHNOLOGIES (Continued)

	FY 1995
Office of Transportation Materials (continued)	
Device or Component Fabrication, Behavior or Testing	$2,541,0000
Advanced Coating Technology (WBS No. 1311)	175,000
Coatings to Reduce Contact Stress Damage of Ceramics (WBS No. 1313)	0
Wear Resistant Coatings (WBS No. 1331)	0
Wear Resistant Coatings (WBS No. 1332)	0
Thick Thermal Barrier Coating Systems for Low Heat Rejection Diesel Engines (WBS No. 1342)	0
Active Metal Brazing PSZ-Iron (WBS No. 1411)	220,000
Surface Durability of Machined Ceramics (WBS No. 1500)	200,000
Next-Generation Grinding Wheel (WBS No. 1501)	392,000
Grindability Test (WBS No. 1502)	0
Chemically Assisted Grinding of Ceramics (WBS No. 1503)	150,000
Grinding Consortium (WBS No. 1503)	150,000
High Speed Grinding (WBS No. 1504)	372,000
Laser-Based NDE Methods (WBS No. 1507)	180,000
Grinding Machine Stiffness (WBS No. 1510)	227,000
Next Generation Grinding Spindle (WBS No. 1511)	225,000
Process Cost Model (WBS No. 1512)	250,000
Office of Propulsion Systems	$12,205,000
Advanced Propulsion Division	$ 7,595,000
Materials Properties, Behavior, Characterization or Testing	$ 100,000
NASA Supporting Research and Technology	100,000
Device or Component Fabrication, Behavior or Testing	$ 7,495,000
Hybrid Vehicle Turbine Engine (HVTE) Technology Support	3,600,000
Ceramic Turbine (CT) Engine Demonstration Project	3,500,000
Advanced Diesel Engine Component Development Project	100,000
Advanced Piston and Cylinder Component Development	70,000
Advanced Piston and Cylinder Component Development	150,000
Microwave Regenerated Particulate Trap	75,000
Electric and Hybrid Propulsion Division	$ 4,610,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 1,025,000
Electrochemical Properties of Solid-State Sodium/Polymer Cells	275,000
Improved Container Electrode Coatings for Sodium/Sulfur Battery Systems	0
The Performance of New Materials for Polymer Electrolyte Batteries	140,000
Novel Polymer Electrolytes for Rechargeable Lithium Batteries	180,000
Novel Solid Polymer Electrolytes for Advanced Secondary Batteries	110,000
Sol-Gel Electrolytes in Lithium Batteries	0
New Cathode Materials	155,000
Development of High Energy Density Cathodes for Sodium/Polymer Cells	165,000

OFFICE OF TRANSPORTATION TECHNOLOGIES (Continued)

	FY 1995
Office of Propulsion Systems (continued)	
Electric and Hybrid Propulsion Division (continued)	
Materials Properties, Behavior, Characterization or Testing	$3,385,000
Surface Morphology of Metals in Electrodeposition/Carbon Electrochemistry	270,000
Fabrication & Testing of Carbon Electrodes as Lithium Intercalation Anodes	200,000
Battery Materials: Structure and Characterization	150,000
In Situ Spectroscopic Applications to the Study of Rechargeable Lithium Batteries	150,000
Polymer Electrolyte for Ambient Temperature Traction Batteries: Molecular Level Modeling for Conductivity Optimization	160,000
Analysis and Simulation of Electrochemical Systems	240,000
Heat Transport and Thermal Management in Advanced Batteries	175,000
Electrode Surface Layers	140,000
Electrode Kinetics and Electrocatalysis	400,000
Effect of Electrocatalyst and Electrolyte Composition on Methanol/Air Fuel Cell Performance	200,000
Poisoning of Fuel Cell Electrocatalyst Surfaces: NMR Spectroscopic Studies	200,000
Fuel Cells for Renewable Applications	1,000,000
Electrocatalysis of Fuel Cell Reactions	100,000
Device or Component Fabrication, Behavior or Testing	$200,000
Zn/NiOOH Cell Studies	0
Applied Research on Secondary Zn/NiOOH Battery Technology	0
Development of a Thin-Film Rechargeable Lithium Battery for Electric Vehicles	0
Na/SRPE Electric Vehicle Batteries	200,000
Lithium-Ion Battery Testing	0
Novel Concepts for an Oxygen Electrode in Secondary Metal-Air Batteries	0

OFFICE OF TRANSPORTATION TECHNOLOGIES

The Office of Transportation Technologies seeks to develop, in cooperation with industry, technologies that are more energy efficient, that will enable the transportation sector to shift to alternative fuels and electricity, and that will minimize the environmental impacts of transportation energy use. Materials research and development within the Office of Transportation Technologies is conducted by the Office of Transportation Materials, the Office of Propulsion Systems, and the Office of Alternative Fuels, each having responsibility for specific technologies and program areas.

OFFICE OF TRANSPORTATION MATERIALS

The overall goal of the Materials Technology Program is to develop, in concert with the United States-based industry, an industrial technology base in cost-effective, advanced transportation-related materials and associated processing of these materials. The timely availability of these materials and processing techniques will enable the development of more energy-efficient transportation technologies capable of utilizing alternative fuels and electricity. Research and development activities focus on: (a) propulsion system materials (specifically cost-effective ceramics which are critical to the development of more efficient advanced heat engines for transportation propulsion); (b) vehicle system materials (specifically lightweight materials that could aggressively reduce the weight and improve the fuel economy of vehicles without compromise to passenger comfort and safety); and (c) operation of the High Temperature Materials Laboratory.

The Propulsion System Materials Program focuses on the development of reliable, cost-effective ceramics to facilitate their commercial introduction in propulsion systems. Program efforts concentrate on reducing the cost of ceramic components and improving their performance. A majority of the research is conducted by industry. The Ceramic Technology Program is managed by the Oak Ridge National Laboratory (ORNL). The DOE Contact is Robert Schulz, (202) 586-8051.

The Vehicle System Materials Program focuses on the development of cost-effective processing and manufacturing of advanced lightweight material components that will, in the near term, continually improve the fuel economy of current production vehicles, and in the long term, allow aggressive weight reductions needed for hybrid and electric vehicles. Lightweight materials will be increasingly important in achieving the energy, economic, and environmental goals for the transportation sector. The DOE Contact is Sidney Diamond, (202) 586-8032.

The High Temperature Materials Laboratory (HTML) at the Oak Ridge National Laboratory is a state-of-the-art research and user facility which supports advanced materials research conducted by the Department of Energy, as well as by industry, universities, and other research and development laboratories. The HTML currently includes six user centers (equipped primarily for characterizing materials), namely: materials analysis, high temperature mechanical properties, high temperature x-ray diffraction, physical properties, ceramic specimen preparation, and residual stress measurements. A seventh center includes instrumentation for conducting sophisticated research on machining of advanced ceramic materials with the goal of working directly with industrial teams to achieve cost-effective manufacturing. The DOE Contact is Debbie Haught, (202) 586-2211.

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

42. **POWDER CHARACTERIZATION (WBS NO. 1118)**
$110,000
DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. R. Johnson, (423) 576-6832
NIST Contact: S. Malghan, (301) 975-2000

This effort is directed toward developing a fundamental understanding of surface chemical changes which take place when silicon nitride powder is attrition milled in an aqueous environment. This project also will demonstrate the use of and establish operating conditions for high energy attrition milling of silicon nitride powder. These tasks will be accomplished by developing measurement techniques and data on the effect of milling variables on the resulting powder. It is expected that information gained from this study will serve in the identification and development of appropriate characterization procedures, process control techniques, and in certification of new Standard Reference Materials.

Keywords: Powder Characterization, Powder Processing, Reference Material, Silicon Nitride

43. **MICROWAVE SINTERING (WBS NO. 1124)**
$400,000
DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. R. Johnson, (423) 576-6832
ORNL Contact: T. N. Tiegs, (423) 574-5173

The objective of this effort is to identify those aspects of microwave processing of silicon nitride that might

(1) accelerate densification, (2) permit sintering to high density using much lower levels of sintering aids, (3) lower the sintering temperature, (4) produce unique microstructures, or (5) contribute to cost-effectiveness of silicon nitride materials.

Early work included investigations of the microstructure development of dense silicon nitride materials annealed in the microwave furnace and the sintering of silicon nitride powder compacts in the 2.45- or 28-GHz units. While improvements were observed in the properties of the materials fabricated, the cost-effectiveness of the microwave processing was marginal. Another approach dealt with the fabrication of sintered reaction-bonded silicon nitride (SRBSN) and was done entirely in the 2.45-GHz microwave furnace. SRBSN is a cost-effective method to fabricate silicon nitride ceramics. Raw materials costs are less than about 1/4 those for high-purity silicon nitride materials, which improves the cost-competitiveness of these materials with metal parts. Conventional SRBSN requires long nitridation times and two-step firing. By using microwave heating, nitridation times are reduced and all firing is performed in a one-step continuous process, simplifying the operation. Current activities involve the scale-up of the microwave process to large quantities of parts.

Keywords: Microwave Sintering, Silicon Nitride, SRBSN

44. **COST-EFFECTIVE SILICON NITRIDE POWDER (WBS NO. 1125)**
$0
DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: S. G. Winslow, (423) 574-0965
Dow Contact: G. A. Eisman, (517) 638-7864

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

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

45. **COST-EFFECTIVE SINTERING OF SILICON NITRIDE CERAMICS (WBS NO. 1127)**
$121,000
DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: T. N. Tiegs, (423) 574-5173
Southern Illinois University (SIU) Contact:
D. E. Wittmer, (618) 453-7006/7924

The objective of this effort is to investigate the potential of cost-effective sintering of Si_3N_4 through the development of continuous sintering techniques and the use of lower cost Si_3N_4 powders and sintering aids. Specifically, the tasks for Phase III are to: (1) continue the evaluation of continuous sintering parameters on properties of selected Si_3N_4 compositions, (2) continue the evaluation of low-cost Si_3N_4 powders, (3) design and construct a prototype belt furnace capable of sintering a large number of parts. The prototype belt furnace has been constructed by Centorr/Vacuum Industries, Inc., and installed and tested at SIU.

Keywords: Cost Effective Ceramics, Silicon Nitride, Sintering

46. **ADVANCED PROCESSING (WBS NO. 1141)**
$0
DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: R. L. Beatty, (423) 574-4536
Norton Contact: D. M. Tracey, (508) 393-5811

The purpose of this task was to develop and demonstrate significant improvements in processing methods, process controls, and nondestructive evaluation (NDE) which can be commercially implemented to produce high-reliability silicon nitride components for advanced heat engine applications at temperatures to 1370°C.

A silicon nitride - 4 wt % yttria composition was used and densification was performed by glass encapsulation hot isostatic pressing. Process demonstration provided data and experience which suggest that the material developed in this program, NCX-5102, truly ranks as a world-class silicon nitride material. The test program established a mean tensile strength of 997 MPa with a fracture toughness approaching 7 $MPa \cdot m^{1/2}$ for the demonstration set of 320 tensile rods.

Keywords: Nondestructive Evaluation, Silicon Nitride, Processing, Processing Controls

47. **IMPROVED PROCESSING (WBS NO. 1142)**
$650,000
DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contacts: D. R. Johnson, (423) 576-6832 and S. D. Nunn, (423) 576-1668

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

Keywords: Powder Processing, Silicon Nitride, Gelcasting

48. **PROCESSING OF SILICON BASED CERAMICS (WBS NO. 1225)**
$267,000
DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. R. Johnson, (423) 576-6832
University of Michigan Contact: T. Y. Tien, (313) 764-9449

The properties of silicon nitride can be optimized by microstructural design, specifically by developing fiber-like β-Si_3N_4 grains and control of the grain-boundary phase. The purpose of this investigation is to optimize the properties of silicon nitride ceramics by microstructure design.

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

49. **IN SITU TOUGHENED SILICON NITRIDE (WBS NO. 1226)**
$353,000
DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: T. N. Tiegs, (423) 574-5173
AlliedSignal Ceramic Components Contact: H. C. Yeh, (213) 618-7449

The purpose of this effort is to develop compositions and processes to obtain high fracture toughness and strength for silicon nitride (Si_3N_4)-based ceramic materials through microstructure control. Under Phase I, an in situ reinforced silicon nitride material (AS800) with elongated grain microstructure was developed. Phase II expanded the AS800 material property database and built on Phase I results to further improve material properties and processing. The objectives of Phase III are to further expand the material properties database, improve high-temperature behavior, and develop cost-effective, advanced fabrication techniques for this material.

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

50. **IN SITU TOUGHENED SILICON NITRIDE (WBS NO. 1231)**
$350,000
DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contacts: D. R. Johnson, (423) 576-6832 and T. N. Tiegs, (423) 574-5173

Significant improvement in the reliability of structural ceramics for advanced engine applications could be attained if the critical fracture toughness (K_{Ic}) were increased without strength degradation. Early results from ORNL research showed that significant increases in fracture toughness could be achieved by manipulating the microstructure to promote toughening mechanisms such as crack bridging. Excellent properties were obtained in this manner for the alumina and mullite matrix systems reinforced with SiC whiskers. In silicon nitride, acicular or elongated grains can be generated by in situ growth and these can provide significant toughening on the same order as the whisker-toughened materials. Microstructural development to promote this type of growth in silicon nitride is the current emphasis of this project.

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

51. **LOW THERMAL EXPANSION CERAMICS (WBS NO. 1243)**
$100,000
DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contacts: D. R. Johnson, (423) 576-6832 and D. P. Stinton, (423) 574-4556

The objective of this effort is to coordinate efforts regarding the application of low-expansion ceramics in advanced heat engines. Contracts have been placed with Golden Technologies, Inc., and LoTEC, Inc., to develop cost-effective processes for the fabrication of portliners. Golden is investigating Al_2TiO_5 and $Ca_{1-x}Mg_xZr_4P_6O_{24}$, while LoTEC is working with $Ba_{1+x}Zr_4P_{6-2x}Si_{2x}O_{24}$ (BaZPS) and $Ca_{1-x}Sr_xZr_4P_6O_{24}$. ORNL is assisting Golden Technologies and LoTEC with the characterization and evaluation of their compositions.

Keywords: Alumina, Beta-eucryptite, Phosphate, Physical/Mechanical Properties, Structural Ceramics, Ultra-low Expansion

52. **NZP COMPONENTS (WBS NO. 1245)**
$0
DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. P. Stinton, (423) 574-4556
LoTEC, Inc. Contact: Santosh Limaye, (801) 277-6940

The overall objective of this effort is to develop sodium-zirconium-phosphate (NZP) ceramic-based, 'cast-in-place, diesel-engine portliners. Specific objectives are: (1) perform materials requirements analyses, (2) successfully demonstrate metal casting around the ceramic, (3) develop a cost-effective process, and (4) develop a high-temperature database (e.g., stability, thermal cycling, thermal shock) for these materials. LoTEC will continue to develop and scale up production of sodium-zirconium-phosphate (NZP) materials developed at Penn State University.

Keywords: Structural Ceramics, Ultra-low Expansion, Zirconia

53. **LOW COST ALUMINUM TITANATE/NZP CERAMICS (WBS NO. 1246)**
$0
DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. P. Stinton, (423) 574-4556

The objective of this work was to develop a low-thermal-conducting, high-thermal-shock-resistant, ceramic portliner which can survive casting in grey iron and diesel engine operation. Golden Technologies worked on developing their own aluminum titanate material and, in addition, on scaling up production of a unique NZP material developed at Virginia Polytechnic Institute and State University.

Keywords: Structural Ceramics, Ultra-low Expansion, Zirconia

54. **ADVANCED MANUFACTURING (WBS NO. 1520)**
$397,000
DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. R. Johnson, (423) 576-6832
Kyocera Contact: E. Kraft, (206) 750-6147

The objective of this program is to develop the cost-effective manufacturing technology required for ceramic turbine rotors for use in turbochargers for heavy duty diesel truck and bus applications. A team, led by Kyocera and including Schwitzer U.S., Inc. and Caterpillar Inc., will develop and demonstrate production readiness for reliable, cost affordable, turbochargers with ceramic turborotors. Program goals include a nominal order of magnitude reduction in cost over the present cost for small quantities, and process capability for critical component attributes which is adequate for the performance and reliability specifications of the application. Silicon nitride SN 235 is the material of choice for this application.

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

55. **ADVANCED CERAMIC MANUFACTURING (WBS NO. 1521)**
$991,000
DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: A. E. Pasto, (423) 574-4956
Norton Contact: Eric Bright, (203) 653-8071

The objectives of this program are to design, develop, and demonstrate advanced manufacturing technology for the production of ceramic exhaust valves for a diesel engine using Norton Advanced Ceramics' NT 451 SiAlON. The component to be developed and tested is the exhaust valve for Detroit Diesel Corporation (DDC)'s Series 149 engine. Specific objectives are to: (1) reduce manufacturing costs by at least an order of magnitude over current levels; (2) develop and demonstrate process capability values of 0.7 or less for all critical component attributes; and (3) to validate ceramic valve performance, durability, and reliability in rig and engine testing.

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

56. **ADVANCED CERAMIC MANUFACTURING (WBS NO. 1522)**
$1,543,000
DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: R. L. Beatty, (423) 574-4536

The objective of this program was to develop a cost-competitive, viable manufacturing process for advanced ceramic engine components. To achieve this goal, two components, utilizing two materials, for two engine companies, were selected. Both components share simple, right-circular geometries and similar manufacturing processes. Key challenges in this program were to meet tight tolerances and yet maintain high yields required to meet cost objectives. Three major activities were to occur in parallel: (1) DDC component design/development, (2) Cummins component design/development, and

(3) intelligent processing and statistical process control development/implementation.

Keywords: Components, Cost Effective Ceramics, Process Control

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

57. **DEVELOPMENT OF STANDARD TEST METHODS FOR EVALUATING THE WEAR PERFORMANCE OF CERAMICS (WBS NO. 2222)**
$30,000
DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contacts: D. R. Johnson, (423) 576-6832 and P. J. Blau, (423) 574-5377

The goal of this effort is to improve consistency in reporting ceramic wear test data by helping to develop one or more standard test methods for quantitatively determining the wear resistance of structural ceramics in reciprocating sliding, a type of motion which is experienced by several types of engine parts. ORNL is working with the American Society for Testing of Materials (ASTM) to meet this objective.

Keywords: Structural Ceramics, Test Procedures, Wear

58. **ADVANCED STATISTICS CALCULATIONS (WBS NO. 2313)**
$0
DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: M. K. Ferber, (423) 576-0818
GE Contact: C. A. Johnson, (518) 387-6421

The design and application of reliable load-bearing structural components from ceramic materials requires a detailed understanding of the statistical nature of fracture in brittle materials. The overall objective was to advance the current understanding of fracture statistics, especially in the areas of optimum testing plans and data analysis techniques, consequences of time-dependent crack growth on the evolution of initial flaw distributions, confidence and tolerance bounds on predictions that use the Weibull distribution and function, strength distributions in multiaxial stress fields, and goodness-of-fit-tests for the Weibull model of strength. The studies were carried out largely by analytical and computer simulation techniques. Actual fracture data were then used as appropriate to confirm and demonstrate the resulting data analysis techniques.

Keywords: Design Codes, Life Prediction, Statistics, Weibull, Fracture, Structural Ceramics, Instrumentation or Technique Development

59. **MICROSTRUCTURAL ANALYSIS (WBS NO. 3111)**
$50,000
DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. R. Johnson, (423) 576-6832
NIST Contact: S. M. Wiederhorn, (301) 975-5772

The objective of this work was to identify the mechanisms of failure in structural ceramics subjected to mechanical loads in various test temperatures and environments. This is a companion project to a related task in which advanced ceramics are characterized in tensile creep. Of particular interest is the damage that accumulates in structural ceramics as a consequence of high temperature exposure to environments and stresses normally present in heat engines. Materials studied included sialons, silicon nitride, and sintered silicon carbide.

Keywords: Corrosion, Engines, Erosion, High Temperature Performance, Structural Ceramics, Silicon Carbide, Creep, SiAlON, Silicon Nitride

60. **MICROSTRUCTURAL CHARACTERIZATION OF SILICON CARBIDE AND SILICON NITRIDE CERAMICS FOR ADVANCED HEAT ENGINES (WBS NO. 3114)**
$200,000
DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contacts: D. R. Johnson, (423) 576-6832 and T. A. Nolan, (423) 574-0811

The purpose of this work is to determine the microstructure of both monolithic and composite ceramics and to relate that microstructure to mechanical properties and material performance. Specifically, the materials of interest are silicon carbides and silicon nitrides developed by U.S. manufacturers as part of this program and the Advanced Turbine Technology Applications Program (ATTAP). A major objective is to use electron microscopy and surface chemistry to characterize the chemistry, crystallography, and morphology of phases present with particular emphasis on the structure and chemistry of grain boundaries and other interfaces.

A second major objective is to relate those microstructural observations to available mechanical test data produced by other participants in the ATTAP and Ceramic Technology programs. Ceramic specimens from foreign sources are also characterized to provide comparative information on microstructural properties. A new initiative began in FY 1995. With increased emphasis being placed on supporting the automotive and diesel industry in the U.S., a program that relates the microstructure of catalysts to catalyst performance has been initiated.

Keywords: Catalyst Performance, Catalysts, Silicon Carbide, Silicon Nitride, Microstructure, Chemical Analysis, Mechanical Properties, Scanning Electron Microscopy

61. **PROJECT DATA BASE (WBS NO. 3117)**
$240,000
DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contacts: D. R. Johnson, (423) 576-6832 and B. L. Keyes, (423) 574-5113

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

Keywords: Database, Mechanical Properties, Structural Ceramics

62. **FRACTURE BEHAVIOR OF TOUGHENED CERAMICS (WBS NO. 3213)**
$290,000
DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contacts: D. R. Johnson, (423) 576-6832 and P. F. Becher, (423) 574-5157

Ceramics with reinforcing microstructures and ceramic composites offer important advantages for heat engine applications. In addition to improved fracture toughness, these materials often exhibit substantial improvement in damage, thermal shock, and slow-crack-growth resistance. In this effort, studies are conducted to determine mechanical properties (e.g., creep, delayed failure, strength, and toughness) at elevated temperatures for these toughened ceramics. Particular emphasis is placed on understanding how microstructure and composition influence the mechanical performance at elevated temperatures and the stability of these properties for extended periods.

Keywords: Toughened Ceramics, Mechanical Properties, Silicon Carbide, Silicon Nitride, Alumina

63. **CYCLIC FATIGUE OF TOUGHENED CERAMICS (WBS NO. 3214)**
$220,000
DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contacts: D. R. Johnson, (423) 576-6832 and K. C. Liu, (423) 574-5116

The objective of this task is to develop and demonstrate the capability of performing uniaxial tension-tension dynamic fatigue testing of structural ceramics at elevated temperature. The effort includes (1) design, fabrication, and demonstration of a load-train column capable of concentric load transfer between grip and specimen at high temperature; and (2) development of the baseline information on the tensile fatigue behavior of structural ceramics at room and elevated temperatures.

Keywords: Cyclic Fatigue, High Temperature Properties, Toughened Ceramics, Tensile Testing, Silicon Nitride

64. **TENSILE STRESS RUPTURE DEVELOPMENT (WBS NO. 3215)**
$300,000
DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contacts: D. R. Johnson, (423) 576-6832 and K. C. Liu, (423) 574-5116

The objective of this task is to develop the test capability for performing uniaxial tensile stress-rupture and creep tests on candidate structural ceramics at high temperature in the range where time-dependent deformation can occur. Creep and creep-rupture design databases will be generated using uniaxial tensile specimens tested in the range of 1150-1370°C. The resulting stress-rupture and creep data will be used to evaluate and refine existing constitutive models. New constitutive models will be developed to facilitate design analyses of high-temperature structural components and improve their reliability.

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

65. **LIFE PREDICTION VERIFICATION (WBS NO. 3216)**
$200,000
DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contacts: D. R. Johnson, (423) 576-6832 and M. K. Ferber, (423) 576-0818

The goal of the proposed research program is to systematically verify life prediction methodologies appropriate for structural ceramic engine components. An emphasis will be to achieve predictability at a level acceptable to end users, in particular, those users associated with the manufacturing of internal combustion engine valves. This effort is comprised of four tasks: (1) characterization of material/mechanical performance using standard testing coupons, (2) life prediction analysis of prototype diesel engine valves, (3) actual mechanical testing of prototype engine valves, and (4) verification of life prediction codes. A valve-testing facility will be specifically developed for static and cyclic tensile testing of the prototype valve geometries at appropriate temperatures.

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

66. **TOUGHENED CERAMICS LIFE PREDICTION (WBS NO. 3217)**
    $200,000
    DOE Contact: Robert B. Schulz, (202) 586-8051
    ORNL Contact: D. R. Johnson, (423) 576-6832
    NASA - Lewis Research Center Contact:
    John P. Gyekenyesi, (216) 433-3210

The purpose of this research is to understand the room-temperature and high-temperature behavior of toughened ceramics as the basis for developing a life prediction methodology. A major objective is to understand the relationship between microstructure and the mechanical behavior within the bounds of a limited number of materials. A second major objective is to determine behavior as a function of time and temperature. Specifically, strength and reliability, fracture toughness, slow crack growth, and creep behavior will be determined as a function of temperature for the as-manufactured material. The same properties will also be evaluated after long-time exposure to various high- temperature isothermal and cyclic environments. These results will provide input for parallel materials development and design methodology programs. Resultant design codes will be verified.

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

67. **LIFE PREDICTION METHODOLOGY (WBS NO. 3222)**
    $0
    DOE Contact: Robert B. Schulz, (202) 586-8051
    ORNL Contact: C. R. Brinkman, (423) 574-5106
    Allison Contact: N. J. Provenzano, (313) 230-3150

The goal of this effort was to develop a methodology which can be used during the design phase to predict the structural behavior of ceramic components. There were four major technical tasks: (1) material database/material characterization, (2) development of nondestructive evaluation technology, (3) development of analytical life-prediction models, and (4) verification. GTE's PY6 injection-molded and hot isotropic pressed silicon nitride was selected for characterization which involved both room- and elevated-temperature tests using a variety of specimen types. Four failure modes were addressed: fast fracture, slow crack growth, creep, and oxidation. The life-prediction models developed as part of this work have been incorporated into NASA's CARES code.

Keywords: Creep, Failure Analysis, Failure Testing, Oxidation, Life Prediction, Nondestructive Evaluation, Silicon Nitride

68. **LIFE PREDICTION METHODOLOGY (WBS NO. 3223)**
    $600,000
    DOE Contact: Robert B. Schulz, (202) 586-8051
    ORNL Contact: C. R. Brinkman, (423) 574-5106
    AlliedSignal Engines Contact: N. Menon,
    (602) 231-1230

This Phase II program will develop the methodology required to adequately predict the useful life of ceramic components used in advanced heat engines. Phase II efforts will concentrate on predictive methodology for time- and cycle-dependent failure modes, as well as proof testing and nondestructive evaluation (NDE) methodology to enhance component reliability through screening out of low-strength components. The life prediction methodologies developed will be generic and hence will be applicable to ceramic components that operate under known temperature and stress conditions. The technical effort has been organized into six areas: (1) material baseline, (2) compressive creep methodology, (3) flaw growth methodology, (4) cyclic fatigue methodology, (5) proof test methodology, and (6) NDE reliability methodology.

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

69. **ENVIRONMENTAL EFFECTS IN TOUGHENED CERAMICS (WBS NO. 3314)**
    $383,000
    DOE Contact: Robert B. Schulz, (202) 586-8051
    ORNL Contact: M. K. Ferber, (423) 576-0818
    University of Dayton Contact: N. L. Hecht,
    (513) 229-4341

The objective of this task is to investigate the effects of environment on the mechanical behavior of commercially available ceramics being considered for heat engine applications.

Keywords: Fatigue, Engines, Structural Ceramics, Environmental Effects, Alumina, Zirconia, Diesel Combustion, Tensile Testing, Time-Dependent, Transformation-Toughened

70. **HIGH TEMPERATURE TENSILE TESTING (WBS NO. 3412)**
$500,000
DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. R. Johnson, (423) 576-6832
North Carolina A&T State University Contact: J. Sankar, (919) 334-7620

The objective of this research is to test and evaluate the long-term mechanical reliability of Si_3N_4 at temperatures up to 1300°C. Microstructural/microchemical analysis of the fracture surfaces using scanning electron microscopy (SEM), transmission electron microscopy (TEM), and energy-dispersive spectral analysis (EDS) is an integral part of this effort.

Keywords: Creep, Fracture, Silicon Nitride, Structural Ceramics, Tensile Testing

71. **STANDARD TENSILE TEST DEVELOPMENT (WBS NO. 3413)**
$125,000
DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. R. Johnson, (423) 576-6832
NIST Contact: S. M. Wiederhorn, (301) 975-5772

This project was concerned with the development of test equipment and procedures for measuring the strength and creep resistance of ceramic materials at elevated temperatures to assist in the development of a reliable data base for use in the structural design of heat engines for vehicular applications. Inexpensive methods of measuring tensile creep of ceramics at elevated temperatures were developed.

Keywords: Creep, High Temperature Properties, Structural Ceramics, Tensile Testing, Test Procedures

72. **NON-DESTRUCTIVE EVALUATION (WBS NO. 3511)**
$335,000
DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contacts: D. R. Johnson, (423) 576-6832 and D. J. McGuire, (423) 574-4835

The purpose of this program is to conduct nondestructive evaluation (NDE) development directed at identifying approaches for quantitative determination of conditions (including both properties and flaws) in ceramics that affect the structural performance. Those materials that have been seriously considered for application in advanced heat engines are all brittle materials whose fracture is affected by structural features whose dimensions are on the order of the dimensions of their microstructure. This work seeks to characterize those features using high frequency ultrasonics and radiography to detect, size, and locate critical flaws and to measure nondestructively the elastic properties of the host material. The studies will also address the problems unique to various fabrication techniques such as sintering, hot isostatic pressing, and gelcasting.

Keywords: Nondestructive Evaluation, Radiography, Structural Ceramics, Ultrasonics

73. **COMPUTED TOMOGRAPHY (WBS NO. 3515)**
$120,000
DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. R. Johnson, (423) 576-6832
Argonne National Lab Contact: W. A. Ellingson, (312) 972-5068

The original objectives of the Phase III work of this project were to: (1) investigate the utilization of high-spatial resolution 3-D X-Ray microcomputed tomography techniques to study density distributions in composite green-state (as-cast) pressure slip cast ATTAP rotors, and (2) correlate destructive density analysis (to be conducted by AlliedSignal Ceramic Components) of the as-cast ATTAP rotors with the 3-D microtomography density data. Because the large ATTAP rotors are no longer of technical interest, a change is being made to refocus the work to the AS-800 Si_3N_4 Series 85 nozzles being produced by AlliedSignal Ceramic Components.

Keywords: Components, Computed Tomography, Nondestructive Evaluation, Silicon Nitride, Structural Ceramics, Green State

74. **NUCLEAR MAGNETIC RESONANCE (NMR) IMAGING (WBS NO. 3516)**
$80,000
DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. R. Johnson, (423) 576-6832
Argonne National Lab Contact: W. A. Ellingson, (312) 972-5068

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

Keywords: Binder, Nondestructive Evaluation, Nuclear Magnetic Resonance, Silicon Nitride

TECHNOLOGY TRANSFER AND MANAGEMENT COORDINATION

75. **MANAGEMENT AND COORDINATION (WBS NO. 111)**
$700,000
DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. R. Johnson, (423) 576-6832

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

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

76. **INTERNATIONAL EXCHANGE AGREEMENT (IEA) (WBS NO. 4115)**
$0
DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contacts: D. R. Johnson, (423) 576-6832 and M. K. Ferber, (423) 576-0818

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

Keywords: International Energy Agency, Powder Characterization, Mechanical Properties

77. **STANDARD REFERENCE MATERIALS (WBS NO. 4116)**
$150,000
DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. R. Johnson, (423) 576-6832
NIST Contact: S. Malghan, (301) 975-5772

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

Keywords: International Energy Agency, Reference Material, Powder Characterization

78. **MECHANICAL PROPERTY STANDARDIZATION (WBS NO. 4121)**
$100,000
DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. R. Johnson, (423) 576-6832
NIST Contact: G. Quinn, (301) 975-5765

The purpose of this effort is to develop mechanical test standards in support of the Ceramic Technology Project and the Advanced Turbine Technology Applications Program.

Keywords: Mechanical Properties, Test Procedures

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

79. **ADVANCED COATING TECHNOLOGY (WBS NO. 1311)**
$175,000
DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contacts: D. R. Johnson, (423) 576-6832 and D. P. Stinton, (423) 574-4556

Sodium corrosion of SiC and Si_3N_4 components in gas turbine engines is a potentially serious problem. The objective of this effort is to develop a coating that will protect the underlying SiC or Si_3N_4 from sodium corrosion and provide simultaneous oxidation protection. To evaluate the behavior of potential materials such as stabilized ZrO_2 or HfO_2, TiO_2, and Ta_2O_5 in sodium-containing atmospheres, the corrosion resistance of hot-pressed samples of these materials will first be evaluated. A chemical vapor deposition (CVD) process will be developed for the application of the most promising coatings. The effect of the combustion environment upon coating characteristics such as microstructure, strength, adherence, and other properties will also be evaluated.

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

80. **COATINGS TO REDUCE CONTACT STRESS DAMAGE OF CERAMICS (WBS NO. 1313)**
$0
DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. R. Johnson, (423) 576-6832
Boston University Contact: V. K. Sarin, (617) 353-2842

The objective of this effort was to develop oxidation/corrosion-resistant, high toughness, adherent coating configurations for silicon-based ceramic substrates for use in advanced gas turbine engines.

Keywords: Adherence, Coatings, Contact Stress, Oxidation, Modeling, Corrosion Resistance, Mullite, Structural Ceramics

81. **WEAR RESISTANT COATINGS (WBS NO. 1331)**
$0
DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. P. Stinton, (423) 574-4556
Caterpillar Contact: M. H. Haselkorn, (309) 578-6624

The goal of this effort is to develop wear-resistant coatings for application to metallic components of low-heat-loss diesel engines, specifically, piston rings and cylinder liners. The following wear-resistant coatings were selected in Phase I: plasma-sprayed high carbon iron-molybdenum, plasma-sprayed chromia-silica, and low temperature arc vapor deposited (LTAVD) chrome nitride. A plasma-sprayed carbon iron-molybdenum and a plasma-sprayed chromia-silica were identified as wear-resistant piston-ring coatings. The three main technical tasks for Phase II are further optimization of the LTAVD chrome nitride and cast iron porcelain enamel wear coatings, process scale-up of wear-resistant plasma coatings for cylinder-liner applications, and simulated engine testing.

Keywords: Coatings, Engines, Friction, Structural Ceramics, Wear

82. **WEAR RESISTANT COATINGS (WBS NO. 1332)**
$0
DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. P. Stinton, (423) 574-4556
Cummins Contact: Malcolm Naylor, (812) 377-7713

The objective of this program is to develop advanced wear-resistant ceramic coatings for in-cylinder components for future, high-efficiency, low-emissions diesel engines. Coatings and substrates (for piston rings and cylinder liners) are to be developed to meet the following requirements:

- low wear as measured in laboratory rig tests which simulate the piston ring-cylinder liner environment near the top ring reversal in a heavy duty diesel engine
- lower friction coefficients than for the conventional system under all test conditions
- high adherence and compatibility with substrate materials
- good thermal shock resistance
- high uniformity and reproducibility

Keywords: Adherence, Coatings, Engines, Friction, Metals, Structural Ceramics, Thermal Conductivity, Wear

83. **THICK THERMAL BARRIER COATING SYSTEMS FOR LOW HEAT REJECTION DIESEL ENGINES (WBS NO. 1342)**
$0
DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. P. Stinton, (423) 574-4556
Caterpillar Contact: M. Brad Beardsley, (309) 578-8514

The objective of this effort is to advance the fundamental understanding of thick thermal barrier coating (TTBC) systems for application to low-heat-rejection diesel engine combustion chambers. Areas of TTBC technology that will be examined include powder characteristics and chemistry; bond coat compositions; coating design, microstructure, and thickness as they affect properties, durability, and reliability; and TTBC "aging" effects (microstructural and property changes) under diesel engine operating conditions.

Keywords: Coatings, Structural Ceramics

84. **ACTIVE METAL BRAZING PSZ-IRON (WBS NO. 1411)**
$220,000
DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contacts: D. R. Johnson, (423) 576-6832 and M. L. Santella, (423) 574-4805

The objective of this task is to develop strong, reliable joints containing ceramic components for applications in advanced heat engines. The overall emphasis is on studying the brazing characteristics of advanced ceramics such as silicon nitride, silicon carbide, and partially stabilized zirconia. The techniques of direct brazing with metallic and nonmetallic filler materials are being used. Vapor coatings are being used where appropriate to circumvent wetting problems associated with braze filler metals. The planned activities during FY 1995 will emphasize the use of structural analysis software to design joints for engine components such as valves and shaft attachments. The objective of this effort will be to identify material combinations and processing that would be feasible for these components, and to produce prototype parts whenever possible.

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

85. **SURFACE DURABILITY OF MACHINED CERAMICS (WBS NO. 1500)**
$200,000
DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contacts: D. R. Johnson, (423) 576-6832 and P. J. Blau, (423) 574-5377

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

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

86. **NEXT-GENERATION GRINDING WHEEL (WBS NO. 1501)**
$392,000
DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: P. J. Blau, (423) 574-5377
Norton Contact: Robert H. Licht, (508) 351-7815

This effort is aimed at the engineering design and development of a next-generation, superabrasive grinding wheel specifically tailored for the cylindrical grinding of silicon nitride and other advanced structural ceramic parts for automotive and truck engine applications. The intent of this effort is to significantly reduce manufacturing cost of ceramic parts and to enhance the competitiveness of U.S. industry by providing an optimized grinding wheel for ceramics. The Phase I objectives to define requirements, and design, develop, and evaluate a next-generation grinding wheel for cost-effective cylindrical grinding of advanced ceramics have been met. A Phase II effort to scale up the new, superabrasive wheel developed in Phase I to larger diameters and conduct additional in-house wheel enhancement is planned.

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

87. **GRINDABILITY TEST (WBS NO. 1502)**
$0
DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: P. J. Blau, (423) 574-5377
Chand Kare Contact: Ronald H. Chand, (508) 793-9814

The objective of this program was to develop a cost-effective method to determine the grindability of ceramics leading to cost-effective methods for machining those materials. Phase I efforts were directed towards a review of literature related to ceramic grinding, development of a variable definition of grindability, design of grindability test experiments, and design of a ceramics grindability test system. The grindability study also included establishment of correlation between the grindability number and conventional grinding practices. Fabrication of the final prototype of the ceramic grindability test system has been completed.

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

88. **CHEMICALLY ASSISTED GRINDING OF CERAMICS (WBS NO. 1503)**
$150,000
DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: P. J. Blau, (423) 574-5377
NIST Contact: Steven M. Hsu, (301) 975-6119

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

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

89. **GRINDING CONSORTIUM (WBS NO. 1503)**
$150,000
DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: P. J. Blau, (423) 574-5377
NIST Contact: Said Jahanmir, (301) 975-6871

The purpose of this effort was to develop guidelines and recommendations for grinding optimization of advanced structural ceramics to achieve minimum cost and maximum reliability. The following steps were taken to achieve the objective: conduct grinding experiments jointly with industrial participants, determine the effect of grinding parameters on machining damage and strength, elucidate mechanisms of material removal and damage formation, evaluate several damage detection techniques, and transfer data and information to industry in computerized database format.

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

90. **HIGH SPEED GRINDING (WBS NO. 1504)**
$372,000
DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: P. J. Blau, (423) 574-5377
Eaton Contact: Joseph A. Kovach, (216) 523-6766

The purpose of this effort is to develop a single-step, rough finishing process suitable for producing high-quality silicon nitride ceramic parts at high material removal rates and at substantially lower cost than traditional, multi-stage grinding processes.

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

91. **LASER-BASED NDE METHODS (WBS NO. 1507)**
$180,000
DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. R. Johnson, (423) 576-6832
Argonne National Lab Contact: J. G. Sun, (708) 252-5169

The primary objective of this effort is to develop a laser-scattering procedure which would provide a direct indication of changes in the subsurface (and surface) during machining-both machining-induced damage such as median crack formation and surface roughness. A second objective is to evaluate dye-penetrant technology as an off-line indicator for surface-breaking cracks.

Keywords: Machining, Nondestructive Evaluation, Structural Ceramics

92. **GRINDING MACHINE STIFFNESS (WBS NO. 1510)**
$227,000
DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: P. J. Blau, (423) 574-5377
University of Connecticut Contact: Bi Zhang, (203) 486-3576

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

Keywords: Machining, Silicon Nitride

93. **NEXT GENERATION GRINDING SPINDLE (WBS NO. 1511)**
$225,000
DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: P. J. Blau, (423) 574-5377
Eaton Contact: J. A. Kovach, (216) 523-6766

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

Keywords: Machining, Structural Ceramics

94. **PROCESS COST MODEL (WBS NO. 1512)**
$250,000
DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: S. G. Winslow, (423) 574-0965
AlliedSignal Ceramic Components Contact:
B. S. Draskovich, (312) 512-5654

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

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

OFFICE OF PROPULSION SYSTEMS

The Office of Propulsion Systems is comprised of the Advanced Propulsion Division and the Electric and Hybrid Propulsion Division. R&D programs focus on developing the technologies that will lead to the production and introduction of advanced heat engine propulsion systems, and electric and hybrid vehicles, in the Nation's transportation fleet. Technology development is conducted in concert with industry through cost-shared contracts. Materials activities of the Office of Propulsion Systems focus on integration of materials into components, and testing of subsystems for advanced vehicle propulsion systems.

ADVANCED PROPULSION DIVISION

The Advanced Propulsion Division consists of two programs: (1) Light Duty Engine Technologies Program, targeting Turbine Engine Technologies and Advanced Piston Engine Technologies; and (2) Heavy Duty Engine Technologies Program, targeting Advanced Diesel Engine Technology. Materials activities are supported by the Advanced Propulsion Division and managed through the NASA Lewis Research Center and the Oak Ridge National Laboratory. The DOE Contacts are: Thomas Sebestyen, (202) 586-8012 for Turbine Engine Technologies; Patrick Sutton, (202) 586-8058 for Automotive Piston Engine Technologies; and John Fairbanks, (202) 586-8066 for Heavy Duty Engine Technologies.

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

95. **NASA SUPPORTING RESEARCH AND TECHNOLOGY**
$100,000
DOE Contact: Thomas Sebestyen, (202) 586-8012
NASA Contact: Thomas Strom, (216) 433-3408

The objective of this program is to evaluate commercially available structural and glass ceramic material specimens exposed to combustion products at temperatures up to 2500°F for periods up to 3,500 hours. Activities include: development of design codes for structural component evaluation; research on non-destructive evaluation of ceramic components to improve reliability; and examination of the effects of corrosive sea salts and other adverse environments on the durability of ceramics.

Keywords: Structural Ceramics, Nondestructive Evaluation, Silicon Carbide, Silicon Nitride, Gas Turbine Engines

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

96. **HYBRID VEHICLE TURBINE ENGINE (HVTE) TECHNOLOGY SUPPORT**
$3,600,000
DOE Contact: Thomas Sebestyen, (202) 586-8012
NASA Contact: Paul Kerwin, (216) 433-3409
Allison Engine Company Contact: Steve Berenyi, (317) 230-6971

The Hybrid Vehicle Turbine Engine (HVTE) Technology Support Program focuses on the DOE Hybrid Vehicle Program turbine engines in the 20-60kW size for hybrid vehicle application. In support of the advanced HVTE, Allison is designing, fabricating, and testing low-emission combustors, ceramic hot section components, a high performance ceramic regenerator core and seal system and cost-effective high temperature insulation system. Test rigs and test bed engines are being used to evaluate full-scale component and subsystem reliability and durability at cyclic operating conditions that are typical of automotive use at up to 2500°F.

Keywords: Structural Ceramics, Component Design, Silicon Carbide, Silicon Nitride, Gas Turbine Engines, Rig and Engine Testing

97. **CERAMIC TURBINE (CT) ENGINE DEMONSTRATION PROJECT**
$3,500,000
DOE Contact: Thomas Sebestyen, (202) 586-8012
NASA Contact: Thomas Strom, (216) 433-3408
AlliedSignal Engine Contact: Jay Smyth, (602) 231-4306

In support of the DOE Hybrid Vehicle Program, this project will provide early ceramic turbine field experience by demonstrating the reliability and durability of ceramic components in actual engine application. To this end, AlliedSignal began introducing ceramic first stage turbine nozzles and blades into its proven, available (all-metal) GTCP 331-200 gas turbine Auxilliary Power Unit (APU) engine. Laboratory and field testing is continuing to address remaining critical design and production concerns related to structural ceramics in gas turbine engines. In addition, efforts are intensified to scale-up and demonstrate commercial engine ceramic component manufacturing in coordination with ceramic suppliers and the Propulsion System Materials element of DOE's Materials Technology Program.

Keywords: Structural Ceramics, Component Design, Fabrication, Gas Turbine Engines, Component Testing

98. **ADVANCED DIESEL ENGINE COMPONENT DEVELOPMENT PROJECT**
$100,000
DOE Contact: John W. Fairbanks, (202) 586-8066
NASA Contact: Mark J. Valco, (216) 433-3717
Detroit Diesel Corporation Contact: Jim Hoelzer, (313) 592-5565

The objective of the project is to develop advanced technology diesel engine components and integrate them into a test bed engine to demonstrate reduced emissions and improved fuel economy. Advanced ceramic and metallic materials are being investigated and used in structural, insulative, and tribological component applications.

Keywords: Structural Ceramics, Low Heat Rejection Diesel Engines, Thermal Barrier Coatings, Component Designs, Composite Materials

99. **ADVANCED PISTON AND CYLINDER COMPONENT DEVELOPMENT**
$70,000
DOE Contact: John W. Fairbanks, (202) 586-8066
NASA Contact: Mark J. Valco, (216) 433-3717
Caterpillar Inc. Contact: G. L. Waltz, (309) 578-6549

The objective of the project is to develop advanced technology diesel engine components and integrate them into a test bed engine to demonstrate reduced emissions and improved fuel economy. Advanced ceramic and metallic materials are being investigated and used in structural, insulative, and tribological component applications. Zirconia coatings are being used on piston crowns and composite pistons are being tested.

Keywords: Structural Ceramics, Low Heat Rejection Diesel Engines, Thermal Barrier Coatings, Component Designs, Composite Materials

100. **ADVANCED PISTON AND CYLINDER COMPONENT DEVELOPMENT**
$150,000
DOE Contact: John W. Fairbanks, (202) 586-8066
NASA Contact: Mark J. Valco, (216) 433-3717
Cummins Engine Contact: T. Yonushonis, (812) 377-7078

The objective of the project is to develop advanced technology diesel engine components and integrate these into a test bed engine to demonstrate reduced emissions and improved fuel economy. Nickel aluminides and Titanium aluminides are being investigated for turbocharger turbine rotors. Cast-in-place titanium nitride exhaust and intake port liners are emerging with improved reliability. Several powder metallurgy parts are being tested and zirconia and mullite coatings are being developed for piston crowns.

Keywords: Structural Ceramics, Low Heat Rejection Diesel Engines, Thermal Barrier Coatings, Component Designs, Composite Materials

101. **MICROWAVE REGENERATED PARTICULATE TRAP**
$75,000
DOE Contact: John W. Fairbanks, (202) 586-8066
ORNL Contact: Ronald Graves, (423) 574-2036

The objective of this project is to develop a particulate trap with fiber-reinforced (SiC) materials which will permit regeneration by heating with microwave energy. This will be done by utilizing a chemical vapor infiltration process to partially densify a thin fibrous substrate and produce a porous filter with high microwave coupling. This project is being performed in collaboration with Cummins, Fleetguard, ReMaxCo and Microwave Materials Technology.

Keywords: Particulate Traps, Microwave Regeneration, Chemical Vapor Infiltration, Silicon Carbide Fibers, Low Heat Rejection Diesel Engines

ELECTRIC AND HYBRID PROPULSION DIVISION

The Electric and Hybrid Propulsion Division has three major programs: Battery Development, Fuel Cell Development, and Systems Development for electric vehicles. The DOE Contact is Kenneth Heitner, (202) 586-2341 for Battery Development; Steve Chalk, (202) 586-3388 for Fuel Cell Development; and Albert Landgrebe, (202) 586-1483 for Exploratory Research in support of Batteries and Fuel Cells.

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

102. **ELECTROCHEMICAL PROPERTIES OF SOLID-STATE SODIUM/POLYMER CELLS**
$275,000
DOE Contact: JoAnn Milliken, (202) 586-2480
Lawrence Berkeley Laboratory Contact:
L. C. De Jonghe, (510) 486-4881

The objective of this project is to investigate the viability of all-solid-state cells based on Na or Na alloy negative electrodes, polymeric electrolytes, and metal oxide positive electrodes. Emphasis is placed on developing a suitable cathode material not only in terms of performance but also in terms of cost and environmental impact. The approach is to synthesize and characterize manganese oxides for use as a cathode in Na/polymer cells and employ AC and DC techniques (e.g., galvanostatic charging and discharging, four probe techniques, and pulse testing) to characterize solid state batteries, as well as the properties of the individual components and interfaces. A full set of transport property measurements for the PEO/Na triflate system was completed. Especially noteworthy was the development of a new method of measuring transference numbers using straightforward electrochemical techniques, and a rigorous theoretical treatment of the results.

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

103. **IMPROVED CONTAINER ELECTRODE COATINGS FOR SODIUM/SULFUR BATTERY SYSTEMS**
$0
DOE Contact: JoAnn Milliken, (202) 586-2480
Environmental Research Institute of Michigan
Contact: T. K. Hunt, (313) 667-2113

The objective of this project was to develop improved corrosion-resistant coatings for high-temperature secondary batteries by sputter-deposition techniques. Research was aimed at determining the utility of titanium films as durable, corrosion protective, conductive coatings for the sulfur electrodes in Na/S batteries. Several series of sputter-deposited TiN coatings were applied to Al coupons and the resulting samples soaked in Na_2S_4 at temperatures up to 390°C for 500 hours. The sputtering conditions were modified during the test series and the latter coatings showed no visible signs of corrosion following the 500 hour exposure. This project has been completed.

Keywords: Coatings, Na/S Batteries, Sputter-Deposition

104. **THE PERFORMANCE OF NEW MATERIALS FOR POLYMER ELECTROLYTE BATTERIES**
$140,000
DOE Contact: JoAnn Milliken, (202) 586-2480
Northwestern University Contact: D. F. Shriver,
(708) 491-5655

The objective of this project is to synthesize polymer electrolytes based on aluminosilicate-polyether hybrid polyelectrolyte with improved low-temperature performance and high cation transport number. These polymer electrolytes should be useful in rechargeable Li/polymer batteries. Initial efforts have focused on cell testing with simple polymer-salt electrolytes. This includes cycling with a cathode consisting of 70 percent Li_xMnO_2, 15 percent carbon, 15 percent polymer electrolyte, and a Li-metal anode. High cell capacity (135 mAh/g active cathode material) can be achieved at low discharge current. Experiments are underway to investigate the cause of the capacity fade that occurs with cycling. The data from these cells will provide a baseline for comparison with more advanced polyelectrolytes such as aluminosilicate-polyether hybrid polyelectrolyte.

Keywords: Polymer Electrolytes, Electrochemical Cells

105. **NOVEL POLYMER ELECTROLYTES FOR RECHARGEABLE LITHIUM BATTERIES**
$180,000
DOE Contact: JoAnn Milliken, (202) 586-2480
Case Western University Contact: M. Litt, (216) 368-4174

The objective of this research is to develop advanced polymeric electrolytes for rechargeable Li batteries. Thin polymeric films are cast and characterized by spectroscopic, nuclear magnetic resonance, thermal and electrochemical techniques. Two types of polymer materials are under investigation: sulfonated and phosphonated polybenzimidazole polymers, and novel poly (4,5-dimethyleneimidazole and hydroxy imidazole) polymers. Currently, efforts are focused on preparing the polymer electrolytes and measuring their conductivities.

Keywords: Polymeric Electrolytes, Li Batteries

106. **NOVEL SOLID POLYMER ELECTROLYTES FOR ADVANCED SECONDARY BATTERIES**
$110,000
DOE Contact: JoAnn Milliken, (202) 586-2480
University of Dayton Contact: D. G. Glasgow, (513) 229-2517

The objective of this research program is to synthesize and characterize new polymer electrolytes that contain crown ethers which could improve the Li-ion transport. The systems proposed are doped polymers with side chains having the ability to form liquid crystalline (LC) mesophases. A novel LC monomer has been prepared and photopolymerized together with a monomer/salt mixture. Studies to align the polymer in an electric field are underway. Future efforts will focus on completing synthesis of polymer electrolytes and characterization of the polymers with respect to ionic conductivity, dimensional stability, and interfacial stability.

Keywords: Polymeric Electrolytes, Li Batteries, Ion Transport

107. **SOL-GEL ELECTROLYTES IN LITHIUM BATTERIES**
$0
DOE Contact: JoAnn Milliken, (202) 586-2480
Rutgers University Contact: L. C. Klein, (908) 932-2096

The objective of this research project was to optimize the synthesis of polymer electrolytes by sol-gel processing of alkali/silicate components, which involves combining the components in liquid form prior to chemically reacting the solution with water to form a gel. These materials should produce solid electrolyte compositions that can be applied directly to electrode materials for rechargeable Li batteries. The approach used in this investigation was to select oxide components that are Li-ion conductors and are thermodynamically stable. Alumina-containing formulations were identified which showed improved thermodynamic stability. This project has been completed.

Keywords: Sol Gel Electrolytes, Li Batteries, Polymer Electrolytes

108. **NEW CATHODE MATERIALS**
$155,000
DOE Contact: JoAnn Milliken, (202) 586-2480
State University of New York Contact: M. S. Whittingham, (607) 777-4623

The objective of this project is to synthesize and evaluate oxides of tungsten, molybdenum, and first-row transition metals for alkali-metal intercalation electrodes which are useful as positive electrodes in advanced nonaqueous rechargeable batteries. Mild hydrothermal techniques are used for the synthesis of molybdenum oxides, or, in cases where the hydrothermal technique does not lead to compounds with the highest oxidation state, electrochemical oxidation from an aqueous alkaline solution is used to drive the cations to their highest oxidation state. Hexagonal Mo oxides were prepared which have a greater capacity for Li intercalation than the normal MoO_3 phase. Layered structures were produced which should allow for rapid diffusion of Li ions. This research will be expanded to synthesize and test vanadium and manganese oxides.

Keywords: Intercalation Electrodes, Rechargeable Batteries

109. **DEVELOPMENT OF HIGH ENERGY DENSITY CATHODES FOR SODIUM/POLYMER CELLS**
$165,000
DOE Contact: JoAnn Milliken, (202) 586-2480
SRI International Contact: S. Smedley, (415) 859-6173

The major objective of this research is to develop high-performance organic polydisulfide positive electrodes for use in low-temperature (ambient to 100°C) Na/polymer cells. This will be achieved by the synthesis and characterization of hexathiobenzene-based compounds and their derivatives for positive electrodes. Specific parameters under investigation include the nature of any heteroatoms or side chains added to the base polymer, the structure of the polymer, the cathode thickness, the voltage stability window of the cathode, the degree of loading of the positive electrode material, the electrode construction technique, and the operating temperature of the cell. A cathode utilization of 164 mAh/g was achieved for poly (hexathiobenzene), with an energy density of 260 Wh/kg at the C/10 rate at 95°C. Optimization of the cathode formulation should significantly improve cathode behavior.

Keywords: Cathodes, Na/polymer Cells, Electrochemical Analysis

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

110. **SURFACE MORPHOLOGY OF METALS IN ELECTRO-DEPOSITION/CARBON ELECTROCHEMISTRY**
$270,000
DOE Contact: JoAnn Milliken, (202) 586-2480
Lawrence Berkeley Laboratory Contacts: K. Kinoshita and C. Tobias, (510) 486-4260

The objective of this project is to develop a pragmatic understanding of the component processes and their interactions in the macrocrystallization of metals necessary for the design and optimization of rechargeable galvanic cells. This project involves investigation of: (1) the role of electric field and solution-side mass transport in the electrocrystallization of metals, mechanisms of initiation, growth and propagation of imperfections, and development of surface textures; (2) the characterization of gases at electrodes with emphasis on their effect on ohmic resistance and mass transfer; and (3) the role of physico-chemical properties of carbonaceous materials on their ability to reversibly intercalate Li. Results have shown that the initial velocity of the interface joining two bubbles depends on the bubble size and surface tension, but not on the electrolyte viscosity. In addition a mathematical model has been completed to understand the hydro-dynamics of flow over protrusions. Analysis of existing data suggests that the mechanism and capacity for intercalation of Li may differ between the highly ordered graphites and less ordered carbons.

Keywords: Macrocrystallization of Metals, Galvanic Cells, Li Batteries

111. **FABRICATION & TESTING OF CARBON ELECTRODES AS LITHIUM INTERCALATION ANODES**
$200,000
DOE Contact: JoAnn Milliken, (202) 586-2480
Lawrence Livermore National Laboratory Contact: R. Pekala, (510) 422-0142

The objectives of this work are to evaluate the performance of carbonaceous materials as hosts for lithium intercalation negative electrodes, and to develop reversible lithium intercalation negative electrodes for advanced rechargeable lithium batteries. The approach is to fabricate electrodes from various commercial carbons and graphites and evaluate them in small lithium-ion cells. Electrode performance will be correlated with carbon structure and properties in collaboration with LBNL. Electrodes fabricated from various Lonza graphites yielded Li intercalation capacities that range from 320 to 365 mAh/g (equivalent to x in Li_xC_6 from 0.85 to 0.95), approaching the theoretical value of 372 mAh/g.

Keywords: Carbon, Li Batteries, Intercalation

112. **BATTERY MATERIALS: STRUCTURE AND CHARACTERIZATION**
$150,000
DOE Contact: JoAnn Milliken, (202) 586-2480
Brookhaven National Laboratory Contact: J. McBreen, (516) 282-4071

The objective of this research is to elucidate the molecular aspects of materials and electrode processes in batteries and to use this information to develop electrode and electrolyte structures with good performance and long life. Current efforts have included *in situ* extended x-ray absorption fine structure (EXAFS) studies of Bi-doped manganese oxides and *ex situ* studies of lithium manganese oxides and nickel oxide electrodes that were cycled in Zn/NiOOH cells. Results have shown that corrosion of Ni plaque is the failure mode for sintered nickel oxide electrodes. No chemical interaction was observed between zincate and nickel hydroxide. Decreases in nickel oxide capacity in zinc/nickel oxide cells are most likely due to pore plugging by ZnO. Future efforts will focus on EXAFS studies of additives in nickel oxide and zinc electrodes as well as studies of molybdenum and tungsten oxide electrodes.

Keywords: Electrodes, Batteries, EXAFS

113. ***IN SITU* SPECTROSCOPIC APPLICATIONS TO THE STUDY OF RECHARGEABLE LITHIUM BATTERIES**
$150,000
DOE Contact: JoAnn Milliken, (202) 586-2480
Case Western Reserve University Contact: D. A. Scherson, (216) 368-5186

The purpose of this project is to use *in situ* spectroscopic techniques to investigate the electrochemical phenomena that occur at Li/electrolyte interfaces during charge/discharge cycling. The approach is to conduct experimental studies under ultrahigh vacuum conditions to examine the reactivity of Li at the Li/polymer and Li/liquid electrolyte interfaces. Attenuated Total Reflection-Fourier Transform Infrared (ATR-FTIR) Spectroscopy indicates that no reaction occurs at the Li/PEO interface. Modifications found in the ATR-FTIR spectrum following Li deposition and stripping are most likely caused by changes in the polymer morphology.

Keywords: Spectrographic Analysis, Electrochemical Phenomena, Electrolytes

114. **POLYMER ELECTROLYTE FOR AMBIENT TEMPERATURE TRACTION BATTERIES: MOLECULAR LEVEL MODELING FOR CONDUCTIVITY OPTIMIZATION**
$160,000
DOE Contact: JoAnn Milliken, (202) 586-2480
Northwestern University Contact: M. A. Ratner, (708) 491-5371

The goal of this research is to apply molecular dynamics (MD) and Monte Carlo simulations to understand the conduction process in polymer electrolytes, and its modification by such parameters as temperature, density, ion species, polymer chain basicity, and interionic correlations. The results of this study should be beneficial in the development of improved polymer electrolytes for rechargeable Li batteries for EV applications. MD simulations have shown that there are very few free ions in polymer/salt electrolytes of the stoichiometry usually measured. Hopping models have demonstrated that the conductivity is fixed by the segmental relaxation of the polymer host and by the number of free ions.

Keywords: Batteries, Electric Vehicles, Polymeric Electrolytes

115. **ANALYSIS AND SIMULATION OF ELECTROCHEMICAL SYSTEMS**
$240,000
DOE Contact: JoAnn Milliken, (202) 586-2480
University of California, Berkeley Contact: J. Newman, (510) 642-4063

The objective of this program is to improve the performance of electrochemical cells used in the interconversion of electrical energy and chemical energy by identifying the phenomena which control the performance of a system. These phenomena are incorporated into a mathematical model which can predict system behavior. The models aid in the recognition of important parameters that are crucial to the optimization of a given electrochemical system. Computer techniques with electrochemical engineering principles permit the calculation of complex interactions without gross mathematical and physical approximations. A model which describes the impedance response of a rechargeable Li battery at open circuit has been developed. The nickel/metal hydride battery has been modeled in both one-dimensional and full two-dimensional form. A model has also been developed which predicts the behavior of electrochemical double layer capacitors under operating conditions.

Keywords: Electrochemical Phenomena, Galvanostatic Charge/Discharge

116. **HEAT TRANSPORT AND THERMAL MANAGEMENT IN ADVANCED BATTERIES**
$175,000
DOE Contact: JoAnn Milliken, (202) 586-2480
University of California, Berkeley Contact: J. W. Evans, (510) 642-3807

This project was initiated in FY 1995 to investigate, by mathematical modeling and experimental measurement, heat generation and transport in advanced secondary batteries for electric vehicle (EV) applications. The objectives of this project are to evaluate the management of the temperature of the battery for optimum performance and to avoid temperature excursions damaging to the battery. Initial investigations were focused on Li/polymer batteries that are under development to operate in the temperature range of approximately 60 to 140°C, which is required to obtain sufficient polymer conductivity and to avoid overheating. A two-dimensional mathematical model revealed that the major resistance to heat transport in a Li/polymer-electrolyte battery is the polymer electrolyte.

Keywords: Thermal Modeling, Advanced Batteries

117. **ELECTRODE SURFACE LAYERS**
$140,000
DOE Contact: JoAnn Milliken, (202) 586-2480
Lawrence Berkeley Laboratory Contact: F. R. McLarnon, (510) 486-4260

Advanced *in situ* and *ex situ* characterization techniques are being used to study the structure, composition, and mode of formation of surface layers on electrodes used in rechargeable batteries. The objective of this research is to identify film properties that improve the rechargeability, cycle-life performance, specific power, specific energy, stability, and energy efficiency of electrochemical cells. Sensitive techniques such as ellipsometry, light scattering, Raman spectroscopy and scanning electron microscopy are utilized to monitor the formation of surface layers on secondary battery electrodes. In addition, foreign ions are incorporated in porous nickel electrodes to improve the cycle performance in an alkaline electrolyte. A newly developed technique for low-energy ion implantation was used to implant Au, Pb, Ta, Ti, W, and Ti_4O_7 in nickel oxide electrodes. Tests showed that the overpotential for oxygen evolution at the surface of a Ti_4O_7-implanted Ni electrode is increased by 50-105 mV, compared with electrodes implanted with other elements.

Keywords: Ion Implantation, Electrodes, Rechargeable Batteries

118. **ELECTRODE KINETICS AND ELECTROCATLYSIS**
$400,000
DOE Contact: JoAnn Milliken, (202) 586-2480
Lawrence Berkeley Laboratory Contact: P. N. Ross and E. J. Cairns, (510) 486-6226

Physically meaningful mechanistic models are essential for the interpretation of electrode behavior and are useful in directing the research on new classes of materials for electrochemical energy conversion and storage devices. The objective of this project is to develop an atomic-level understanding of the processes taking place in complex electrochemical reactions at electrode surfaces. Researchers are employing low energy electron diffraction (LEED) to study single crystals; high resolution electron microscopy (HREM) for carbon electrode materials; and X-ray absoption fine structure (EXAFS) for organometallic catalysts. Low Energy Ion Scattering (LEIS) and Auger Electron Spectroscopy (AES) are being utilized to study the composition of sputtered and UHV-annealed polycrystalline Pt-Ru bulk alloys for methanol electrocatalysis. It was found that the property of Ru atoms to nucleate oxygen-containing species at low potentials produced a strong enhancement in the catalytic activity of sputter-cleaned Pt-Ru alloy electrodes compared to pure Pt, thereby supporting the concept of the bifunctional character of the oxidation process of these alloys.

Keywords: Spectrographic Analysis, Electrocatalysts, Electrooxidation

119. **EFFECT OF ELECTROCATALYST AND ELECTROLYTE COMPOSITION ON METHANOL/AIR FUEL CELL PERFORMANCE**
$200,000
DOE Contact: JoAnn Milliken, (202) 586-2480
Lawrence Berkeley Laboratory Contact: E. J. Cairns and P. N. Ross, (510) 486-6226

There is a strong need to develop a fuel cell that can electrochemically oxidize liquid fuels, and the successful development of a direct-methanol fuel cell (DMFC) would represent a major advance for fuel-cell-powered vehicles. However, some major obstacles such as oxidation rate must be addressed before acceptable performance can be attained. The objective of this project is to elucidate the mechanism of methanol electrooxidation on electrocatalysts for DMFCs. Results have shown that the optimum surface composition of Pt-Ru varied with temperature and the shift in optimum composition with temperature can be attributed to a shift in the rate-determining step from CH_3OH adsorption/dehydrogenation at room temperature to the surface reaction between the dehydrogenated intermediate and surface oxygen at 60°C. Fuel cells with 20-cm^2 electrodes were designed and fabricated. Studies of the direct electrochemical oxidation of methanol and hydrocarbon fuels in liquid alkali carbonate and Solid Polymer Electrolytes (SPEs), respectively, are underway.

Keywords: Electrooxidation, Fuel Cells

120. **POISONING OF FUEL CELL ELECTROCATALYST SURFACES: NMR SPECTROSCOPIC STUDIES**
$200,000
DOE Contact: JoAnn Milliken, (202) 586-2480
Lawrence Berkeley Laboratory Contact: E. J. Cairns, (510) 486-5028

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

Keywords: NMR, Electrooxidation, Fuel Cells

121. **FUEL CELLS FOR RENEWABLE APPLICATIONS**
$1,000,000
DOE Contact: JoAnn Milliken, (202) 586-2480
Los Alamos National Laboratory Contact: S. Gottesfeld, (505) 667-0853

The primary focus of this program is to develop efficient and cost-effective polymer electrolyte fuel cells (PEFC) for transportation applications. The specific goals of the program are to: (1) reduce the cost of the Pt catalyst and ionomeric membrane, (2) increase the efficiency and power density of the PEFC, (3) optimize the system for operation on reformed organic fuels and air, (4) achieve stable, efficient, long-term operation, and (5) solve key technical issues that impede the development of the DMFC. For the first time, limiting currents significantly in excess of 2 A/cm^2 were obtained for hydrogen/air PEM fuel cells under ordinary operating conditions. Efforts will continue to focus on improving the performance and life of PEM and DM fuel cells and identifying new low-cost components for these fuel cells.

Keywords: Fuel Cells, Proton Exchange Membranes, Methanol Oxidation

122. **ELECTROCATALYSIS OF FUEL CELL REACTIONS**
$100,000
DOE Contact: JoAnn Milliken, (202) 586-2480
Brookhaven National Laboratory Contact: J. McBreen, (516) 282-4513

The purpose of this project is to increase the understanding of electrocatalysis on a molecular level and to apply this knowledge to improve the performance of fuel cells for transportation applications. The goals are to reduce the Pt requirements for solid PEFCs, to develop non-Pt catalysts for oxygen reduction, and to identify catalysts for the direct oxidation of methanol. The approach is to use X-ray absorption (XAS) to study the chemical/electrochemical properties of fuel cell electrocatalysts. XAS results have shown that the electrocatalysis of small organic molecules on Pb-modified Pt cannot be attributed to adsorption of oxygen species on Pb, but rather depend on the disordered nature of the Pb adlayer. This project has been completed.

Keywords: Fuel Cells, Electrocatalysts, X-Ray Absorption

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

123. **Zn/NiOOH CELL STUDIES**
$0
DOE Contact: JoAnn Milliken, (202) 586-2480
Lawrence Berkeley Laboratory Contact: E. Cairns and F. McLarnon, (510) 486-4260

The purpose of this project was to investigate the behavior of Zn electrodes in alkaline Zn/NiOOH cells to improve their lifetime and performance. Zn/NiOOH batteries would provide superior performance and lower life-cycle costs compared to Cd/NiOOH and MH/NiOOH batteries. The approach of this project was to determine the performance and cycle life of alkaline Zn/NiOOH cells using realistic cell components and operating conditions as well as utilize analytical instruments such as X-ray diffraction analysis and XAS to understand changes to cell components resulting from charge/discharge cycling. X-ray photoelectron spectroscopy results have shown that the NiOOH electrode in the Zn/KOH/NiOOH cells do not chemically react with the Zn species under cycling conditions with a KOH-KF-K_2CO_3 electrolyte. A CRADA has been established with Energy Research Corporation to further technology transfer.

Keywords: Electrodes, Batteries, Electric Vehicles

124. **APPLIED RESEARCH ON SECONDARY Zn/NiOOH BATTERY TECHNOLOGY**
$0
DOE Contact: JoAnn Milliken, (202) 586-2480
Acme Electric Corporation Contact: M. Anderman, (602) 921-0470

The objectives of this project were to evaluate the Lawrence Berkeley Laboratory (LBL) electrolyte composition for extending the cycle life of Zn/NiOOH cells, and to develop these cells for EV applications. Cells containing the LBL electrolyte were fabricated and results have shown that 175 charge/discharge cycles were completed. A visual examination of the electrodes showed a drastic improvement (reduction) in electrode shape change compared to the electrodes cycled in the standard, highly-alkaline electrolyte. This project has been completed.

Keywords: Electrodes, Batteries, Electric Vehicles

125. **DEVELOPMENT OF A THIN-FILM RECHARGEABLE LITHIUM BATTERY FOR ELECTRIC VEHICLES**
$0
DOE Contact: JoAnn Milliken, (202) 586-2480
Oak Ridge National Laboratory Contact: J. B. Bates, (615) 574-4143

The objective of this research is to identify methods for depositing acceptable thin-film electrodes for rechargeable Li batteries. These methods are being applied to develop solid-state Li/$Li_xMn_2O_4$ rechargeable thin-film Li batteries for EV applications. The batteries are expected to have several important advantages as power sources: high specific energy and energy density, long cycle lifetimes, and a wide temperature range of operation. Accomplishments have included fabrication of Li/Li_x/Mn_2O_4 cells in which the cathode was deposited at temperatures below 150°C by rf magnetron sputtering and fabrication of thin-film cells capable of sustaining current densities of several mA/cm^2, having a specific power of 30 W/g at an 85 C discharge rate. Cells exhibited less than 0.05 percent capacity loss per cycle after hundreds of cycles when discharged to 2-3 volts (~C/1). Efforts will focus on improving the performance of $Li_xMn_2O_4$ cathode films deposited at low temperatures and investigate the performance of a hybrid solid-state Li-$Li_xMn_2O_4$ cell.

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

126. **NA/SRPE ELECTRIC VEHICLE BATTERIES**
$200,000
DOE Contact: JoAnn Milliken, (202) 586-2480
PolyPlus Battery Company Contact: May-Ying Chu, (510) 841-4313

The purpose of this project is to demonstrate the cycling capability of cells containing Na negative and organosulfur-based positive electrodes, and develop a low-cost high-performance Na/polymer cell that utilizes an organosulfur-based positive electrode. The proposed batteries will be mechanically sturdy, have a reliable electrical performance, operate between 50 and 80°C, and are expected to be immune to thermal cycling. To date, approximately 80 laboratory Na/Solid Redox Polymer Electrolyte (SRPE) cells have been constructed and testing has been initiated. Maximum single discharge of 450 Wh/kg of cathode vs. Na and peak power of 800 W/kg of cathode vs. Na have been demonstrated. Limited cycling of 5 cycles above 250 Wh/kg and 20 cycles above 100 Wh/kg was achieved.

Keywords: Electrodes, Batteries, Electric Vehicles

127. **LITHIUM-ION BATTERY TESTING**
$0
DOE Contact: JoAnn Milliken, (202) 586-2480
Lawrence Livermore National Laboratory Contact: S. Mayer, (510) 423-4897

The objective of this project was to evaluate the performance of Li-ion cells to determine their cycle life and energy/power characteristics under controlled conditions. In this study, cells manufactured by the Sony Corporation for use in portable electronic devices were tested. The capacity and specific energy of cells that were charged to 4.2 V were about 1 Ah and >94 Wh/kg, respectively. Cycle life exceeded 300 cycles under Dynamic Stress Test at 100 percent Depth of Discharge (DOD), and 2800 cycles at 44 percent DOD. This project has been completed.

Keywords: Li Batteries, Dynamic Stress Testing

128. **NOVEL CONCEPTS FOR AN OXYGEN ELECTRODE IN SECONDARY METAL-AIR BATTERIES**
$0
DOE Contact: JoAnn Milliken, (202) 586-2480
Eltech Research Corporation Contact: E. J. Rudd, (216) 357-4073

The objective of this research was to develop improved bifunctional air electrodes for electrically rechargeable Zn/air cells. The successful development of bifunctional air electrodes depends on selecting electrochemically stable support materials and electrocatalysts for O_2 reduction and evolution, and the fabrication of suitable porous structures that are capable of extended operation. In this program, the properties of corrosion-resistant substrates such as semi-graphitic carbon, graphite or non-carbon materials were investigated. Results show that electrodes with a graphitized acetylene black for the support and $NiCo_2O_4$ and either CoTMPP or $La_{0.6}Ca_{0.4}CoO_3$ as electrocatalysts have operated for over 100 cycles in 35 percent KOH at room temperature. This project has been completed.

Keywords: Metal-Air Batteries, Bifunctional Air Electrodes, Zn/Air Cells

OFFICE OF UTILITY TECHNOLOGIES

	FY 1995
Office of Utility Technologies - Grand Total	$33,740,000
Office of Solar Energy Conversion	$15,200,000
Photovoltaic Energy Technology Division	$15,200,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$11,600,000
Amorphous Silicon for Solar Cells	3,500,000
Polycrystalline Thin Film Materials for Solar Cells	7,500,000
Deposition of III-V Semiconductors for High-Efficiency Solar Cells	600,000
Materials Properties, Behavior, Characterization or Testing	$ 1,800,000
Materials and Device Characterization	1,800,000
Device or Component Fabrication, Behavior or Testing	$ 1,800,000
High-Efficiency Crystal Silicon Solar Cells	1,800,000
Office of Renewable Energy Conversion	$ 540,000
Geothermal Division (GD)	$ 540,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 90,000
Thermally Conductive Composites for Heat Exchangers	90,000
Materials Properties, Behavior, Characterization or Testing	$ 450,000
Advanced High Temperature Geothermal Well Cements	300,000
Corrosion Mitigation in Highly Acidic Steam Condensates	100,000
Advanced Coating Materials	50,000
Office of Energy Management	$18,000,000
Advanced Utility Concepts Division	$18,000,000
Superconductivity Systems Program	$18,000,000
Device or Component Fabrication, Behavior or Testing	$18,000,000
Wire Technology Project	4,000,000
Systems Technology	6,000,000
Superconductivity Partnership Initiative	8,000,000

OFFICE OF UTILITY TECHNOLOGIES

OFFICE OF SOLAR ENERGY CONVERSION

PHOTOVOLTAIC ENERGY TECHNOLOGY DIVISION

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

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

129. **AMORPHOUS SILICON FOR SOLAR CELLS**
$3,500,000
DOE Contact: Richard King, (202) 586-1693
NREL Contact: Bolko von Roedern, (303) 384-6480

This project performs applied research upon the deposition of amorphous silicon alloys to improve solar cell properties. Efficient solar energy conversion is hindered by improper impurities or undesired structure in the deposited films and the level of uniformity of the films over large (1000 cm^2) areas. The films are deposited by plasma enhanced chemical vapor deposition (glow discharge), thermal chemical vapor deposition and sputtering. The long term goal of this effort is to develop the technology for 12 percent efficient solar cells with an area of about 1000 cm^2. Achieving that goal should enable amorphous silicon to be a cost-effective electrical generator.

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

130. **POLYCRYSTALLINE THIN FILM MATERIALS FOR SOLAR CELLS**
$7,500,000
DOE Contact: Richard King, (202) 586-1693
NREL Contact: Kenneth Zweibel, (303) 384-6441

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

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

131. **DEPOSITION OF III-V SEMICONDUCTORS FOR HIGH-EFFICIENCY SOLAR CELLS**
$600,000
DOE Contact: Richard King, (202) 586-1693
NREL Contact: John Benner, (303) 384-6496

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

Keywords: Semiconductors, Chemical Vapor Deposition, Solar Cells

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

132. **MATERIALS AND DEVICE CHARACTERIZATION**
$1,800,000
DOE Contact: Richard King, (202) 586-1693
NREL Contact: Larry Kazmerski, (303) 384-6600

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

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

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

133. **HIGH-EFFICIENCY CRYSTAL SILICON SOLAR CELLS**
$1,800,000
DOE Contact: Richard King, (202) 586-1693
NREL Contact: John Benner, (303) 384-6496

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

Keywords: Semiconductors, Solar Cells, Crystal Silicon

OFFICE OF RENEWABLE ENERGY CONVERSION

GEOTHERMAL DIVISION (GD)

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 long-term high risk GD-sponsored materials research and development.

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

134. **THERMALLY CONDUCTIVE COMPOSITES FOR HEAT EXCHANGERS**
$90,000
DOE Contact: R. LaSala, (202) 586-4198
BNL Contact: L. E. Kukacka, (516) 282-3065

This project is investigating thin thermally conductive polymer-based composites for use as corrosion and scale-resistant liner materials on carbon steel tubing used in shell and tube heat exchangers in binary geothermal processes or for bottoming cycles in multi-stage flash plants. Corrosion and scaling on the brine side of carbon steel tubing in shell and tube heat exchangers have been major problems in the operation of geothermal processes. Compared to the cost of high alloy steels, a considerable economic benefit could result from the utilization of a proven corrosion resistant polymer concrete material if sufficient heat transfer and anti-fouling properties can be derived. The work consists of determinations of the effects of compositional and processing variables on the thermal and fouling properties of the composite, and measurements of the physical and mechanical properties after exposure to hot brine in the laboratory and in plant operations. The effects of anti-oxidant additives on the fouling coefficient and scale adherence are also being evaluated. Results to date from field tests performed in FY 1994 and FY 1995 with flowing hypersaline brine under heat exchange conditions indicate heat transfer coefficients similar to those for high alloy stainless steels. The liner provided excellent corrosion protection to the carbon steel substrate, and no deterioration or disbondment of it were apparent. Improvements in the fouling coefficients by the inclusion of anti-oxidants are anticipated.

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

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

135. **ADVANCED HIGH TEMPERATURE GEOTHERMAL WELL CEMENTS**
$300,000
DOE Contact: R. LaSala, (202) 586-4198
BNL Contact: L. E. Kukacka, (516) 282-3065

Lightweight (<1.2 g/cc), environmentally benign, chemically and thermally resistant well cements are needed to reduce the potential for lost circulation problems during well completion operations and to insure long-term well integrity. Materials designed for temperatures >400 °C will be needed as higher temperature resources are developed. Cements resistant to brines containing high concentrations of CO_2 at temperatures >150 °C are also needed. Emphasis is being placed on high temperature rheology, phase chemistry, and the mechanical, physical, and chemical resistance properties of the cured materials. Retarding admixtures required to maintain pumpability during placement operations are also being identified. To date, phosphate bonded calcium aluminate cement formulations containing hollow aluminosilicate microspheres appear to meet the design criteria and preparations for large-scale mixing and field placement are underway.

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

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

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

Keywords: Polymers, Polymer Matrix Composites, Acid, Durability, Fabrication Techniques, Field Tests

137. **ADVANCED COATING MATERIALS**
$50,000
DOE Contact: R. LaSala, (202) 586-4198
BNL Contact: L. E. Kukacka, (516) 282-3065

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

Keywords: Polymers, Polymer Matrix Composites, Placement Techniques, Field Tests

OFFICE OF ENERGY MANAGEMENT

ADVANCED UTILITY CONCEPTS DIVISION

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

SUPERCONDUCTIVITY SYSTEMS PROGRAM

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

138. **WIRE TECHNOLOGY PROJECT**
$4,000,000
DOE Contact: Jim Daley, (202) 586-1165
Argonne National Laboratory: U. Balachandran, (708) 252-4250
Brookhaven National Laboratory: David Welch, (516) 282-3517
Los Alamos National Laboratory: Dean Peterson, (505) 665-3030
National Renewable Energy Laboratory: Richard Blaugher, (303) 384-6518
Oak Ridge National Laboratory: Robert Hawsey, (615) 574-8057
Sandia National Laboratory: Peter Roth, (505) 845-9301
American Superconductor Contact: G. N. Riley, (508) 836-4200
Intermagnetics General Contact: Paradeep Haldar, (518) 782-1122

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

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

a. Green state texturing of superconductors - To increase the J_c of BSCCO superconductors by a coated-wire-in tube (CWIT) method. In this approach, fine silver (Ag) wires are coated with BSCCO-2223 superconductor powder loaded into an Ag tube and processed by the powder-in-tube (PIT) method.

b. High temperature superconductor (HTS) current leads for superconducting storage devices - The goal of this project is to develop prototype HTS leads that will be used commercially in the storage device. Developed initial specifications for a pair of vapor-cooled HTS current leads based on the requirements of superconducting storage device.

c. Thallium based HTS coils - This project has produced Tl-1223 multifilament tapes exhibiting $J_c(77K)$ ~ 10,000 A/cm^2 in short lengths, which only decreases by a factor of 4 in magnetic fields above 8T. This J_c value is superior to analogous values for BSCCO tapes at 77K and high magnetic fields.

d. Fabrication and testing of HTS wires and coils - The purpose of this project is development of necessary conductor and provision of a pre-prototype demonstration that HTS can be substituted for the NbTi winding presently used in the ORNL quadruple motor. The proposed work will augment work already in place.

e. Development of high current density superconducting wires - The objective of this project is to develop and demonstrate the technology necessary for high critical current density, oxide powder-in-tube wires using the Tl-1223 and Tl-1212 composition. Tasks to involve preparation of aerosol-derived powders, fabrication of superconducting wires, deformation processing experiments, and statistical studies to optimize the texture, phase formation, and overall superconducting properties of the wires.

f. Study of magnetic flux motion and pining in HTS - Understanding of the vortex configuration and dynamics in HTS for applied fields that are not parallel to any of the principal axes is still insufficient. As a complementary study to those related to the alignment effects by columnar defects, the response of unirradiated HTS to inclined fields will be investigated. Completed initial characterization of energetic, Tl-1223 wires.

g. Aerosol powder synthesis - The objective of this agreement is to transfer the process of forming superconducting powder precursors via the aerosol pyrolysis technique. Refined the aerosol pyrolysis technique to control Pb-BSCCO powder particle size and phase assemblage. Evaluated the effects of chemical doping of the precursor materials prior to or during the atomization process on flux pinning.

Keywords: Superconductor, Coated-Wire-in-Tube Method, Thallium, Fabrication, Current Density, Magnetic Flux, Aerosol Powder

139. **SYSTEMS TECHNOLOGY**
$6,000,000
DOE Contact: Jim Daley, (202) 586-1165
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Brookhaven National Laboratory: David Welch, (516) 282-3517
Los Alamos National Laboratory: Dean Peterson, (505) 665-3030
National Renewable Energy Laboratory: Richard Blaugher, (303) 384-6518
Oak Ridge National Laboratory: Robert Hawsey, (615) 574-8057
Sandia National Laboratory: Thomas Bickel, (505) 845-9301
American Superconductor Contact: G. N. Riley, (508) 836-4200
Intermagnetics General Corp. Contact: Paradeep Haldar, (518) 782-1122
General Electric Research & Development Contact: J. E. Tkaczyk, (518) 387-5004
Oxford Instruments, Inc. Contact: K. R. Marken, (908) 541-1300

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

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

a. Bearing and Flywheels - The purpose of the HTS bearing scale-up project is to establish the technology base for improved flywheel energy storage systems through efficiency enhancements made possible by incorporation of HTS magnetic bearings. A critical issue is to demonstrate that low-loss HTS bearings can be scaled up to sizes of interest for flywheel energy storage applications. The project is a continuation of the effort started in calendar year 1994.

b. Processing of Bi 2223 superconducting tape for power application - Studies of approaches to optimize phase behavior and mechanical properties in order to achieve high critical current densities in longer lengths up to 1 meter are the focus of the agreement. Active exchanges of precursor powders and silver clad tapes for further processing and characterization as well as experimental results have been an important part of this agreement.

c. BSCCO HTS working group - The objective of this project is to develop the technology necessary for commercialization of oxide powder-in-tube conductors for electric power applications. Tasking included oxide powder development using aerosol pyrolysis to develop HTS aerosol spray pyrolysis powder process and system technology for use in PIT wires.

d. Thallium-based deposited conductor development - The objective of this project is to determine the sequence of events leading to formation of textured Tl-1223 with colony microstructure during vapor phase thallination of spray-pyrolyzed deposits. Completed to reproduce on buffeted metallic and other flexible metallic substrate the high critical current property with field and temperature dependence of that obtained on polycrystalline yttria-stabilized zirconia (YSZ) substrates.

e. Development of thallium-oxide superconducting materials for electric power - Performed the collaborative studies in the two-zone thallium oxide vapor reactor processing of precursor films deposited by low-cost methods to produce Tl-based HTS conductors.

Keywords: Thallium Conductor, Composite Conductors, Long Length Wire, Bearing, Flywheels, Superconducting Tape

140. **SUPERCONDUCTIVITY PARTNERSHIP INITIATIVE**
$8,000,000
DOE Contact: Jim Daley, (202) 586-1165
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Lockheed Martin Contact: Eddie Leung, (619) 974-1166
Reliance Electric Company Contact: Rich Schiferl, (216) 266-6253
Electric Power Research Institute Contact: Don Von Dollen, (415) 855-2679

The Superconductivity Partnership Initiative (SPI) is an industry-led venture between the Department of Energy and four industrial consortia intended to accelerate the use of high temperature superconductivity in energy applications. Each SPI team includes a vertical integration of non-competing companies that represent the entire spectrum of the R&D cycle. That is, the teams include the ultimate user of the technology-the electric utilities-as well as a major manufacturing company and a small company supplier of superconducting components. Each team also includes one or more national laboratories who perform specific tasks defined by the team. The SPI goal is to design cost-effective HTS systems for electricity generation, delivery and use. The funding amount below includes the Department's share of the SPI design activities as well as parallel HTS technology development that directly supports the SPI teams. In FY 95, projects are underway for a superconducting 100 MVA generator (General Electric), fault-current limiter (General Dynamics), and 100 HP motor (Reliance, Electric Company). In addition, a transmission cable project, led by the Electric Power Research Institute and Pirelli Cable, was funded in FY 1995. All of these projects will incorporate high-temperature superconducting wire. Four Department of Energy National Laboratories are currently directly supporting the Superconductivity Partnership Projects: Argonne, Los Alamos, Oak Ridge, and Sandia. Project subtasks are as follows:

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

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

c. Motor - Electrical and mechanical design and thermal analysis completed. In addition, the construction of the components for a motor prototype will be nearly completed, with assembly and testing. Supercond-ucting motors can have a large impact on electrical energy utilization through reduced losses and size compared to conventional iron core motors. The reduced losses and smaller size will be the driving forces for the commercial introduction of super-conducting motors in industrial applications.

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

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

OFFICE OF ENERGY RESEARCH

	FY 1995
Office of Energy Research - Grand Total	$358,555,719
Office of Basic Energy Sciences	$295,610,365
Division of Materials Sciences	$275,708,000
Division of Chemical Sciences	$ 5,800,000
Division of Engineering and Geosciences	$ 6,559,365
Engineering Sciences Research	$ 4,114,376
Materials Properties, Behavior, Characterization or Testing	$ 4,114,376
Bounds on Dynamic Plastic Deformation	194,411
Continuous Damage Mechanics - Critical States	50,945
An Investigation of the Effects of History Dependent Damage in Time Dependent Fracture Mechanics	23,000
Micromechanical Viscoplastic Stress-Strain Model with Grain Boundary Sliding	0
Micromechanical Viscoplastic Stress-Strain Model with Grain Boundary Sliding	0
An Analytical-Numerical Alternating Method for 3-D Inelastic Fracture and Integrity Analysis of Pressure-Vessels and Piping at Elevated Temperatures	61,325
In-Flight Measurement of the Temperature of Small, High Velocity Particles	436,000
Intelligent Control of Thermal Processes	224,000
Elastic-Plastic Fracture Analysis Emphasis on Surface Flaws	687,000
Modeling of Thermal Plasma Processes	210,000
Nondestructive Evaluation of Superconductors	180,000
Stress Induced Phase Transformations	67,419
Pulse Propagation in Inhomogeneous Optical Waveguides	0
Multivariable Control of the Gas-Metal/Arc Welding Process	152,609
Metal Transfer in Gas-Metal Arc Welding	123,688
Modeling and Analysis of Surface Cracks	191,628
Thermal Plasma Processing of Materials	0
Development of Measurement Capabilities for the Thermophysical Properties of Energy-Related Fluids	416,000
Low Resistivity Ohmic Contacts Between Semiconductors and High-T_c Superconductors	86,000
Thin Film Characterization and Flaw Detection	91,537
Experiments on the Gas Dynamics of the High Velocity Oxy-Fuel (HVOF) Thermal Spray Process	94,981
Transport Properties of Disordered Porous Media from the Microstructure	101,185
Effect of Forced and Natural Convection on Solidification of Binary Mixtures	103,571
Inelastic Deformation and Damage at High Temperature	0
Flux Flow, Pinning and Resistive Behavior in Superconducting Networks	70,519
Stability and Stress Analysis of Surface Morphology of Elastic and Piezoelectric Materials	135,000
Optical Techniques for Superconductor Characterization	145,000
Degenerate Four-Wave Mixing as a Diagnostic of Plasma Chemistry	0

OFFICE OF ENERGY RESEARCH (Continued)

	FY 1995
Office of Basic Energy Sciences (continued)	
Division of Materials Sciences (continued)	
Division of Engineering and Geosciences (continued)	
Engineering Sciences Research (continued)	
Materials Properties, Behavior, Characterization or Testing (continued)	
Effective Elastic Properties and Constitutive Equations for Brittle Solids Under Compression	0
3-D Experimental Fracture Analysis at High Temperature	69,975
Simulation and Analysis of Dynamic Failure in Ductile Materials	98,919
Dynamic Failure Characterization of Ductile Steels	99,664
Geosciences Research	$ 2,444,989
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 335,679
An Investigation of Organic Anion-Mineral Surface Interactions During Diagenesis	199,500
Transition Metal Catalysis in the Generation of Petroleum and Natural Gas	136,179
Materials Structure and Composition	$ 639,587
Reaction Mechanisms of Clay Minerals and Organic Diagenesis: An HRTEM/AEM Study	125,696
Infrared Spectroscopy and Hydrogen Isotope Geochemistry of Hydrous Silicate Glasses	123,000
Biomineralization: Systematics of Organic-Directed Controls on Carbonate Growth Morphologies and Kinetics Determined by In Situ Atomic Force Microscopy	90,891
Reactions and Transport of Toxic Metals in Rock-Forming Silicates at 25°C	200,000
The Crystal Chemistry and Structural Analysis of Uranium Oxide Hydrates	100,000
Materials Properties, Behavior, Characterization or Testing	$ 1,469,723
Cation Diffusion Rates in Selected Silicate Minerals	95,000
Shear Strain Localization and Fracture Evolution in Rocks	85,404
Oxygen and Cation Diffusion in Oxide Materials	171,000
Dissolution Rates and Surface Chemistry of Feldspar Glass and Crystal	114,700
Thermodynamics of Minerals Stable Near the Earth's Surface	150,000
Three-Dimensional Imaging of Drill Core Samples Using Synchrotron-Computed Microtomography	177,200
Transport Phenomena in Fluid-bearing Rocks	139,680
Structure and Reactivity of Ferric Oxide and Oxyhydroxide Surfaces: Quantum Chemistry and Molecular Dynamics	142,500
Micromechanics of Failure in Brittle Geomaterials	184,239
Cation Chemisorption at Oxide Surfaces and Oxide-Water Interfaces: X-Ray Spectroscopic Studies and Modeling	210,000

OFFICE OF ENERGY RESEARCH (Continued)

	FY 1995
Office of Basic Energy Sciences (continued)	
Division of Advanced Energy Projects	$ 7,543,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 3,574,000
Combustion Synthesis and Engineering of Nanoparticles for Electronic, Structural and Superconductor Applications	196,000
Creation and Destruction of C_{60} and Other Fullerene Solids	302,000
Synthesis and Properties of High Strength Nanolayered Composites	330,000
Optimally Controlled Interior Manipulation of Solids	299,000
Photorefractive Liquid Crystals: New Materials for Energy-Efficient Imaging Technology	320,000
Rapid Melt and Resolidification of Surface Layers Using Intense, Pulsed Ion Beams	300,000
'Off Diagonal' Thermoelectricity for Cooling and Power Generation	170,000
Evaporation Through Tungsten to Achieve High-Rate Vapor Phase Processing of Intermetallics	291,000
Ultrasonic and Dielectric Noninvasive Diagnostics for Sintering of Ceramic Composites	342,000
Compact MeV Ion Implantation	319,000
Thermoelectric Quantum Wells	350,000
Porous Carbons: Controlling Structure, Composition and Performance	355,000
Materials Properties, Behavior, Characterization or Testing	$1,644,000
Feasibility of a Novel Approach for Fast, Economical Determination of Radiation Damage in Nuclear Reactor Cores	149,000
Hot Carrier Solar Cells	330,000
Atomic and Nanoscale Engineering of Thermophotovoltaic Semi-conductors Using Scanning Probe Microscopy Techniques	552,000
Fabrication and Characterization of Micron Scale Ferromagnetic Features	133,000
Photochemical Solar Cells	150,000
Semiconductor Broadband Light Emitters	330,000
Device or Component Fabrication, Behavior or Testing	$ 2,325,000
Energy Related Applications of Selective Line Emitters	291,000
Photo-Induced Electron Transfer From a Conducting Polymer to Buckminsterfullerene: A Molecular Approach to High Efficiency Photovoltaic Cells	446,000
Superconducting Bitter Magnets	300,000
Blue-Emitting Devices Based on Gallium Nitride	340,000
Solid State Multi-Layered Batteries	296,000
PV-Powered, Electrochromic Windows	330,000
A Novel Tandem Homojunction Solar Cell: An Advanced Technology for High Efficiency Photovoltaics	322,000

OFFICE OF ENERGY RESEARCH (Continued)

	FY 1995
Office of Basic Energy Sciences (continued)	
Office of Fusion Energy	$22,870,000
Materials Properties, Behavior, Characterization or Testing	$22,870,000
Structural Materials Development	1,552,000
Repair Welding of Fusion Reactor Components	100,000
Insulating Ceramics for Fusion	435,000
Modeling Irradiation Effects in Solids	100,000
Fusion Systems Materials	3,815,000
Structural Materials for Fusion Systems	1,613,000
Development of Radiation-Hardened Ceramic Composites for Fusion Applications	60,000
Radiation Effects and Micromechanics of SiC/SiC Composites	115,000
Damage Analysis and Fundamental Studies for Fusion Reactor Materials Development	225,000
Development of Lithium-Bearing Ceramic Materials for Tritium Breeding in Fusion Reactors	200,000
Post-Irradiation Examination of Lithium-Bearing Ceramic Materials for Tritium Breeding in Fusion Reactors	400,000
ITER Materials Development for Plasma Facing Components	5,500,000
ITER Structural Materials Development	250,000
ITER Ceramic Materials	335,000
Radiation Hardened Fiber Optics for ITER Fusion Diagnostic Systems	75,000
ITER Materials Evaluation	1,505,000
ITER Structural Materials Evaluation	490,000
Development of Nb_3Sn Superconducting Wire for the ITER Magnet Program	5,000,000
Structural Materials Development for the Conduit of ITER Cable-in-Conduit-Conductors	1,100,000
Small Business Innovation Research Program	$39,175,749
Materials Preparation, Synthesis, Deposition, Growth or Forming	$15,756,575
Phase I Projects	$ 3,323,903
Low Cost, Contamination-Tolerant Electrocatalysts for Low-Temperature Fuel Cells	75,000
Laser Consolidation of Silicon Carbide/Titanium Metal Composite Turbine Rings	75,000
Solid Free-Body Formed Alumina-Tungsten Electrode Insulators for Heavy Ion Fusion Accelerators	75,000
High Current Density High Temperature Superconductor Composite Conductors	75,000
Superconducting Wires for Alternating Current Magnet Applications	75,000
A Low Cost, High Temperature Superconductor Wire Manufacturing Technology	75,000
A Low Cost Receiver Plate Manfacturing Process for High Concentration Photovoltaic Systems	60,000
Gallium Phosphide Ultraviolet Diode Arrays	75,000
An Intumescent Mat Material for Joining of Ceramics to Metals at High Temperatures	75,000
A New Alloy for Refiner Plates in the Pulp and Paper Industry	75,000
Development of Modulator Quality Rubidium Titanyl Arsenate Crystals for Remote Sensing Laser Systems	74,953
Slicing of Silicon Ingots with Reduced Kerf	75,000

OFFICE OF ENERGY RESEARCH (Continued)

	FY 1995
Small Business Innovation Research Program (continued)	
Phase I Projects (continued)	
Materials Properties, Behavior, Characterization or Testing (continued)	
A Novel Method to Recycle Thin Film Semiconductor Materials	75,000
Development of Novel Iron-Chromium-Silicon Alloys for Use in Kraft Recovery Boilers	67,068
High Capacity Carbon Anodes for Lithium Ion Batteries	74,500
Refractory Coatings for Improved Papermaking	75,000
An Improved Material and Low-Cost Fabrication Options for Candle Filters	74,960
An Integrated Catalyst/Collector Structure for Regenerative Proton-Exchange Membrane Fuel Cells	75,000
Pseudo-Porous Zirconium Carbide Fiber Coating for Environmentally Durable Silicon Carbide/ Silicon Carbide Composites	68,955
A Resistive Fault Current Limiter Based on Highly Directional Superconductor Thick Film Conductors	74,953
A Low Cost, Windable Yttrium-Barium-Copper-Oxide Conductor by Continuous Ion Beam Assisted Deposition/Metal Organic Chemical Vapor Deposition on a Metallic Substrate Tape	74,921
In-Situ Removal and Recycling of Copper Indium Selenide from Thin-Film Solar Cells	75,000
Conformal Source Ion Implantation	74,796
Synthesis and Application of a Novel Electrode Material for Use in Proton-Exchange-Membrane Fuel Cells Capable of Using Simple Organic Fuels and Fuel Reformate	75,000
A Novel Tritium Collection Technology Using Fullerence Tritides	75,000
A Steam-Resistant Hydrogen Selective Ceramic Membrane for Fuel Cell Applications	74,684
Low-Cost Durable Tooling for High Production Rate Structural Reaction Injection Molding/Resin Transfer Molding Processing	75,000
Silicon Hexaboride Reinforced Aluminum Ingot Material Development for the Transportation Industry	75,000
An Advanced Scintillator for Medical Imaging	74,765
Nanostructured Interstitial Alloys as Catalysts for Direct Energy Applications	75,000
Nanostructured Thermal Barrier Coatings for Natural Gas-Fired Advanced Turbines	75,000
Aggressive, Abrasion-Resistant Cutters for Hard Rock Drill Bits	74,907
An Integrated Catalyst/Substrate for Catalytic Combustion	75,000
Cesium Iodide Bromide and Cesium Iodide Chloride Scintillators for High-Rate Applications	74,564
Environmentally Responsible Recycling of Thin-Film Cadmium Telluride Modules	75,000
Low-Cost, Large-Area, High-Resistivity Substrates for Gas Microstrip Detectors	74,800
Bonding of Ceramic Composites for Structural Applications in Fusion Energy Systems	74,517
An Energy Efficient Design for a Surface Treatment Process which Improves Wear Properties of Materials	55,597
Fabrication of a Flexible Reacted Niobium Tin Cable for Applications in React and Wind Magnets	74,979
Low Temperature Fabrication of Copper Swirl Tubes for the International Thermonuclear Experimental Reactor	75,000
Fabrication of Copper-Backed Dense Tungsten Plasma Facing Component Armor	75,000
A Novel Fabrication Process to Enable Joining of Ceramics and Intermetallics	75,000
An Economic Sorbent for the Removal of Mercury, Chlorine, and Hydrogen Chloride from Coal Combustion Flue Gases	75,000
A Discontinuous Fiber Composite Interlayer for Increased Brazed Joint Reliability	75,000
Controlled Shear Strength Oxidation-Resistant Interfacial Coatings	74,984

OFFICE OF ENERGY RESEARCH (Continued)

	FY 1995
Small Business Innovation Research Program (continued)	
Materials Preparation, Synthesis, Deposition, Growth or Forming (continued)	
Phase II Projects (First Year)	$4,039,290
A Ceramic Material and Process for Use in Monolithic Ceramic Cross-Flow Filters	617,274
Jet Vapor Deposition of Multilayer and Nanocluster Thick Film Targets for Radioactive Nuclear Beams and Medical Applications	750,000
Design and Applications of Close-Spaced Thermionic Converters with Novel Isothermal Electrodes	750,000
A Multilayer Silicon Carbide Fiber Coating for Toughened, Neutron Radiation-Resistant Silicon Carbide/Silicon Carbide Composites	422,016
Economical and Reliable Niobium-Tin Conductors via Innovations in Stabilizers	750,000
Carbon-Carbon to Copper Joining for Fusion Reactor Applications	750,000
Phase II Projects (Second Year)	$8,393,382
Multi Layer, Quantum Well Layer Film Thermoelectrics	595,070
Production of Carbon Materials from Biomass	599,988
Oxide Dispersion Strengthened Silver for Use in High Temperature Superconductor Composite Wires	600,000
Low Temperature Deposition of Titanium Nitride	599,677
Coated Micrograin Carbides for Wear Resistance	599,577
Composite Plasma-Polymer Membranes	599,916
Improved Coated-Metal Hydrogen Extraction Membranes	599,314
Methods of Improving Internal-Tin Niobium-Tin for Fusion Applications	600,000
Advanced Nondestructive Evaluation for Quality Assurance of Divertor Plate Armor Tiles in Plasma Fusion Reactors	600,000
Dense, High Conductivity, Copper/Aluminum/Beryllium Functionally Gradient Plasma Facing Components	599,995
Flexible Electrochromic Window Materials Based on Poly(Diphenyl Amine) and Related Conducting Polymers	599,893
Advanced Window Materials Based on Conducting Polymer/Sol-Gel Composites	600,000
An Innovative Approach for the Formation of Silicon Carbide/Silicon Carbide Composites	599,952
Doping of Chemically Vapor Infiltrated Silicon Carbide to Enhance Thermal Conductivity	600,000
Materials Properties, Behavior, Characterization or Testing	$5,970,599
Phase I Projects	$1,195,953
Low Cost, Novel Precursors to Beta Alumina Solid Electrolyte	75,000
A Nanolayer Coating for Dry Machining	74,761
Development of a Process Management Technology for the Manufacture of High Temperature Superconductors to Improve Conductor Quality	75,000
An In-Process Quality Monitoring System for High Temperature Superconducting Wire Manufacturing	75,000
Low Cost, High Conductivity Plasma Facing Components	74,934
Structure-Property Relationships of Internal-Tin Niobium Tin	75,000
Nondestructive Characterization of Radiation Embrittlement in Fusion Structural Materials Using Laser Ultrasound	75,000

OFFICE OF ENERGY RESEARCH (Continued)

	FY 1995
Small Business Innovation Research Program (continued)	
Materials Preparation, Synthesis, Deposition, Growth or Forming (continued)	
Silicides for Space Power and Waste Heat Applications	75,000
Rotating, In-Plane Magnetization and Magneto-Optic Imaging of Cracks under Coatings on Ferromagnetic Metals	75,000
A Modular Inspection System for Complete In-Service Examination of a Nuclear Reactor Pressure Vessel, Including the Beltline Region	74,948
Development of Laser Materials and Rugged Coatings as Components for Tunable Ultraviolet Laser Systems	71,476
A Modified Natural Clay Sorbent for Control of Mercury from Coal Fired Combustors	74,912
Improved Solid Oxide Fuel Cell Seals	74,928
A Cost Efficient Method for Producing Ceramic Composites for Coal-Fired Furnace Applications	75,000
Application of Raman Spectroscopy to Identification and Sorting of Post-Consumer Plastics for Recycling	74,994
A Sensor for Automated Plastics Sorting	75,000
Phase II Projects (First Year)	$4,174,974
An Apparatus for Structural Analysis of High Temperature Materials Using Synchrotron Radiation	750,000
A Novel High Strength Ceria-Zirconia Toughened Alumina Ceramic with Superior High Temperature Corrosion and Erosion Resistance	425,165
Improvement in the Characteristics of Ternary Niobium Titanium Tantalum Alloys	750,000
X-Ray Absorption Spectroscopy for Trace Analysis of Chemical Phase and Composition	749,809
High-Temperature Thermally-Stable Multi-Layer Quantum Well Films	750,000
A Long Life Zinc-Oxide-Titanium-Oxide Sorbent	750,000
Phase II Projects (Second Year)	$ 599,672
A Testing Process to Define Electrode Current Wear Mechanisms and Develop Improved Electrodes	599,672
Device or Component Fabrication, Behavior or Testing	$17,448,575
Phase I Projects	$2,618,188
A Highly Efficient and Low Emission Catalytic Radiant Burner	75,000
Light Emitting Devices Based on Germanium Quantum Crystals in a Direct Bandgap Matrix (Aluminum Nitride)	74,995
A Two Dimensional Semiconductor Imaging Array for Scattered Cold Neutrons	75,000
A Thermal Neutron Detector Based upon a Lanthanum Boron Germanate Scintillator	74,947
Advanced Silicon Carbide and Beryllium/Aluminum Alloy Integrally Cooled X-ray Synchrotron Mirrors	74,992
A New Type of Acoustical Sensor for Chemical Measurements	75,000

OFFICE OF ENERGY RESEARCH (Continued)

	FY 1995
Small Business Innovation Research Program (continued)	
Device or Component Fabrication, Behavior or Testing (continued)	
Phase I Projects (continued)	
Chemically Resistant Gas Separation Perfluoromembranes	75,000
Advanced Chemiresistor Devices as Micron Size Sensors for the Rapid, On-Line Measurement of Chemical Vapors	73,005
Interactive Particle Detector Teaching Aids Based on Plastic Scintillators	75,000
A Thermally Stable Iron Core Permanent Magnet Dipole Utilizing a Flux Shunt	74,972
Enhanced Flux Pinning at High Fields in Niobium-Titanium-Tantalum by Magnetic Artificial Pinning Centers	75,000
Development of Artificial Pinning Center Niobium-Titanium Superconductors with Very High Residual Resistivity Ratio Aluminum Stabilizers	75,000
A High Resolution Multi-hit Time to Digital Converter Integrated Circuit	71,402
A Segmented Deep Depletion Depth Silicon Detector and Application Specific Integrated Circuits Signal Conditioning Systems for Physics Research	75,000
Microporous Alumina Microchannel Plates	74,987
Manufacturing Technologies, Improved Performance, and Cost Reduction of Superconducting Radiofrequency Resonant Niobium Cavities	74,994
A High Brightness Cold Cathode Electron Beam Source	74,994
A High Conductance Thermal Interface	75,000
A Helium-Cooled Faraday Shield Using Porous Meatl Cooling	74,929
Low Cost Fabrication of Large Silicon Carbide/Silicon Carbide Composite Structures	74,966
Accurate Broadband Detectors for Plasma Diagnostics	74,955
Bandgap-Engineered Thermophotovoltaic Devices for High Efficiency Radioisotope Power	74,918
Ion-Selective Ceramic Membranes for Separation of Radioactive Wastes	74,981
Removal and Concentration of Heavy Metals and Radionuclides from Polluted Groundwater	75,000
Rugged, Tunable Infrared Laser Sources	75,000
A Mid-Infrared Laser for Remote Sensing of Chemicals	74,994
A Membrane-Based Process for the Removal of Nitrogen from Natural Gas	74,912
Electrochemical Activation of Natural Gas Constituents to Alcohols Using Bimetallic Anode Electrocatalysts	74,995
An Innovative Membrane and Process for Removal and Recovery of Natural Gas Liquids	75,000
A Tubular Intermediate Temperature Natural Gas Fuel Cell Incorporating a Perovskite Solid Electrolyte	74,995
A Lower Cost Molten Carbonate Matrix	74,858
Fabrication of Multi-layer Molten Carbonate Fuel Cell Composites	74,470
Low Cost Molten Carbonate Fuel Cell Anodes	74,982
Abrasive-Waterjet Machining Techniques for Ceramic-Material Coal-Based Power System Components	74,945
Advanced Hot Gas Filter Development	75,000

OFFICE OF ENERGY RESEARCH (Continued)

	FY 1995
Small Business Innovation Research Program (continued)	
Device or Component Fabrication, Behavior or Testing (continued)	
Phase II Projects (First Year)	$5,970,753
Economical Photochromic Films Based on Metal Oxides	736,720
A Continuous Cryopump/Pellet-Fabrication Apparatus for Fusion	748,826
Development of Expansive Cements Using Dry Flue Gas Desulfurization (FGD) Solid Wastes	748,476
Highly Selective Membranes for the Separation of Organic Vapors Using Super-Glassy Polymers	750,000
A Long Life Perovskite Oxygen Electrode for Calcium and Lithium Oxide Processing in Nuclear Fuel Cycles	749,994
Fullerene-Based Catalysts for Heavy Oil Upgrading	750,000
A Low Emission Alkali Metal Thermal to Electric Converter Automotive Power System	749,857
An Acoustic Plate Mode Sensor for Aqueous Mercury	736,880
Phase II Projects (Second Year)	$8,859,634
Glass-Ceramic Construction Tile from Coal-Fired Boiler Flyash	599,861
A High Repetition-Rate, High Power, All-Solid-State Pulsed Driver for Electrodes Inductive Thrusters	599,937
Demonstration of an Integrated Carbon Dioxide/Thermal Management System for Carbonate Fuel Cells	599,968
Porous Aluminum Nitride Part Fabrication to Support Advanced Battery Development	599,703
Capacitive Energy Storage Using High Surface Area Transition Metal Compounds	600,000
Advanced Ceramic Fibers for a Carbonate Fuel Cell Matrix	599,950
An In-Situ Particle Sensor for Metal Forming Processes	595,070
Development of a High Spatial Resolution Neutron Detector	472,688
A High Resolution Scintillator-Based Neutron Detector	600,000
On-Chip Infrared-Spectral Sensors By Superconducting Detector Arrays	592,568
Radiation Resistant Radio Frequency Feedthrough Insulators for Fusion Applications	600,000
Helium-Cooled Divertors with Low- Activation Materials and Simple Fabrication Techniques	599,918
Niobium-Tin Superconducting Wire with Built-in Niobium Surface Coating to Limit Inter-Strand Eddy Currents in Cables	599,978
Ceramic Filters for Ultrafine Particulate Separation in Combustion Gas Environments	600,000
A Carbonate Fuel Cell Monolith for Low-Cost and High Power Density Operation	599,993
Small Business Technology Transfer Program	$899,605
Materials Preparation, Synthesis, Deposition, Growth or Forming	$599,697
Phase I Projects	$599,697
Laser Processing of Thermal Sprayed Beryllium Plasma Facing Components	99,975
Amorphous Silicon/Crystalline Silicon Heterojunctions for Nuclear Radiation Detector Applications	99,786
An Investigation to Determine the Commercial Feasibility of Vanadium-Hafnium-Zirconium Laves Phase C-15 Superconductor	100,000

OFFICE OF ENERGY RESEARCH (Continued)

	FY 1995
Small Business Technology Transfer Program (continued)	
Materials Preparation, Synthesis, Deposition, Growth or Forming (continued)	
Phase I Projects (continued)	
Production of Jelly-Roll Process Niobium-Aluminum Superconducting Wire Using Low Oxygen Niobium Foils and Special Softening Techniques During Deformation	99,936
Catalysts for Heterogeneous Alkene Hydroformylation	100,000
Low Loss Sapphire Windows for High Power Microwave Transmission	100,000
Device or Component Fabrication, Behavior or Testing	$299,908
Phase I Projects	$299,908
An Advanced X-ray Detector and Detector Array	99,998
Environmentally Benign Manufacturing of Compact Disk Stampers	100,000
Improved Strained-Layer Photocathodes for Spin-Polarized Electrons	99,910

OFFICE OF ENERGY RESEARCH

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

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

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

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

OFFICE OF BASIC ENERGY SCIENCES

The Office of Basic Energy Sciences supports research to advance the scientific and technical knowledge and skills needed to develop and use new and existing energy resources in an economically viable and environmentally sound manner. The largest portion of materials-related research is carried out through the Division of Materials Sciences.

Basic Energy Sciences carries out basic materials research that underpins the energy mission and Strategic Plan of the Department at all nine DOE multiprogram laboratories, two single program laboratories and one specific-mission laboratory. The multiprogram laboratories are Argonne National Laboratory, Brookhaven National Laboratory, Idaho National Engineering Laboratory, Lawrence Berkeley National Laboratory, Los Alamos National Laboratory, Oak Ridge National Laboratory, Pacific Northwest National Laboratory, and Sandia National Laboratories in New Mexico and California. The multiprogram laboratories conduct significant research activities for other DOE programs such as Energy Efficiency, Fossil Energy, Nuclear Energy, Environmental Management and Defense Programs.

The single program laboratories are Ames Laboratory at Iowa State University and the National Renewable Energy Laboratory. The specific-mission laboratory is the Stanford Synchrotron Radiation Laboratory.

The Division of Materials Sciences also funds a program which consists of 50 research projects at the University of Illinois Frederick Seitz Materials Research Laboratory.

DIVISION OF MATERIALS SCIENCES

The Materials Sciences subprogram supports energy related fundamental scientific research in materials and the operation of national scientific user facilities. Specific information on the Materials Sciences sub-program is contained in the DOE publication DOE/ER-0682 Materials Sciences Programs FY1995 (published May 1996). This 157-page publication contains program descriptions for 438 research programs that were funded in Fiscal Year 1995 by the Division of Materials Sciences. Five cross-cutting indices identify all 438 programs according to Principal Investigator(s), Materials, Techniques, Phenomena and Environment. Other contents include identification of the Division of Materials Sciences Staff structure and expertise; a bibliographical listing of 50 scientific workshop, topical, descriptive, Research Assistance Task Force and research facilities reports on select topics that identify materials sciences research needs and opportunities; a descriptive summary of the DOE Center of Excellence for the Synthesis and Processing of Advanced Materials; a descriptive summary and access information on 14 National

Research User Facilities including synchrotron light sources, neutron beam sources, electron beam microcharacterization instruments, materials preparation and combustion research; and an analytical summary of research funding levels.* Limited copies may be obtained by calling (301) 903-3427 and requesting DOE publication DOE/ER-0682.

Materials Science enables technology. 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. This research seeks to understand the synergistic relationship between the synthesis, processing, structure, properties, behavior, performance in energy technology applications and recycling of materials. Such understanding is necessary in order to develop the cost-effective capability to discover technological and economically desirable new materials and cost-competitive and environmentally acceptable methods for their synthesis, processing, fabrication, quality manufacture and recycling. The subprogram 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.

NATIONAL USER FACILITIES UNDER THE OFFICE OF BASIC ENERGY SCIENCES

The goal of the National User Facilities supported by the Office of Basic Energy Sciences is to provide experimental capabilities, which are not otherwise available in individual laboratories, for the pursuit of research of interest to the Department. These facilities are constructed and operated to support energy-related research, but are available to all qualified scientists based on the merit of their proposed experiments.

There were 4,900 users of Basic Energy Sciences supported National User Facilities in Fiscal Year 1995. 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.

They 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 Basic Energy Sciences 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 Basic Energy Sciences national user facilities have been constructed within cost, on schedule, and with rigorous compliance to all environmental, safety and health regulations.

DIVISION OF CHEMICAL SCIENCES

The Division of Chemical Sciences supports research important to fossil chemistry, combustion, advanced fusion concepts, photoconversion, catalysis, separations chemistry, actinide and lanthanide chemistry, thermophysical properties of complex fluids, nuclear waste processing, and environmental remediation. Research related to materials is carried out in the areas of heterogeneous catalysis, advanced battery technology, and materials precursor chemistry. The operating budget for FY 1995 for materials-related programs was $5,800,000 and was allocated to 43 projects in heterogeneous catalysis, advanced batteries and materials precursor chemistry.

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

*Operating funds for FY 1995 for the Office of Materials Science were $275,708,000.

This area is closely tied to alloy physics. Finally, the reactive decomposition chemistry of chlorocarbons on single crystals has a strong relationship to corrosion and lubrication.

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

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

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

For information about specific programs the DOE contact is William S. Millman, (301) 903-3285. The reader also is referred to DOE publication Summaries of FY 1995 Research in the Chemical Sciences (DOE/ER-0144/13 dated September 1995) for summaries of all funded programs, summaries of Small Business Innovation Research programs; and descriptions of major user and other special facilities. Limited copies may be obtained by calling (301) 903-5804.

DIVISION OF ENGINEERING AND GEOSCIENCES

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

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

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

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

ENGINEERING SCIENCES RESEARCH

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

141. **BOUNDS ON DYNAMIC PLASTIC DEFORMATION**
$194,411
DOE Contact: Oscar P. Manley, (301) 903-5822
Argonne National Laboratory Contact:
C. K. Youngdahl, (312) 972-6149

Analytical studies are being performed to develop load correlation parameters which can be used in approximating or bounding the dynamic plastic deformation of structures. In many applications where the load is transmitted to the structure through a fluid, details of the load history and spatial distribution significantly affect the final plastic deformation. The objective of the program is to devise load correlation parameters based on various weighted integrals of the time-space load distributions which can be used to characterize the effects of the load without resorting to detailed numerical analysis. These load correlation parameters have three important uses: to perform design and safety analyses of structures over a wide range of design variables and loadings; to validate computer programs which have a nonlinear dynamic plasticity capability; and to correlate experimental simulations with actual or predicted events. The dynamic plastic deformation of some basic structural configurations will be analyzed for loadings which vary both in magnitude and region of application with time. Load correlation parameters will be hypothesized and their usefulness in predicting final plastic deformation will be determined. The analyses will be based initially on a rigid, perfectly plastic material model and small deformation response, but will be extended to include strain hardening, and initial elastic response period, and large deformation interactions.

Keywords: Plastic Deformation

142. **CONTINUOUS DAMAGE MECHANICS - CRITICAL STATES**
$50,945
DOE Contact: Oscar P. Manley, (301) 903-5822
Arizona State University Contact: D. Krajcinovic,
(602) 965-8656

The research during the fourth, and last, year of the research was focused almost entirely on the two tasks: (1) response of microcrack weakened solids in the vicinity of the critical state, and (2) initial exploration of the use of Preisach model in fatigue analyses.

The studies of critical states were concentrated on fundamental issues such as the determination of the proximity parameter, universal parameters, order parameter and differences between the elastic and traditional (conduction) percolation problems. It was demonstrated that the second order phase (connectivity) transition takes place only in stress (load) controlled conditions. In contrast, localization (emergence of shear bands) of the deformation occurs in the strain (displacement) controlled tests.

Initial exploration of the Preisach model were focused on ductile behavior using parallel bar models. Important conclusions were related to the thermodynamics of the process, including differences between locked-in and dissipated work.

Keywords: Metals: Ferrous, Fracture, Fatigue, Creep

143. **AN INVESTIGATION OF THE EFFECTS OF HISTORY DEPENDENT DAMAGE IN TIME DEPENDENT FRACTURE MECHANICS**
$23,000
DOE Contact: Oscar P. Manley, (301) 903-5822
Battelle Memorial Institute Contact: F. Brust,
(614) 424-5034

The demands for structural systems to perform reliably under severe operating conditions continue to increase. Modern energy production facilities experience degradation and damage because they operate in severe high-temperature environment where time dependent straining and damage may lead to structural failures. The goal of this research is to study the high temperature damage and failure processes and to further develop a method for predicting this behavior in an effort to increase structural life. In particular, we focus on time dependent damage which occurs under history-dependent loading conditions, i.e., transient conditions.

The types of time dependent (creep) damage considered in this program include: sustained load creep, variable load creep, and variable load creep with thermal gradients. During the first year of this study, the implications of using Norton's creep law on various integral parameters used to characterize crack tip phenomena were evaluated as a function of time. Other constitutive laws for time dependent materials such as those of Murakami and Ohno are being implemented into the finite element code. In addition, constitutive property data and high temperature creep crack growth data are being obtained on stainless steel. These experiments will be used to verify analytical predictions and characterize time and history dependent damage during crack nucleation and growth.

The results from this work will be used by practicing engineers to enhance the life of high temperature structural systems during the design phase.

Keywords: Fracture Mechanics, History Dependent Damage, High Temperature

144. **MICROMECHANICAL VISCOPLASTIC STRESS-STRAIN MODEL WITH GRAIN BOUNDARY SLIDING**
$0
DOE Contact: Oscar P. Manley, (301) 903-5822
University of Connecticut Contact: E. H. Jordan, (203) 486-2371

The first part of this project has focused on developing and experimentally verifying methods of predicting the deformation response of polycrystalline metals from models of single crystal deformation, based on crystallographic slip. In the ongoing research, the goal is to try to predict the degree of heterogeneity of deformation and verify these predictions experimentally. The existing self-consistent model is to be completed by a second model based on periodicity which is expected to be both more realistic and more computationally burdensome. The degree of heterogeneity of deformation will be studied by different experimental techniques. Neutron diffraction experiments are planned in which diffraction from a few grains at a time is studied to determine lattice strains in individual grains. Many grains will be surveyed to get a statistical measure of heterogeneity of grains including no surface grains. The Moire strain analysis will alsc be done on large grained samples. The material studied is the same one used in the first phase, so that all the single crystal mechanical properties are accurately known. The data collected will provide a unique complete set of data to test the ability of the models in this program and other models with respect to their ability to predict the degree of heterogeneity of deformation. Comparison of the Moire data and the neutron diffraction data will also provide insight into the difference between surface grain behavior and interior grain behavior. Developing models that realistically predict grain to grain heterogeneity and verifying those models is a basic element in modeling mechanical behavior. Heterogeneity is particularly important to fatigue in which the most unfavorably oriented grain is the site of failure.

Keywords: Micromechanical, Viscoplasticity, Grain Boundary, Crystallographic Slip, High Temperature, Experiments

145. **MICROMECHANICAL VISCOPLASTIC STRESS-STRAIN MODEL WITH GRAIN BOUNDARY SLIDING**
$0
DOE Contact: Oscar P. Manley, (301) 903-5822
Engineering Science Software, Inc., Contact: K. P. Walker, (401) 231-3182

This project is joint with the University of Connecticut project described above. See the previous paragraph for a description.

Keywords: Micromechanical, Viscoplasticity, Grain Boundary, Crystallographic Slip, High Temperature, Constitutive Model

146. **AN ANALYTICAL-NUMERICAL ALTERNATING METHOD FOR 3-D INELASTIC FRACTURE AND INTEGRITY ANALYSIS OF PRESSURE-VESSELS AND PIPING AT ELEVATED TEMPERATURES**
$61,325
DOE Contact: Oscar P. Manley, (301) 9903-5822
Georgia Institute of Technology Contact: S. Atluri, (404) 894-2758

This research effort involves the application of highly efficient and accurate analytical-numerical alternating methods for the non-linear analysis of surface-flawed pressure vessels and piping under (1) elastic-plastic fracture, (2) high-temperature creep and viscoplastic fracture, and (3) pressurized thermal shock conditions. These procedures are highly efficient because only the uncracked structure is modeled numerically (finite element and boundary element approaches) and the severity of the stress state due to the presence of the 3-dimensional flaw is accounted for entirely analytically. This procedure is a novel application of the Schwartz-Neumann alternating method, which is a superposition method for linear problems, being extended to the nonlinear problems of elastoplasticity and creep through the generalized mid-point radial return mapping procedures which return the elastic estimates of stress in the cracked body to the appropriate yield surface. This effort is being conducted in collaboration with researchers at the University of Washington where some seminal experimental work is being conducted to verify and validate the analytical work done at Georgia Tech.

Keywords: Fracture, Failure Analysis

147. **IN-FLIGHT MEASUREMENT OF THE TEMPERATURE OF SMALL, HIGH VELOCITY PARTICLES**
$436,000
DOE Contact: Oscar P. Manley, (301) 903-5822
Idaho National Engineering Laboratory Contact:
J. R. Fincke, (208) 526-2031

The measurement of temperature, velocity, enthalpy, and species concentration in high temperature gases such as weakly ionized thermal plasmas has considerable importance in the areas of plasma thermal spray and the thermal plasma synthesis of materials. In particular, the dynamics of the plasma, the interaction of the plasma with its surroundings and the behavior of particles immersed in the plasma surrounding it are important in the understanding, development and optimization of plasma process that involve fine powders. Laser based measurement techniques have been developed at this laboratory and are being applied to the study of thermal plasmas. In addition to the laser techniques enthalpy probes coupled to a mass spectrometer also provide temperature, velocity and concentration information. The experimental data produced is used to benchmark the modeling work done under a related program in "Modeling of Thermal Plasma Processes" (see J. Ramshaw, INEL).

Keywords: Plasma Processing, Particle/Plasma Interaction

148. **INTELLIGENT CONTROL OF THERMAL PROCESSES**
$224,000
DOE Contact: Oscar P. Manley, (301) 903-5822
Idaho National Engineering Laboratory Contacts:
H. B. Smartt, (208) 526-8333 and J. A. Johnson, (208) 526-9021

This project addresses intelligent control of thermal processes as applied to materials processing. Intelligent control is defined as the combined application of process modeling, sensing, artificial intelligence, and control theory to process control. The intent of intelligent control is to produce a good product without relying on post-process inspection and statistical quality control procedures. The gas metal arc welding process is used as a model system; considerable fundamental information on the process has been developed at INEL and MIT during the past six years. Research is being conducted on an extension of the fundamental process physics, application of neural network-like dynamic controllers and signal/image processors, and development of noncontact sensing techniques.

Tasks include physics of nonlinear aspects of molten metal droplet formation, transfer, and substrate thermal interaction; understanding substrate thermal interaction; understanding the relationship of neural network structure and associated learning algorithm to model development and learning dynamics in neural networks with the objective of obtaining a fundamental understanding of network transfer functions; and advanced sensing, including the propagation and interaction of ultrasound in metallic solid and liquid media.

Keywords: Welding, Ultrasonic Sensing, Optical Sensing

149. **ELASTIC-PLASTIC FRACTURE ANALYSIS EMPHASIS ON SURFACE FLAWS**
$687,000
DOE Contact: Oscar P. Manley, (301) 903-5822
Idaho National Engineering Laboratory Contact:
W. G. Reuter, (205) 526-0111

The objective is to improve design and analytical techniques for predicting the integrity of flawed structural components. The research is primarily experimental, with analytical evaluation guiding the direction of experimental testing. Tests are being conducted on a material (a modified ASTM A-710) exhibiting a range of fracture toughness but essentially constant yield and ultimate tensile strength. As test temperature increases, the specimen configuration-fracture toughness relationship complies initially with requirements for linear elastic-fracture mechanics and extends beyond the range of a J-controlled field. Presently, compact tension and bend specimens are being used to develop state-of-the-art fracture mechanics.

Metallographic techniques are being used to measure crack tip opening displacement and remaining ligament size for comparison with analytical models. Other techniques including microphotography and the replicating of the crack tip region, for future metallographic examination, are being used to complement the above measurements to identify limits and capabilities of each technique. Moire interferometry techniques are being used to evaluate and quantify the deformation in the crack region. These data are being used to experimentally measure J and CTOD for standard (CT and SENB) specimens as well as for specimens containing surface cracks.

The above tests have been supplemented by using specimens fabricated from aluminum (dimple rupture only) and titanium. The titanium specimens are being used to study the fracture behavior and the ability of existing models to predict failure for weldments. Moire interferometry techniques are being used to study the local constitutive behavior and the fracture process at the crack tip region of the weldment.

Keywords: Fracture, Metals: Ferrous

150. **MODELING OF THERMAL PLASMA PROCESSES**
$210,000
DOE Contact: Oscar P. Manley, (301) 903-5822
Idaho National Engineering Laboratory Contacts:
J. D. Ramshaw, (208) 526-9240 and
C. H. Chang, (208) 526-2886

Optimization of thermal plasma processing techniques requires a better understanding of the space- and time-resolved flow and temperature distributions in the plasma plume and of the interaction between the plasma and a particulate phase. This research is directed toward the development of a comprehensive computational model of thermal plasma processes and plasma-particle interactions capable of providing such information. The model is embodied in the LAVA computer code for two- or three-dimensional transient or steady state thermal plasma simulations. LAVA uses a rectangular mesh with an excluded volume function to represent geometrical obstructions and volume displaced by particles. Simple highly vectorizable numerics are utilized, with rapid steady state and low-speed flow options. The plasma is represented as a multicomponent fluid governed by the transient compressible Navier-Stokes equations. Real gas physics is allowed for by temperature-dependent specific heats and transport properties. Multicomponent diffusion is calculated in a self-consistent effective binary diffusion approximation, including ambipolar diffusion of charged species. Both k-epsilon and subgrid-scale turbulence models are included. Dissociation, ionization, and plasma chemistry are represented by means of general kinetic and equilibrium chemistry routines. Discrete particles interacting with the plasma will be represented by a stochastic particle model similar to that previously used to model liquid sprays. This model allows for spectra of particle sizes, shapes, temperatures, etc., thereby capturing the important statistical aspects of the problem. It will include sub-models for the various plasma-particle and particle-particle interaction processes, including melting, evaporation, condensation, nucleation, agglomeration, and coalescence.

Keywords: Plasma Processing, Optimization, Computational Model

151. **NONDESTRUCTIVE EVALUATION OF SUPERCONDUCTORS**
$180,000
DOE Contact: Oscar P. Manley, (301) 903-5822
Idaho National Engineering Laboratory Contact:
K. L. Telschow, (208) 526-1264

The purpose of this task is to perform fundamental research which will lead to the development and application of new nondestructive evaluation (NDE) techniques and devices for the characterization of high-temperature superconducting materials. In the near future, application of these new superconductors will require NDE methods for evaluating the properties of wires, tapes and coatings. Microstructural and, particularly, superconducting properties must be measured noninvasively in a manner capable of providing spatial information so that fabrication processes can be optimized. Although the fabrication of these ceramic materials is being pursued by many different techniques at present, there is enough similarity in the different superconducting materials and the fabricated forms to begin research into NDE measurement techniques. In FY89 this project began identifying techniques that can determine critical superconducting properties on a local scale. This has resulted in the use of AC induced currents in conjunction with DC transport currents to determine critical currents and dissipation locally. The analysis of these measurements is being carried out with the aid of the London and "Critical State" models for supercurrent flow in these materials. These results are being correlated with material microstructure information and other measurement techniques.

Keywords: NDE, Superconductors

152. **STRESS INDUCED PHASE TRANSFORMATIONS**
$67,419
DOE Contact: Oscar P. Manley, (301) 903-5822
University of Illinois Contact: H. Sehitoglu,
(217) 333-4112

Understanding stress-induced phase transformations is of paramount importance in modeling the behavior of engineering materials and components. From the material behavior standpoint, transformations generate internal (micro) stresses which alter the constitutive behavior, and from the component standpoint transformation strains may result in dimensional changes and alteration of macroscopic stress fields. The transformation strains are strong functions of the applied stress state since favorably oriented planes transform in the course of loading. Several unique experiments under combined shear stress-hydrostatic pressure are conducted on steels, containing retained austenite, in order to measure and study anisotropic transformation strains. Test specimens are subjected to externally applied pressures in excess of 700 MPa. The compressive hydrostatic stresses would increase the extrinsic ductility of the material, and hence permit high magnitudes of the stress-induced and strain-induced transformations. Based on these experiments, the work will set the background to evaluate the theories proposed, and lay the foundation for new ones with particular emphasis on complex changes in transformation strains. The basic information obtained from the work will generate improved understanding of transformation under contact loadings and transformation toughening phenomenon in metallic and non-metallic materials.

Keywords: Phase Transformation, Stress, Strain

153. **PULSE PROPAGATION IN INHOMOGENEOUS OPTICAL WAVEGUIDES**
$0
DOE Contact: Oscar P. Manley, (301) 903-5822
University of Maryland Contact: C. Menyuk, (301) 455-3501

Our research, which was originally focused on light propagation in inhomogeneous optical fibers, has broadened in scope to include studies of solid state rib waveguides and Y-junctions which are used to guide and switch light. The work on optical fibers is divided into two research projects.

The first project concerns long-distance communication using solutions. We have been particular concerned with the effects of randomly varying birefringence, and we have shown that its effect is benign. From the basic equations we were able to show from an appropriate ordering expansion that the nonlinear Schrodinger equation is the lowest order equation and, hence, we expect its behavior to dominate the soliton evolution even in a highly birefringent fiber, as long as the birefringence is rapidly varying. We have also studied optical fiber soliton switches based on trapping and dragging. To do the work on optical fibers, we have collaborated with scientists at AT&T Bell Laboratories. The first solid state project was to find the effect of a quantum well on the propagation characteristics of a rib waveguide. Using a planar guide as reference, we were able to show that the effect of the real geometry is qualitatively small but can have a significant quantitative effect.

The second solid-state project is to determine the effect of dry-etching on the mode-holding characteristics of the device. As a consequence of the etching, the height at which the junction splits can vary. We showed that the rounding has a very small effect, in contrast to blunting which occurs when the materials are chemically wet etched.

Keywords: Optical Fibers, Pulse Propagation, Inhomogeneities, Imperfections

154. **MULTIVARIABLE CONTROL OF THE GAS-METAL/ARC WELDING PROCESS**
$152,609
DOE Contact: Oscar P. Manley, (301) 903-5822
MIT Contact: David E. Hardt, (617) 253-2429

The Gas-Metal Arc Welding Process (GMAW) is a highly productive means for joining metals and is being used increasingly for structures and pressure vessels. The overall objective of this work is to examine the problem of simultaneous regulation of all real-time attributes of a weld. Past work has established the viability of independent control of thermal characteristics and the present work is examining the geometric aspects of weld pool control.

One objective of this work is to develop basic process modeling and control schemes to allow independent regulation of the weld bead width and height. A control model relating wirefeed and travel speed to width and height was developed using transfer function identification techniques applied to a series of step welding tests. We are developing a control system to independently regulate the weld bead width and the width of the heat affected zone. Initial work is concentrating on simulation of wide seam welding using an analytical heat transfer model as well as a finite difference process model. A key issue in the problem is the strong coupling between the inputs (current and travel speed) and the outputs. The use of high frequency transverse motion of the torch is being investigated as a means of overcoming this coupling. Once the control latitude is increased, a two variable control scheme based on both video and infrared sensing will be implemented.

Finally, the depth of penetration of a weld is the most important indicator of weld strength, yet it is the one variable that is essentially impossible to measure directly. A real-time depth estimator has been developed based on solution of an inverse heat transfer problem. Surface temperature measurements from the top and bottom of the weld have shown accurate and rapid convergence and development of a depth control system based on this estimator is now being processed.

This project is a collaborative program with INEL.

Keywords: Welding, Control

155. **METAL TRANSFER IN GAS-METAL ARC WELDING**
$123,688
DOE Contact: Oscar P. Manley, (301) 903-5822
MIT Contacts: T. W. Eagar and J. Lang, (617) 253-3229

The present research is part of a cooperative program among faculty at MIT and staff at the Idaho National Engineering Laboratory (INEL) to develop a sound understanding of the arc welding process and to develop sensing and control methods that can be used to automate the gas-metal arc process.

The research during the current year has reviewed methods of filtering the voltage and current waveforms during pulsed current welding in order to extract signals which can be used to control the process. A new process control system has been developed and integrated with the welding equipment. Work has begun to study methods of mechanically controlling droplet detachment from the welding electrode.

Keywords: Welding, Control

156. **MODELING AND ANALYSIS OF SURFACE CRACKS**
$191,628
DOE Contact: Oscar P. Manley, (301) 903-5822
MIT Contacts: David M. Parks, (617) 253-0033 and F. A. McClintock, (617) 253-2219

This research focuses on the analysis of ductile crack initiation, growth and instability in part-through surface-cracked plates and shells. The overall approach consists of careful calculations of crack front stress and deformation fields, and correlation of cracking with experimental observations being conducted at the Idaho National Engineering Laboratory. Recently, significant progress has been achieved in developing and applying a two-parameter description of crack front fields.

Simplified engineering applications of surface crack analysis are being developed in the context of the line-spring model. Specific enhancements include improved elastic-plastic procedures for the practically important case of shallow surface cracks, as well as simple methods for calculating the T-stress along surface cracks fronts.

Detailed elastic-plastic stress analyses of cracked structural geometries provide a basis for interpreting experimental observations, for quantitatively assessing inherent limitations of nonlinear fracture mechanics methodology, and for extending these boundaries through development of two-parameter characterization of crack tip fields. Simplified but accurate analytical methods are also under development for analysis of surface-cracked plates and shells. Emphasis is placed on better understanding complex three-dimensional features of elastic-plastic crack tip fields.

Keywords: Fracture

157. **THERMAL PLASMA PROCESSING OF MATERIALS**
$0
DOE Contact: Oscar P. Manley, (301) 903-5822
University of Minnesota Contact: E. Pfender, (612) 625-6012

The objective of this research project is to study analytically and experimentally specific thermal plasma processes for materials treatment. Processes of interest include the synthesis of ultrafine ceramic powders and of films.

During the past year our efforts have concentrated on characterizing the thermal plasma chemical vapor deposition (TPCVD) process of diamond films onto various substrates. Modeling of the situation close to the substrate indicates extremely steep temperature and concentration gradients pointing to the important of thermal diffusion.

Very high diamond deposition rates up to 1 mm/hr have been observed with a plasma reactor with recirculation eddies. A series of diagnostic studies have been initiated to facilitate an understanding of the main reasons for the observed high deposition rates.

Keywords: Plasma Processing, Plasma Diagnostics

158. **DEVELOPMENT OF MEASUREMENT CAPABILITIES FOR THE THERMOPHYSICAL PROPERTIES OF ENERGY-RELATED FLUIDS**
$416,000
DOE Contact: Oscar P. Manley, (301) 903-5822
National Institute of Standards and Technology Contacts: R. Kayser, (301) 975-2483 and J. M. H. Sengers, (301) 975-2463

The major objective of this project is to develop state-of-the-art experimental apparatus that can be used to measure the thermophysical properties of a wide range of fluids and fluid mixtures important to the energy, chemical, and energy-related industries and to carry out carefully selected benchmark measurements on key systems. The research is being done jointly by two groups within the Thermophysics Division of the NIST Chemical Science and Technology Laboratory; one group is located in the Gaithersburg, MD, laboratories and the other at the Boulder laboratories. The specific measurement capabilities to be developed in this project include new apparatus for transport properties (thermal conductivity and viscosity), for thermodynamic properties (pressure-volume-temperature data and enthalpy), for phase equilibria properties (vapor-liquid equilibria, coexisting densities, and dilute solutions), and for dielectric properties (dielectric constant). These new apparatus will extend significantly the existing state of the art for properties measurements and make it possible to study a wide range of complex fluid systems (e.g., highly polar, electrically conducting, and reactive fluids) under conditions which have been previously inaccessible. This project also includes benchmark experimental measurements on systems containing alternative refrigerants, on aqueous solutions, and on carefully selected systems with species of diverse size and polarity that are important to the development of predictive models for energy-related fluids.

Keywords: Thermophysical Properties, Mixtures, Fluids, High Temperature, High Pressure

159. **LOW RESISTIVITY OHMIC CONTACTS BETWEEN SEMICONDUCTORS AND HIGH-T_c SUPERCONDUCTORS**
$86,000
DOE Contact: Oscar P. Manley, (301) 903-5822
National Institute of Standards and Technology Contacts: J. Moreland, (303) 497-3641 and J. W. Ekin, (303) 497-5448

The purpose of this project is to fabricate and characterize high-T_c superconductor/semiconductor contacts. Developing a method for optimizing the current capacity of such contact will extend the application of high-T_c superconductors to hybrid superconductor/semiconductor technologies. These technologies include integrated circuit interconnects (both on-chip and package) and proximity superconductor/semiconductor/superconductor SNS Josephson junctions. Presently, these are among the most promising high-T_c superconductor applications, but an essential first step is the development of reliable, stable, ohmic contacts between semiconductors and the high-T_c oxide superconductors.

The initial phase of this program is to determine the compatibility of various metals and alloys (Au and Al alloys and W, for example) as contact materials for superconducting YBCO and other high T_c materials. Once a good combination has been established, patterned YBCO/normal metal contacts will be deposited onto semiconductor wafer surfaces. We have purchased a sputter co-deposition system for YBCO thin films and have adapted three other vacuum systems for contact deposition including two sputtering systems and an evaporator.

Keywords: High-Tc Superconductors, Semiconductors, Contact, Low Resistivity

160. **THIN FILM CHARACTERIZATION AND FLAW DETECTION**
$91,537
DOE Contact: Oscar P. Manley, (301) 903-5822
Northwestern University Contact: J. D. Achenbach, (312) 491-5527

The work on this project is concerned with applications of the scattered field approach to the detection and characterization of cracklike flaws. The work is both analytical and numerical in nature.

The efficacy of ultrasonic methods to detect and characterize a crack depends on topographical features of the crack faces, the presence of inhomogeneities in the crack's environment, and on the mechanical properties in the near-crack region. In this work the effects on the scattered ultrasonic field of various features of fatigue and stress corrosion cracks, such as partial crack closure, the presence of microcracks and microvoids, and near-tip zones of different mechanical properties have been investigated. Most of the results have been obtained by formulating a set of singular integral equations for the fields on the boundaries of the scattering obstacles. These equations have been solved numerically by the boundary element method, and the scattered fields have subsequently been obtained by using representation integrals.

For the configurations examined in this work, crack closure has the most significant effect on far-field scattering.

Keywords: Non-Destructive Evaluation, Superconductors, Scattering

161. **EXPERIMENTS ON THE GAS DYNAMICS OF THE HIGH VELOCITY OXY-FUEL (HVOF) THERMAL SPRAY PROCESS**
$94,981
DOE Contact: Oscar P. Manley, (301) 903-5822
Pennsylvania State University Contact: G. Settles, (814) 863-1504

This reseaarch program involves an experimental study of the gas dynamics of high-velocity oxy-fuel (HVOF) thermal sprays, a promising new technology in the fields of materials, manufacturing, and the extension of the useful life of large equipment. HVOF relies on combustion to melt and propel solid particles at high speeds onto a surface to be coated. The principles of gas dynamics govern the expansion of this gas/particle stream from high stagnation conditions to produce a supersonic jet. The current scientific basis of the HVOF process is poorly understood; dramatic improvements in the HVOF thermal spray are likely by applying the principles of gas dynamics which is a well-developed field in the disciplines of high-speed aerodynamics and propulsion. The specific approach is to use a properly-shaped nozzle and an appropriate pressure ratio to demonstrate that a perfectly-expanded supersonic jet constitutes the central physical principle upon which the HVOF thermal spray can be based. In such case the temperature-time history of the sprayed particles can be tailored to achieve coatings with specific properties, and to minimize oxidation due to mixing with the surrounding air.

Keywords: Surface Coatings, HVOF Sprays

162. **TRANSPORT PROPERTIES OF DISORDERED POROUS MEDIA FROM THE MICROSTRUCTURE**
$101,185
DOE Contact: Oscar P. Manley, (301) 903-5822
Princeton University Contact: S. Torquato, (609) 258-4600

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

Both theoretical and computer-simulation techniques have been employed to quantitatively characterize the microstructure and compute the transport properties of disordered media.

Keywords: Disordered Media

163. **EFFECT OF FORCED AND NATURAL CONVECTION ON SOLIDIFICATION OF BINARY MIXTURES**
$103,571
DOE Contact: Oscar P. Manley, (301) 903-5822
Purdue University Contact: F. Incropera, (317) 494-5688

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

The primary objective of current studies is to determine the manner in which externally imposed forces influence thermo-solutal convection in the mushy and liquid regions during solidification of a binary mixture. A special goal is to determine means by which the forces may be used to offset or dampen thermo/solutal convection, thereby reducing macrosegregation and attendant casting defects. Separate consideration is being given to the effects of magnetic and centrifugal forces on solidification in binary metallic alloys and aqueous salt solutions, respectively. Predictions based on the continuum model are being compared with measurements obtained for metallic (Pb-Sn) and aqueous (NH_4Cl-H_2O) systems.

Keywords: Solidification, Convection, Binary Alloys, Salt Solutions, Magnetic Fields, Centrifugal Forces

164. **INELASTIC DEFORMATION AND DAMAGE AT HIGH TEMPERATURE**
$0
DOE Contact: Oscar P. Manley, (301) 903-5822
Rensselaer Polytechnic Institute Contact: Erhard Krempl, (518) 266-6432

A combined theoretical and experimental investigation is performed to study the biaxial deformation and failure behavior of engineering alloys under low-cycle fatigue conditions at elevated temperature. The purpose is to characterize the material behavior in mathematical equations which are ultimately intended for use in inelastic stress analysis and life prediction. Creep-fatigue interaction and ratchetting are of special concern. The long-term goal is the development of a finite element program that can directly calculate the life-to-crack initiation of a component under a given load history.

Keywords: Fracture, Damage

165. **FLUX FLOW, PINNING AND RESISTIVE BEHAVIOR IN SUPERCONDUCTING NETWORKS**
$70,519
DOE Contact: Oscar P. Manley, (301) 903-5822
University of Rochester Contact: S. Teitel, (716) 275-4039

The motion of vortex structures, in response to applied currents, is a major source of resistance in superconducting networks in magnetic fields. Systems of interest include regular Josephson junction arrays and type II superconductors, such as the new granular high T_c ceramics. Numerical simulations of finite temperature, current carrying networks will be carried out to provide a characterization of vortex response in non-equilibrium situations. For periodic networks, current-voltage (I-V) characteristics will be computed and compared with experimental results. The effects on resistivity of transitions from pinned to unpinned or to melted vortex structures, will be investigated. For disordered networks, the effects of pinning in producing metastable vortex structures leading to glassy behavior will be explored.

To date, simulations have been carried out for the "fully frustrated" two dimensional regular Josephson junction array. I-V characteristics were computed and reasonable agreement found with experiment. Behavior was explained within a simple physical model, in which correlations between vortices is crucial for producing the critical excitations leading to vortex flow resistance.

Keywords: Flux Flow, Pinning, Vortex Motion, Superconductors

166. **STABILITY AND STRESS ANALYSIS OF SURFACE MORPHOLOGY OF ELASTIC AND PIEZOELECTRIC MATERIALS**
$135,000
DOE Contact: Oscar P. Manley, (301) 903-5822
Stanford University Contact: H. Gao, (415) 725-2560

The goal of this research is to investigate the mechanical effects of surface morphology of elastic dielectric and piezoelectric materials. In particular, the project will study the stability of a flat surface against diffusional perturbations and the stress concentration caused by slightly undulating surfaces.

The surface morphology of materials will be studied by using a unified perturbation procedure based on the notion of thermodynamic forces and the energy momentum tensor. The thermodynamic forces on material inhomogeneities such as interfaces and inclusions are a measure of the rate at which the total energy of a physical system varies with the configurational change of these inhomogeneities. Within the general methodology, any type of material and loading condition can be studied as long as the proper forces can be identified. By using corresponding material conservation laws discovered previously, a systematic analysis of surfaces of piezoelectric solids will be made. Preliminary studies have shown that under sufficiently large stresses, surfaces of materials become unstable against a range of diffusional perturbations bounded by two critical wave lengths. Even a slight undulation caused by these unstable diffusional perturbations, such as micro-level bumps and troughs, can result in a significant stress concentration along a material surface. These concentrations may lead to mechanical failures along the surface and may have more consequences for piezoelectric materials where the deformation is coupled to an applied electric field. There are also suggestions that the stress distributions in a body may be sensitive to the surface morphology.

Keywords: Stress Analysis, Surface Morphology, Elastic, Dielectric, Piezoelectric Materials

167. **OPTICAL TECHNIQUES FOR SUPERCONDUCTOR CHARACTERIZATION**
$145,000
DOE Contact: Oscar P. Manley, (301) 903-5822
Stanford University: G. S. Kino, (415) 497-0205

The aim of this project is to develop a photothermal microscope for noncontact testing of materials. Techniques of this kind are particularly well suited to the determination of thermal parameters, and anisotropy of small samples.

One example of the work is the measurement of high temperature superconductors over a range of temperatures from room temperature through the critical temperature T_c down to 20°K. A modulated laser beam, focused to less than 1 m diameter, impinges through a sapphire window onto a sample of Bi-Ca-Sr-Cu-O in a helium cryostat and periodically modulates its temperature. This process excites a thermal wave, which can be detected by the variation in reflected signal amplitude of a second focused laser beam, due to the change of refractivity with temperature. The sample can be rotated under the beams and the thermal diffusion coefficient, its anisotropy and its magnitude can be measured from the phase delay of the thermal wave. By measuring the amplitude of the thermal wave, material phase changes associated with superconductivity can be measured. A pronounced peak in amplitude is seen at the critical temperature T_c. Even stronger effects of this type are observed with charge density waves in a variety of materials.

Keywords: Nondestructive Evaluation, Acoustic Sensors

168. **DEGENERATE FOUR-WAVE MIXING AS A DIAGNOSTIC OF PLASMA CHEMISTRY**
$0
DOE Contact: Oscar P. Manley, (301) 903-5822
Stanford University Contact: R. Zare, (415) 723-3062

A need exists for *in situ* nonintrusive diagnostics for probing trace and highly reactive radical intermediates in nonequilibrium plasma used for chemical vapor deposition. We propose applying a novel nonlinear spectroscopic technique, degenerate four-wave mixing (DFWM). The DFWM signal is a coherent scattered beam at frequency which is generated by the nonlinear response of the medium to the interaction of three incident waves at the same frequency. The signal is enhanced by a resonant transition and offers a form of Doppler-free spectroscopy with extremely high spectral, spatial, and temporal resolution. Signal detection is remote and does not suffer from background interference from the bright plasma source. In addition, the phase conjugate nature of the signal eliminates optical aberration. The environment we propose to study is an atmospheric-pressure rf-inducively-coupled plasma and the target radicals include CH, CH_2, C_2, C_2H, and CH_3 that are important in plasma synthesis of diamond thin films. The spatial sensitivity of DFWM will be used to study the coupling of gas-phase and gas-surface chemistry by measuring temperature and concentration profiles. The proposed research will advance diagnostic techniques for plasma environments and provide a better understanding of the plasma chemistry of diamond synthesis.

Keywords: Plasma, Four-Wave Mixing

169. **EFFECTIVE ELASTIC PROPERTIES AND CONSTITUTIVE EQUATIONS FOR BRITTLE SOLIDS UNDER COMPRESSION**
$0
DOE Contact: Oscar P. Manley, (301) 903-5822
Tufts University Contact: Mark Kachanov, (617) 628-5000, ext. 2821

The knowledge of effective elastic properties of solids with cracks appears to be of increasing engineering importance. Extensive microcracking in structural elements working under conditions of high temperatures or irradiation, microcracking in composite materials under fatigue conditions may noticeably reduce the stiffness of the material and make it anisotropic. Understanding and prediction of these changes are essential for proper design and strength and lifetime assessments.

A new approach to many crack problems based on interrelating the average tractions on individual cracks is introduced. Its advantages are that it yields simple analytical results which are quite accurate up to very high crack densities and that it can be applied to crack arrays or arbitrary geometry. Relation between deterioration of elastic properties and "damage" is discussed.

Keywords: Fracture, Elasticity

170. **3-D EXPERIMENTAL FRACTURE ANALYSIS AT HIGH TEMPERATURE**
$69,975
DOE Contact: Oscar P. Manley, (301) 903-5822
University of Washington Contact: Albert Kobayashi, (206) 543-5488

This research deals with a detailed experimental investigation of the nonlinear deformation and failure of surface-flawed pressure vessels and piping. It includes (1) elastic-plastic fracture, and (2) high-temperature creep and viscoplastic fracture. The objective of this effort is to acquire an understanding of the mechanics of the initial phases of failure and, thereby, provide better designs and life assessments of critical structural parts. This effort is being conducted in collaboration with Georgia Institute of Technology which is performing the theoretical research of the overall and crack-tip fields.

Keywords: Fracture, Failure Analysis

171. **SIMULATION AND ANALYSIS OF DYNAMIC FAILURE IN DUCTILE MATERIALS**
$98,919
DOE Contact: Oscar P. Manley, (301) 903-5822
Brown University Contact: B. Freund, (401) 863-1157

This mainly theoretical effort is a part of a joint program with the California Institute of Technology, where Professor Rozakis, under a separate grant, contributes the necessary data obtained by novel measurement techniques.

Dynamic crack initiation and growth in ductile metals is still poorly understood, in spite of the fact that many energy structures are built using such materials. Unlike static considerations of crack propagation in brittle materials, the corresponding dynamical crack evolution is intrinsically three dimensional and, until recently, beyond experimental and computational capabilities. Recent advances reported in the literature have shown the feasibility of carrying out the proposed research with existing or readily accessible resources.

The specific objectives of this project include: study of the plain strain deformation of a thick-walled cylinder subjected to suddenly applied pressure or equivalent loading; detailed examination and modeling of a ductile failure process including three dimensional effects as exhibited in the data to be obtained by Professor Rosakis at Caltech; the interaction of dynamically growing cracks in ductile materials, leading up to structural failure under intense loading conditions.

Keywords: Fracture, Ductility, Dynamic

172. **DYNAMIC FAILURE CHARACTERIZATION OF DUCTILE STEELS**
$99,664
DOE Contact: Oscar P. Manley, (301) 903-5822
California Institute of Technology Contact: A. Rozakis, (818) 395-4523

This mainly experimental effort is a part of a joint program with Brown University, where Professor B. Freund contributes his theory and modeling efforts.

Dynamic crack initiation and growth in ductile metals is still poorly understood, in spite of the fact that many energy structures are built using such materials. Unlike static considerations of crack propagation in brittle materials, the corresponding dynamical crack evolution is intrinsically three dimensional and, until recently, beyond experimental and computational capabilities. Recent advances reported in the literature have shown the feasibility of carrying out the proposed research with existing or readily accessible resources.

The specific objectives of this project include: damage models for deformation of stainless steels as a function of strain, strain rate and temperature; novel optical and IR techniques for observing crack initiation and evolution under a range of loading rates; 3-D aspects of crack initiation; determination of the criteria for crack initiation, growth and arrest; numerical simulation of dynamic failure experiments including thermomechanics of damage evolution.

Keywords: Fracture, Ductility, Dynamic

GEOSCIENCES RESEARCH

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

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

173. **AN INVESTIGATION OF ORGANIC ANION-MINERAL SURFACE INTERACTIONS DURING DIAGENESIS**
$199,500
DOE Contact: W. C. Luth, (301) 903-5822
SNL Contacts: Patrick Brady, (505) 844-7216 and Randall Cygan, (505) 844-7216

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

Key Words: Surface Reactions, Aluminosilicate Minerals, Adsorption Mechanisms

174. **TRANSITION METAL CATALYSIS IN THE GENERATION OF PETROLEUM AND NATURAL GAS**
$136,179
DOE Contact: W. C. Luth, (301) 903-5822
Rice University Contact: Frank D. Mango, (713) 527-4880

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

Keywords: Transition Metals, Catalysis, Petroleum

MATERIALS STRUCTURE AND COMPOSITION

175. **REACTION MECHANISMS OF CLAY MINERALS AND ORGANIC DIAGENESIS: AN HRTEM/AEM STUDY**
$125,696
DOE Contact: W. C. Luth, (301) 903-5822
Arizona State University Contact: P. R. Buseck, (602) 965-3945

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

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

176. **INFRARED SPECTROSCOPY AND HYDROGEN ISOTOPE GEOCHEMISTRY OF HYDROUS SILICATE GLASSES**
$123,000
DOE Contact: W. C. Luth, (301) 903-5822
Caltech Contacts: S. Epstein, (818) 356-6100 and E. Stolper, (818) 356-6504

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

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

177. **BIOMINERALIZATION: SYSTEMATICS OF ORGANIC-DIRECTED CONTROLS ON CARBONATE GROWTH MORPHOLOGIES AND KINETICS DETERMINED BY *IN SITU* ATOMIC FORCE MICROSCOPY**
$90,891
DOE Contact: W. C. Luth, (301) 903-5822
Georgia Inst. of Technology Contact: P. Dove, (404) 894-6043

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

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

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

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

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

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

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

Keywords: Uranium Oxide Hydrates, Crystal Chemistry, Structural Topology

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

180. **CATION DIFFUSION RATES IN SELECTED SILICATE MINERALS**
$95,000
DOE Contact: W. C. Luth, (301) 903-5822
Sandia National Laboratory Contacts: Randall T. Cygan, (505) 844-7216 and H. R. Westrich, (505) 844-9092

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

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

181. **SHEAR STRAIN LOCALIZATION AND FRACTURE EVOLUTION IN ROCKS**
$85,404
DOE Contact: W. C. Luth, (301) 903-5822
Northwestern University Contact: J. W. Rudnicki, (708) 491-3411

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

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

182. **OXYGEN AND CATION DIFFUSION IN OXIDE MATERIALS**
$171,000
DOE Contact: W. C. Luth, (301) 903-5822
LLNL Contact: F. J. Ryerson, (510) 422-6170
University of California at Los Angeles Contact: K. D. McKeegan, (310) 825-3580

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

Keywords: Diffusion, Minerals, Plastic Deformation

183. **DISSOLUTION RATES AND SURFACE CHEMISTRY OF FELDSPAR GLASS AND CRYSTAL**
$114,700
DOE Contact: W. C. Luth, (301) 903-5822
Penn State Contact: S. Brantley, (814) 863-1739

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

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

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

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

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

185. **THREE-DIMENSIONAL IMAGING OF DRILL CORE SAMPLES USING SYNCHROTRON-COMPUTED MICROTOMOGRAPHY**
$177,200
DOE Contact: W. C. Luth, (301) 903-5822
BNL Contact: Keith Jones, (516) 282-4588
SUNY, Stony Brook Contact: W. B. Lindquist, (516) 632-8361

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

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

186. TRANSPORT PHENOMENA IN FLUID-BEARING ROCKS
$139,680
DOE Contact: W. C. Luth, (301) 903-5822
Renssalaer Polytechnic Institute Contact:
E. B. Watson (518) 276-6475

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

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

187. STRUCTURE AND REACTIVITY OF FERRIC OXIDE AND OXYHYDROXIDE SURFACES: QUANTUM CHEMISTRY AND MOLECULAR DYNAMICS
$142,500
DOE Contact: W. C. Luth, (301) 903-5822
PNNL Contacts: Jim Rustad and Andrew Felmy, (509) 376-1134

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

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

188. MICROMECHANICS OF FAILURE IN BRITTLE GEOMATERIALS
$184,239
DOE Contact: W. C. Luth, (301) 903-5822
SUNY, Stony Brook Contact: Teng-Fong Wong, (516) 632-8240
SNL Contact: Joanne Fredrich, (505) 846-0965

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

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

189. CATION CHEMISORPTION AT OXIDE SURFACES AND OXIDE-WATER INTERFACES: X-RAY SPECTROSCOPIC STUDIES AND MODELING
$210,000
DOE Contact: W. C. Luth, (301) 903-5822
Stanford University Contacts: G. E. Brown and G. A. Parks, (415) 723-9168

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

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

DIVISION OF ADVANCED ENERGY PROJECTS

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

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

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

190. **COMBUSTION SYNTHESIS AND ENGINEERING OF NANOPARTICLES FOR ELECTRONIC, STRUCTURAL AND SUPERCONDUCTOR APPLICATIONS**
$196,000
DOE Contact: Walter M. Polansky, (301) 903-5995
Alfred University Contact: Gregory C. Stangle, (607) 871-2798

The investigation will: (1) produce nanoparticles of multicomponent oxide ceramic materials by a combustion synthesis technique that is readily scaled up; (2) apply proven, in-house grain-boundary engineering methods to fine-tune microstructure evolution during densification; (3) use conventional and rapid sintering techniques to densify consolidated nanoparticle compacts; and (4) characterize the material at each stage. Expected results include: (a) the synthesis of nanoparticles of complex composition for use in several applications (such as $YBa_2Cu_3O_{7-x}$, a high-temperature superconductor with uses, e.g., in magnetic flux trapping and high-speed capacitor applications; yttria-stabilized zirconia for, e.g., high surface toughness materials for high-temperature applications; and $BaTiO_3$, a material expected to possess superparaelectric properties when nanocrystalline); (b) the development and reduction to practice of a generic, widely applicable process; and (c) the evaluation of the energy efficiency and commercialization potential of the process. The proposed study will enlist three U.S.-based companies to aid in focusing the research toward the commercialization of successful research results.

Keywords: Nanoparticles, Ceramics, Superconductors, Electronic Materials

191. **CREATION AND DESTRUCTION OF C_{60} AND OTHER FULLERENE SOLIDS**
$302,000
DOE Contact: Dr. Walter M. Polansky, (301) 903-5995
University of Arizona Contact: Donald R. Huffman, (602) 621-4804

This work will focus on the creation and destruction of fullerenes to produce new materials of interest to the Department of Energy. It is now known that, besides the famous C_{60} molecule (buckminsterfullerene), hundreds of other fullerenes, with masses of up to 600 carbon atoms, are also synthesized in the Krätschmer-Huffman process. The physics underlying the creation of the fullerenes is poorly understood and the major portion of this work will be a systematic study of the process. This will involve construction of a new, fully-instrumented smoke-chamber, that will be used in a methodical exploration of fullerene yield versus production conditions. Recent reports of the successful seeding of chemical vapor deposition (CVD)-grown diamond films using thin films of C_{70}, and of the room-temperature conversion of solid C_{60} into diamond powder via non-hydrostatic compression, indicate that some of the first important commercial applications of the fullerenes may involve their destruction as a means of synthesizing high-performance materials. This work will include a systematic study of the destruction and modification of the various fullerenes by chemical reaction, electromagnetic radiation, and electron bombardment.

Keywords: Fullerenes, Diamond Powders, Buckyballs

192. **SYNTHESIS AND PROPERTIES OF HIGH STRENGTH NANOLAYERED COMPOSITES**
$330,000
DOE Contact: Walter M. Polansky, (301) 903-5995
Los Alamos National Laboratory Contact:
Michael Nastasi, (505) 667-7007

The objective of this project is to synthesize and evaluate ultra high strength vapor-deposited nanoscale materials both in the monolithic and composite form. Such materials have been shown to posses strengths that are within a factor of three or four of the theoretical shear strength $\approx\mu/15$, where μ is the shear modulus. Synthesis of nanoscale materials presents the opportunity to develop a basic understanding of the deformation and fracture mechanisms that operate close to the theoretical limit of strength of materials to enable a new technological breakthrough, namely mechanical miniaturization. The availability of the fine-scale ultra high strength materials would provide the basis for fabricating, among others, miniature activators, springs, and diaphragms, for biomedical or sensor applications. The primary performance task will be to synthesize ductile materials with ultra high strength for application in mechanical miniaturization.

Keywords: Nanostructures, Composites, Mechanical Miniaturization

193. **OPTIMALLY CONTROLLED INTERIOR MANIPULATION OF SOLIDS**
$299,000
DOE Contact: Walter M. Polansky, (301) 903-5995
Princeton University Contact: Herschel Rabitz, (609) 258-3917

This project is concerned with the development of a technique for modification of the interior solids without the necessity of opening up the material. The technique is based on the concept of designing and creating temporally and spatially tailored laser pulses that deposit energy on the surface for the purpose of launching an intense acoustic wave that focuses within the solid. Taking account of the relatively large illumination area on the surface and the focusing nature of the acoustic waves, it should be possible to minimally disrupt the surface while still attaining significant degrees of interior modification at the target volume. A central feature of this new materials processing method is its reliance on destructive and constructive interference between the ensuing shear and compressional acoustic waves. The research will include a theoretical design component. An established capability for interior manipulation of solids would open up many opportunities including interior annealing, induced phase transitions, induced chemical reactions, crack arresting, controlled defect site generation, and interior welding.

Keywords: Interior Processing of Materials, Acoustic Manipulation

194. **PHOTOREFRACTIVE LIQUID CRYSTALS: NEW MATERIALS FOR ENERGY-EFFICIENT IMAGING TECHNOLOGY**
$320,000
DOE Contact: Walter M. Polansky, (301) 903-5995
Argonne National Laboratory Contact:
Gary P. Wiederrecht, (708) 252-6963

This project will develop a new class of materials that will be used to produce energy-efficient image processing micro-devices. These materials will exploit the photorefractive effect, a light-induced change in the refractive index of a nonlinear optical materials that results from photogeneration of a space charge field caused by directional charge transport over macroscopic distances within a solid. Both frequency and phase information contained in light that has passed through a distorting medium can be recovered noise-free using photorefractive materials. The only high quality photorefractive materials commercially available today are expensive single crystals of inorganic materials such as barium titanate. This project will develop a completely new approach that combines cheap, easily processed organic materials with a built-in method of achieving the solid state order necessary to achieve photorefractivity comparable to that seen in inorganic crystals. The new approach uses organic molecules that undergo a phase transition above ambient temperatures to a liquid crystalline phase. These thin solid films have the potential to possess greater photorefractive sensitivity and faster responses times that any material developed to date.

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

195. **RAPID MELT AND RESOLIDIFICATION OF SURFACE LAYERS USING INTENSE, PULSED ION BEAMS**
$300,000
DOE Contact: Walter M. Polansky, (301) 903-5995
Sandia National Laboratories Contact:
Regan W. Stinnett, (505) 845-7488

This project will develop a surface processing technology based on new, repetitively pulsed ion beams. Rapid solidification is known to greatly improve metal surface properties such as corrosion, wear, and fatigue resistance, but the lack of an economic and effective way to apply this technique to surfaces has prevented its use except in high value applications. Intense, pulsed, high energy ion beams treat surfaces to produce non-equilibrium microstructures, nanocrystalline phases, and extended solid solutions leading to improved corrosion and friction properties of metals, as well as surface smoothing and defect healing, grain refinement, and modification of surface layer hardness. The low cost and in-depth deposition of high energy pulsed ion beams gives pulsed ion beam technology important advantages over laser treatment. The project will determine the capabilities and limitations of rapid melt and resolidification using pulsed ion beams. It will document the non-equilibrium micro-structures produced in treated layers and their effect on metal surface properties and will do the initial process development needed to show how this technique can be applied to commonly used metals. If successful, this will enable new ways to modify surfaces for enhanced properties and lifetimes with greatly improved energy efficiency and cost-effectiveness and will enable a significant reduction in the use of heavy metal and solvent-based surface treatment coating processes.

Keywords: Surface Processing, Pulsed Ion Beams, Rapid Solidification

196. **'OFF DIAGONAL' THERMOELECTRICITY FOR COOLING AND POWER GENERATION**
$170,000
DOE Contact: Walter M. Polansky, (301) 903-5995
TecOne Contact: Louis R. Testardi, (904) 562-9789

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

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

197. **EVAPORATION THROUGH TUNGSTEN TO ACHIEVE HIGH-RATE VAPOR PHASE PROCESSING OF INTERMETALLICS**
$291,000
DOE Contact: Walter M. Polansky, (301) 903-5995
General Electric Company Contact: David W. Skelly, (518) 387-6534

Modification of current practice of electron beam processes has been found to enhance chemistry uniformity and deposition rates through the addition or tungsten to the evaporation pool to permit much higher pool temperatures and stable pool dynamics. The objective of this research is to define optimum operating conditions for achieving economic deposition of controlled-chemistry, controlled-thickness Ni-base superalloys, NbTi-base metallic materials, and high strength, high temperature intermetallic phases. The approach will be to: evaluate process stability during prolonged evaporation through a tungsten-rich liquid pool; measure the effect of tungsten concentration in the pool on the evaporation process; characterize the influence of electron beam scan rate and scan pattern on the deposit chemistry and deposition rate; characterize the influence of the source temperature profile on deposit chemistry and deposition rate; determine evaporation conditions for Ni-base alloys containing Ta and Mo; and extend the electron beam evaporation-through-tungsten processing to higher melting intermetallic phases and NbTi-base metals. The understanding derived from this investigation will have significant impact on the ability to fabricate advanced designs of turbine blades.

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

198. **ULTRASONIC AND DIELECTRIC NONINVASIVE DIAGNOSTICS FOR SINTERING OF CERAMIC COMPOSITES**
$342,000
DOE Contact: Walter M. Polansky, (301) 903-5995
Johns Hopkins University Contact: Moshe Rosen, (410) 516-8678

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

Keywords: Microwave Sintering, Ceramics, Noninvasive Diagnostics

199. **COMPACT MEV ION IMPLANTER**
$319,000
DOE Contact: Walter M. Polansky, (301) 903-5995
Lawrence Berkeley Laboratory Contact:
Simone Anders, (510) 486-6745

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

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

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

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

Keywords: Quantum Wells, Thermoelectric Devices

201. **POROUS CARBONS: CONTROLLING STRUCTURE, COMPOSITION AND PERFORMANCE**
$355,000
DOE Contact: Walter M. Polansky, (301) 903-5995
Lawrence Livermore National Laboratory Contact:
Richard W. Pekala, (510) 422-0152

This research examines the synthesis and processing conditions necessary to tailor the local structure and composition of porous carbons for potential applications in energy storage devices. Carbon aerogels are being formed from resorcinol-formaldehyde and phenolic-furfural precursors. These porous carbons have low electrical resistivity, an ultrafine pore size distribution, high surface area (400 to 1100 square meters per gram, roughly the size of one or two basketball courts), and a solid matrix composed of interconnected particles or fibers. Preliminary data show that these materials are attractive electrodes for double layer capacitors. The project investigates sol-gel polymerization of multifunctional organic monomers, the phase separation of polymer/solvent mixtures, the formation of porous composites, intrinsic chemical doping, and pyrolysis in controlled atmospheres. A variety of characterization tools are being used to study the structure and properties of porous carbons. The overall objective is to develop a fundamental understanding of how morphology, chemical composition, and local order affect the electrochemical performance of porous carbons. The potential payoff from this research is the development of new energy storage devices with superior performance.

Keywords: Porous Carbons, Energy Storage Devices

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

202. **FEASIBILITY OF A NOVEL APPROACH FOR FAST, ECONOMICAL DETERMINATION OF RADIATION DAMAGE IN NUCLEAR REACTOR CORES**
$149,000
DOE Contact: Walter M. Polansky, (301) 903-5995
University of Michigan Contact: Gary S. Was, (313) 763-4675

The objective of this project is to determine the feasibility of using proton irradiation as a radiation damage tool, resulting in order-of-magnitude savings in time and cost over current methods to study radiation damage. The feasibility will be established through the application of proton irradiation to the determination of the mechanism of irradiation assisted stress corrosion cracking (IASCC) in light water reactors (LWRs). The emphasis of the technical program will be on the role of grain boundary chemistry and microstructural changes on IASCC. High energy proton irradiation has recently been shown to produce grain boundary segregation of the major alloying elements and impurities, and a microstructure that is comparable to that produced by neutron irradiation in a fraction of the time and at a fraction of the cost. This program is designed to uncover the effects of grain boundary impurity segregation, chromium depletion, and the irradiated microstructure on IASCC. It involves both experimental and computational efforts. The plan also calls for investigation of the dose, dose rate, temperature and injected hydrogen effects and comparison with available neutron irradiation data.

Keywords: Radiation Damage, Stress Corrosion Cracking, Irradiated Microstructures

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

This project is focused on the development and understanding of a new kind of high efficiency solar cell, called a Hot Carrier Solar Cell (HCSC), which may have the potential to double the maximum efficiency of conventional solar cells. The ultimate thermodynamic conversion efficiency of an optimized HCSC is 66 percent, compared to 31 percent for an optimized conventional single bandgap solar cell. This project will attempt to utilize the excess kinetic energy of higher energy (hot) carriers generated by the absorption of high energy photons in the solar spectrum, which is normally unavailable for useful work. The HCSC employs a new superlattice structure to absorb the solar photons and to inhibit hot carriers from cooling in the photovoltaic device. Hot carriers from the superlattice region are collected in high bandgap contacts to produce a higher photovoltage. With this combination, the photocurrent and photovoltage of the cell can be separately controlled and optimized. This project will synthesize HCSCs, measure their performance and properties, compare them to appropriate conventional solar cells, and develop a theoretical model for predicting the device characteristics of the HCSC.

Keywords: Hot Carrier Solar Cells, High Efficiency Energy Conversion

204. **ATOMIC AND NANOSCALE ENGINEERING OF THERMOPHOTOVOLTAIC SEMICONDUCTORS USING SCANNING PROBE MICROSCOPY TECHNIQUES**
$552,000
DOE Contact: Walter M. Polansky, (301) 903-5995
National Renewable Energy Laboratory Contact: Lawrence L. Kazmerski, (303) 275-3711

This project uses scanning probe microscopies for the atomic-scale engineering of semiconductors leading to advances in understanding their improvement, and their use in energy-conversion thermophotovoltaic (TPV) structures and devices. This project consists of three interrelated segments: (1) preparation of selected GaInAs and GaInAsP alloy surfaces having suitable compositions; (2) use of modern electronic structure theory to predict the properties of these semiconductor surfaces before and after atomic-scale engineering takes place and to provide guidance for the experiments; and the central and primary activity, (3) evolution of the novel atomic processing microscope to image, process (including atom removal and placement), and characterize these semiconductors with the same nanoscale spatial resolutions and to produce nanometer-scale optimized TPV structures for the next generation of these energy conversion devices.

Keywords: Thermophotovoltaics, Atomic Force Microscopy

205. **FABRICATION AND CHARACTERIZATION OF MICRON SCALE FERROMAGNETIC FEATURES**
$133,000
DOE Contact: Walter M. Polansky, (301) 903-5995
University of Nebraska Contact: Peter A. Dowben, (402) 472-9838

This is a project to study micro scale features of ferromagnetic nickel, cobalt, cobalt-palladium alloys and cobalt-palladium heterostructures fabricated by "direct writing," i.e., by selective area deposition from organometallic compounds. Two goals for this research program are: (1) making magnetic features smaller and smaller, in a variety of different shapes to elucidate the influence of defects on magnetization reversal and coercivity; (2) the project will determine if there is any coupling between small ferromagnetic features (approximately 1 micron), possibly substrate mediated, on the length scale of 1000 angstroms smaller. Polarized light microscopy will be used to image micron scale features and coercivity. A microscope will be used to make polar Kerr rotation measures and obtain spacially selective magnetic information. Spin polarized inverse photoemission with both longitudinal and transverse spin polarization will also be used for probing electronic structures. A new technique for fabricating micro-scale ferromagnetic features involves organometallic chemical vapor deposition techniques to deposit pure metal features with excellent spacial resolution, developed at this laboratory. These techniques allow selective deposition of features as small as 0.2 microns, and as thin as a few monolayers or as thick as 10 microns. The approach is superior to techniques employing ion beams or conventional lithography and is inexpensive and compatible with the fabrication of the next generation of optical and magnetic recording media.

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

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

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

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

207. **SEMICONDUCTOR BROADBAND LIGHT EMITTERS**
$330,000
DOE Contact: Walter M. Polansky, (301) 903-5995
Sandia National Laboratories Contact: Paul Gourley, (505) 844-5806

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

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

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

208. **ENERGY RELATED APPLICATIONS OF SELECTIVE LINE EMITTERS**
$291,000
DOE Contact: Walter M. Polansky, (301) 903-5995
Auburn University (Space Power Institute) Contact:
M. Frank Rose, (334) 844-5894

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

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

209. **PHOTO-INDUCED ELECTRON TRANSFER FROM A CONDUCTING POLYMER TO BUCKMINSTER-FULLERENE: A MOLECULAR APPROACH TO HIGH EFFICIENCY PHOTOVOLTAIC CELLS**
$446,000
DOE Contact: Walter M. Polansky, (301) 903-5995
University of California, Santa Barbara Contact:
Paul Smith, (805) 893-8104

The recently-discovered photoinduced electron transfer, with subpicosecond transfer rate, in composites of a conducting polymer, MEH-PPV, and a molecular acceptor, buckminsterfullerene, C_{60}, opens a new opportunity for photovoltaic research. Since the charge transfer takes place ~1000 times faster than the radiative and/or non-radiative decay of photoexcitations, the quantum efficiency for charge transfer and charge separation is near unity. Photoinduced electron transfer across the donor-acceptor rectifying heterojunction offers potential for solar cell applications, using materials that exhibit a unique combination of properties: electronic and optical properties of semiconductors and metals in combination with the attractive mechanical properties and the processing advantages of polymers. The potential advantages of an all-polymer heterojunction solar cell include low cost, large area, and flexibility. The goal of the proposed research is to build upon this novel molecular approach to photo-induced charge separation and charge transfer, with quantum efficiency approaching unity, and to create a capability to efficiently produce flexible, "plastic" solar cells for large areas.

Keywords: Fullerenes, Photovoltaics, Solar Cells

210. **SUPERCONDUCTING BITTER MAGNETS**
$300,000
DOE Contact: Walter M. Polansky, (301) 903-5995
Massachusetts Institute of Technology Contact:
Leslie Bromberg, (617) 253-6919

A novel process for manufacturing high temperature superconducting magnets, using thick-film superconducting material on structural plates, is described. The technique is similar to that used in constructing Bitter magnets. The superconductor is manufactured in the required shape, avoiding the need to develop ductile wires. The structural metal plate serves as the material as well as the quench protector. A dielectric with high electrical resistivity is placed between the conductor and the metal plate (copper, aluminum, composite materials). This method can be utilized for manufacturing solenoidal, toroidal, saddle, and other types of magnets with both high-T_c and low-T_c superconductors. This project will address issues faced in this type of magnet construction (quench protection, materials compatibility, stability, and cooling). Interaction with the manufacturers to improve the performance of superconducting materials for this application will be maintained. It is expected that in the final phase of this program, magnets will be constructed and tested. The project is in collaboration with the Plasma Fusion Center at the Massachusetts Institute of Technology and the Superconductivity Technology Center at Los Alamos National Laboratory.

Keywords: Bitter Magnets, Superconductivity

211. **BLUE-EMITTING DEVICES BASED ON GALLIUM NITRIDE**
$340,000
DOE Contact: Walter M. Polansky, (301) 903-5995
Lawrence Berkeley Laboratory Contact:
Michael D. Rubin, (510) 486-7124

The purpose of this project is to convert the recent breakthroughs in growth of gallium nitride (GaN) into practical ultraviolet and blue light emitting diodes and lasers. Short-wavelength semiconductor devices based on GaN are needed for many important applications such as energy-efficiency illumination, high-density optical data storage, flat-screen color displays, underwater communications, and high-temperature electronics. One of the principal technical problems that limits device applications has been achieving controllable properties with addition of Mg. It was discovered that good quality material could be readily obtained by a variety of doping methods including ion implantation, diffusion and co-evaporation of Mg. The defect studies which guide the improvements in the growth process will be continued. The technology will be transferred to Hewlett-Packard, where it will be reproduced in a large-scale commercial growth system.

Keywords: Gallium Nitride, Blue-Emitting Devices

212. **SOLID STATE MULTI-LAYERED BATTERIES**
$296,000
DOE Contact: Walter M. Polansky, (301) 903-5995
Lawrence Livermore National Laboratory Contact:
Richard M. Bionta, (510) 423-4846

The purpose of this project is to develop thin film solid-electrolyte batteries fabricated by the advanced multilayer sputtering techniques developed for X-ray optics. This technique allows the battery to be constructed *in situ* by depositing the anode, electrolyte, and cathode as distinct layers. Solid-electrolyte batteries have long been attractive because of their shelf-life and compatibility with severe environments. Recently, rechargeable lithium cells that operate at ambient temperature have been developed based on ionically conducting solid polymer electrolytes. This project will concentrate on the development of thin-film solid-electrolyte cells constructed of lithium based inorganic materials fabricated by multilayer sputtering. The ability of this fabrication technique to discretely layer or compositionally grade thin films provides a unique opportunity to investigate the effect of electrode-electrolyte interface structure on cell performance. Finally, the computer control associated with this fabrication technique will allow the deposition of multiple cells in a bipolar configuration with either series or parallel connection. It is anticipated that this research will directly lead to power sources for modern electronic circuits (i.e., microsensors, memory elements, displays, and timers).

Keywords: Solid State Batteries, Solid Electrolyte Batteries, Multilayer Fabrication

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

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

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

214. A NOVEL TANDEM HOMOJUNCTION SOLAR CELL: AN ADVANCED TECHNOLOGY FOR HIGH EFFICIENCY PHOTOVOLTAICS

$322,000
DOE Contact: Walter M. Polansky, (301) 903-4\5995
Colorado State University Contact:
Henryk Temkin, (303) 491-6018

The semiconductor, $ZnSnP(2)$, meets many criteria for large-scale photovoltaic applications. It is isoelectronic with the III-V alloy InGaP(2), but has the advantage, for photovoltaic applications, of not containing expensive and rare group III elements. In addition, this material does not contain toxic heavy metals such as are found in CdTe and CuInSe(2)/CdS thin film solar cells. The absorption coefficient for this material is also very high. The bandgap of ZnSnP(2) has the additional interesting and useful property of ranging from 1.24 to 1.66 eV, depending on the preparation conditions. There is no *a priori* reason that the electronic properties of these materials cannot be made as good as III-V materials, since very high mobilities were only achieved in III-V's after the development of modern epitaxial growth techniques. State-of-the-art metal-organic molecular beam epitaxy (MOMBE) will be used to grow epitaxial layers of ZnSnP(2) on lattice matched GaAs substrates. When the conditions can be established for preparing a material of a given bandgap, a "tandem homojunction" solar cell will be fabricated by variation of growth conditions in the MOMBE chamber in the appropriate way. This device should show significant efficiency advances over a single material device or tandem heterojunction devices where lattice mismatch produces recombination promoting interface states.

Keywords: Tandem-Homojunction Solar Cell, Photovoltaics, Molecular Beam Epitaxy

OFFICE OF FUSION ENERGY

The mission of the Office of Fusion Energy (OFE) is to develop fusion as an environmentally attractive, commercially viable, and sustainable energy source for the Nation and the world. This mission will be accomplished by parallel activities to develop the science and technology base for fusion, the conduct of large-scale experiments to explore the physics and demonstrate the components of fusion technologies, and the construction and operation of fusion power plants that will culminate in a demonstration power plant.

A significant component of the fusion energy program is the development and validation of the materials required for the fusion systems. Materials must be developed that will meet the unique requirements of fusion, as well as the standard requirements of a high efficiency, high reliability power generating system. The unique requirements of fusion are the result of the intense neutron environment, dominated by the 14 MeV neutrons characteristic of the deuterium-tritium fusion reaction. For performance, the materials must have slow and predictable degradation of properties in this neutron environment. For safety and environmental considerations, materials must be selected with activation products that neither decay too rapidly (affecting such safety factors as system decay heat) nor too slowly (affecting the waste management concerns for end-of-life system components). Materials that meet these requirements are referred to as "Low Activation Materials." Programs to develop the materials for plasma-facing components, for diagnostic and control systems, for structures in the high neutron flux regions, for the production of tritium in the blanket, and for the superconducting magnets required for confinement are sponsored by OFE.

The fusion program in the United States is conducted with a high degree of international cooperation. Of particular importance is the International Thermonuclear Experimental Reactor (ITER) engineering design activity, conducted in partnership with the European Union, Japan, and the Russian Federation. Approximately half of the materials work sponsored by OFE is in support of the ITER collaboration.

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

215. STRUCTURAL MATERIALS DEVELOPMENT

$1,552,000
DOE Contact: F. W. Wiffen (301) 903-4963
ANL Contact: D. L. Smith (708) 252-4837

This program is directed at the development of advanced, low activation structural materials for application in fusion power system first wall and blankets. Emphasis at ANL is on the development of vanadium-base alloys and on chemical corrosion/compatibility of the structural materials with other system materials. The vanadium alloy development is focused on the V-Cr-Ti system, with the goals of identifying promising candidate compositions, determining the properties of candidate alloys, and evaluating the response to irradiation conditions that simulate anticipated fusion system operation. The compatibility studies include vanadium and other candidate structural materials, and focus on the effects of exposure to projected coolants, especially liquid lithium.

Keywords: Vanadium, Compatibility, Lithium, Irradiation Effects, Alloy Development

216. **REPAIR WELDING OF FUSION REACTOR COMPONENTS**
$100,000
DOE Contact: F. W. Wiffen, (301) 903-4963
Auburn University Contact: B. A. Chin, (334) 844-3322

Repair welding of metal components that have been in service under neutron irradiation is limited by the tendency of the material to crack during welding. This program is identifying the mechanisms of the weld cracking and the association with transmutation-produced helium. Experiments on the effects of stress state on the growth of helium bubbles is expected to lead to methods to mitigate the weld cracking problem in irradiated steels.

Keywords: Steels, Welding, Irradiation Effects

217. **INSULATING CERAMICS FOR FUSION**
$435,000
DOE Contact: F. W. Wiffen, (301) 903-4963
LANL Contact: E. H. Farnum, (505) 665-5223

The goals of this project are to determine the changes in electrical, optical and structural properties of ceramic insulators in predicted fusion service, especially the effects of neutron irradiation. An understanding of the effects of radiation and of the controlling mechanisms are used to select or develop materials capable of extended life for use in fusion systems.

Keywords: Ceramics, Electrical Properties, Irradiation Effects

218. **MODELING IRRADIATION EFFECTS IN SOLIDS**
$100,000
DOE Contact: F. W. Wiffen, (301) 903-4963
LLNL Contact: T. Diaz de la Rubia, (510) 422-6714

Large scale computer simulation and experimental data on irradiation effects are combined to extend the understanding of the primary damage processes in solids. Special attention is given to the energy range appropriate for the 14 MeV neutrons produced in D-T fusion, and to the materials of interest for fusion systems.

Keywords: Modeling, Irradiation Effects

219. **FUSION SYSTEMS MATERIALS**
$3,815,000
DOE Contact: F. W. Wiffen, (301) 903-4963
ORNL Contacts: E. E. Bloom, (423) 574-5053 and A. F. Rowcliffe, (423) 574-5057

This program is directed at the development and qualification of structural materials and insulating ceramics for use in components of fusion power systems exposed to the intense neutron flux. Candidate low activation structural material systems include ferritic/martensitic steels, vanadium alloys and SiC/SiC composites. Investigations focus on the most critical questions or limiting properties in each of these systems: ferritic/martensitic steels - DBTT transition shifts and fracture toughness, vanadium alloys - welding processes, effects of irradiation on fracture toughness, and compatibility in proposed coolant systems, SiC/SiC composites - definition of the effects of irradiation on properties and structure. The insulating ceramic activity is initially developing an understanding of irradiation effects in alumina, spinel, and other materials. The greatest concern is to establish the permanent and transient changes in electrical properties, requiring measurement while the specimen is under irradiation. Work on these material classes involves irradiation in fission reactors, including HFIR, HFBR, and other test reactors, as partial simulation of the fusion environment.

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

220. **STRUCTURAL MATERIALS FOR FUSION SYSTEMS**
$1,613,000
DOE Contact: F. W. Wiffen, (301) 903-4963
PNNL Contact: R. H. Jones, (509) 376-4276

The goal of this program is to develop an understanding of radiation effects that provides a basis for development of irradiation insensitive materials. The objective is low activation materials for use as structures in divertor, first wall, and blanket components of fusion systems. Irradiation in fission reactors is used to simulate fusion conditions, with measurement of physical and mechanical properties used to track irradiation effects. A modeling activity complements the experimental measurements. The ultimate goal is optimized ferritic steels, vanadium alloys, and SiC/SiC composite materials for fusion power plant use.

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

221. **DEVELOPMENT OF RADIATION-HARDENED CERAMIC COMPOSITES FOR FUSION APPLICATIONS**
$60,000
DOE Contact: F. W. Wiffen, (301) 903-4963
RPI Contact: D. Steiner, (518) 276-4016

This research is directed at furthering the understanding of the effects of irradiation on the SiC/SiC composite system, as the basis for developing superior composite materials for fusion structural applications. The focus of the work is on the evaluation of improved fibers and alternative interface layer materials.

Keywords: Silicon Carbide, Composites

222. **RADIATION EFFECTS AND MICROMECHANICS OF SiC/SiC COMPOSITES**
$115,000
DOE Contact: F. W. Wiffen, (301) 903-4963
UCLA Contact: N. M. Ghoniem, (310) 825-4866

The goal of this program is to develop an understanding of the basic processes of neutron damage production, microstructural evolution, chemical compatibility, and micromechanics of fracture in SiC/SiC composite materials. This basic knowledge of materials behavior is used to model the effects of irradiation and the service performance of SiC/SiC components in fusion power systems. The critical goal is helping to evaluate the feasibility of using SiC/SiC in this application.

Keywords: Silicon Carbide, Composites, Modeling, Irradiation Effects

223. **DAMAGE ANALYSIS AND FUNDAMENTAL STUDIES FOR FUSION REACTOR MATERIALS DEVELOPMENT**
$225,000
DOE Contact: F. W. Wiffen, (301) 903-4963
UCSB Contacts: G. R. Odette, (805) 893-3525 and G. E. Lucas, (805) 893-4069

This research is directed at developing a fundamental understanding of both the basic damage process and microstructural evolution that take place in a material during neutron irradiation. This understanding is used with empirical data to develop physically-based models of irradiation effects. The focus is on the fracture properties of vanadium alloys, austenitic and ferritic stainless steels, including helium effects, to (a) develop an integrated approach to integrity assessment, (b) develop advanced methods of measuring fracture properties, and (c) analyze the degradation of the mechanical properties of austenitic stainless steels. The program contributes to the assessment of the feasibility of using these alloys in ITER and other fusion systems.

Keywords: Vanadium, Steels, Irradiation Effects, Fracture

224. **DEVELOPMENT OF LITHIUM-BEARING CERAMIC MATERIALS FOR TRITIUM BREEDING IN FUSION REACTORS**
$200,000
DOE Contact: S. Berk, (301) 903-4171
ANL Contact: C. Johnson, (708) 252-7533

Research activities are focused on critical issues of ceramic breeder blankets for fusion reactors, including ceramic breeder material tritium retention and release, ceramic breeder and beryllium irradiation response, chemical compatibility of ceramic breeder materials and beryllium with blanket coolant and structural materials, and heat transfer and temperature control in ceramic breeder materials. Small-scale laboratory experiments are performed to study tritium transport characteristics and to benchmark computer models of tritium transport. Computer models are tested against data on irradiation of lithium-oxide and lithium-zirconate materials in a fast-spectrum fission reactor. There is good agreement between model predictions and experimental data in the area of transient tritium release.

Keywords: Ceramics, Compatibility, Tritium Release, Modeling, Lithium Ceramics

225. **POST-IRRADIATION EXAMINATION OF LITHIUM-BEARING CERAMIC MATERIALS FOR TRITIUM BREEDING IN FUSION REACTORS**
$400,000
DOE Contact: S. Berk, (301) 903-4171
PNNL Contact: G. Hollenberg, (509) 376-5515

Research activities are for post-irradiation examinations (PIE) of the ceramic breeder materials irradiated in the Fast Flux Test Facility. The PIE is conducted as part of the BEATRIX-II program under an International Energy Agency agreement between the US, Japan, and Canada. PIE involves capsule disassembly, neutron radiography, plenum gas analysis, photography, mensuration characterization, tritium inventory measurements, microstructural characterization, and thermal conductivity measurements. PIE for specimens from the BEATRIX-II Phase 1 irradiation (lithium-oxide irradiated to 5 percent lithium atom burnup) and the Phase 2 irradition (lithium-oxide and lithium-zirconate irradiated to 5 percent lithium atom burnup) have been completed.

Keywords: Ceramics, Lithium Ceramics, Tritium Release

226. **INTERNATIONAL THERMONUCLEAR EXPERIMENTAL REACTOR (ITER) MATERIALS DEVELOPMENT FOR PLASMA FACING COMPONENTS**
$5,500,000
DOE Contact: M. M. Cohen, (301) 903-4253
SNL Contact: M. Ulrickson, (505) 845-3020

Research activities include: improved techniques for joining beryllium to copper alloys, determination of the tritium retention of beryllium, improvement of the thermal conductivity of plasma sprayed beryllium, development of radiation damage resistant carbon-fiber composites, determination of erosion rates of beryllium, tungsten and carbon under normal and disruption conditions, and thermal fatigue testing of beryllium and carbon-fiber composites. The joining techniques being investigated include diffusion bonding, induction brazing, electroplating, and inertial welding. Tritium retention and permeation measurements have been conducted on the Tritium Plasma Experiment. The improvements in the plasma spray technique are centered on improving the beryllium powder and selection of the proper powder sizes. Highly oriented pitch based carbon fibers have been used to produce carbon-fiber composite for neutron irradiation. The erosion rates are measured on both plasma simulators and tokamaks. The thermal fatigue testing is carried out on electron beam test systems.

Keywords: Plasma-Facing Components, Beryllium, Carbon-Fiber Composite, Joining, Erosion, Thermal Fatigue

227. **ITER STRUCTURAL MATERIALS DEVELOPMENT**
$250,000
DOE Contact: F. W. Wiffen, (301) 903-4963
ANL Contact: D. L. Smith, (708) 252-4837

The ITER structural materials program is working toward the establishment of a database on the main candidate materials for use in the divertor, first wall, blanket and shield structures. The ANL program is evaluating candidate vanadium alloys. The early stages of this work are concentrating on baseline properties, irradiation effects, and compatibility with coolant fluids. Issues of fabrication, joining, and protective coatings are being incorporated as the program progresses.

Keywords: Vanadium, Irradiation Effects, Compatibility

228. **ITER CERAMIC MATERIALS**
$335,000
DOE Contact: F. W. Wiffen, (301) 903-4963
LANL Contact: E. H. Farnum, (505) 665-5223

The ITER will require ceramic materials in a number of the heating, current drive, and diagnostic elements of the plant. Behavior of these systems can be limited by their electrical, optical and/or structural properties. A program of in situ and post irradiation measurements to determine the effects of irradiation on these properties is conducted at LANL and other sites, with the goals of developing the properties database on candidate materials that will allow system designers to effectively include these components in the ITER plant.

Keywords: Ceramics, Electrical Properties, Optical Properties, Irradiation Effects

229. **RADIATION HARDENED FIBER OPTICS FOR ITER FUSION DIAGNOSTIC SYSTEMS**
$75,000
DOE Contact: F. W. Wiffen, (301) 903-4963
NRL Contact: D. L. Griscom, (202) 404-7087

This work evaluates the effects of fusion system irradiation on optical fibers and selects and/or develops fibers that are radiation resistant in use in diagnostic applications. Experiments on available fibers use gamma sources, spallation neutron sources, and fission reactors to characterize degradation of optical properties during and after irradiation. The most resistant fibers will be studied in more detail, and the data used to formulate potentially more resistant fiber compositions.

Keywords: Optical Fibers, Optical Properties, Irradiation Effects

230. **ITER MATERIALS EVALUATION**
$1,505,000
DOE Contact: F. W. Wiffen, (301) 903-4963
ORNL Contact: E. E. Bloom, (423) 574-5053 and A. F. Rowcliffe, (423) 574-5057

ITER requires structural materials and insulating ceramics for use in a range of system components exposed to the neutrons produced by the fusion reaction. ORNL's part of the ITER materials program is directed at the selection of promising compositions of austenitic stainless steels, copper alloys, and vanadium alloys and assisting in the development of the database needed for the use of these materials. Irradiation effects, compatibility and weldability of these materials are under study. The insulating ceramics work is focused on the electrical properties under irradiation, and the in situ measurement techniques to determine this response are being developed. The work at ORNL emphasizes the use of the HFIR to perform the irradiations in support of the ITER materials development and evaluation.

Keywords: Steels, Copper, Vanadium, Ceramics, Irradiation Effects, Electrical Properties

231. **ITER STRUCTURAL MATERIALS EVALUATION**
$490,000
DOE Contact: F. W. Wiffen, (301) 903-4963
PNNL Contact: R. H. Jones, (509) 376-4276

Materials systems of interest to ITER for use as structural materials in the divertor, first wall, and blankets are under evaluation to select the most attractive candidates in each system, and to develop the property database on these. The PNNL program is evaluating copper alloys, stainless steels, and vanadium alloys for the ITER program. While the emphasis is on irradiation effects, especially on fracture properties, the program at PNNL also is examining hydrogen effects and compatibility with water cooling.

Keywords: Steels, Copper, Vanadium, Irradiation Effects, Compatibility

232. **DEVELOPMENT OF Nb_3Sn SUPERCONDUCTING WIRE FOR THE ITER MAGNET PROGRAM**
$5,000,000
DOE Contact: M. M. Cohen, (301) 903-4253
MIT Contact: J. Minervini, (617) 253-5503

Activities include development of Nb_3Sn superconducting wire primarily for use in the high field magnets of the ITER model coils. Aggressive target specifications for high critical current density in the 12-13 tesla magnetic field range have been set and an industrial development program has begun to produce large quantities of this wire. U.S. superconducting wire industries involved include Intermagnetics General Corp./Advanced Superconductors Inc., and Teledyne Wah Chang Albany. Characterization of critical superconducting properties and ac losses has been carried out with measurements in university and national laboratories, including establishment of standardized samples and test procedures.

Keywords: Superconductors, Magnet Materials, Nb_3Sn

233. **STRUCTURAL MATERIALS DEVELOPMENT FOR THE CONDUIT OF ITER CABLE-IN-CONDUIT-CONDUCTORS**
$1,100,000
DOE Contact: M. M. Cohen, (301) 903-4253
MIT Contact: J. Minervini, (617) 253-5503

Activities include fabrication of conduit for the conductors of the central solenoid and toroidal field model coils for ITER. The conduit material, Incoloy alloy 908, was developed via collaboration of INCO Alloys International and MIT. Work is proceeding on development of the database for this material. Alloy 908 has a low coefficient of expansion and minimizes the compressive strain in the Nb_3Sn superconductor upon cool down from the heat treatment temperature of approximately 1000 K to the operation temperature of 4 K. Industrial processing by various methods to finished conduit shape has been a priority.

Keywords: Conduit, Incoloy, Magnet Materials

SMALL BUSINESS INNOVATION RESEARCH PROGRAM

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

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

The work supported in this program represents high-risk research, but the potential benefits are also high if the objectives are met. Brief descriptions of all DOE SBIR projects (not just those of interest in materials research) are given in the following publications: Abstracts of Phase I Awards, 1995 (DOE/ER-0654), Abstracts of Phase II Awards, 1995 (DOE/ER-0655), and Abstracts of Phase II Awards, 1994 (DOE/ER-0628). Copies of these publications may be obtained by calling Mrs. Kay Etzler on (301) 903-5867.

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

PHASE I PROJECTS

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

Laser Consolidation of Silicon Carbide/Titanium Metal Composite Turbine Rings - DOE Contact Cynthia Carter, (301) 5997; Cordec Corporation Contact Mrs. Helen Pierides, (703) 550-8044

Solid Free-Body Formed Alumina-Tungsten Electrode Insulators for Heavy Ion Fusion Accelerators - DOE Contact Mark A. Wilson, (301) 903-5048; Advanced Ceramics Research, Inc. Contact Mr. Mark Angier, (602) 792-2616

High Current Density High Temperature Superconductor Composite Conductors - DOE Contact James Daley, (202) 586-1165; American Superconductor Corporation Contact Mr. Ramesh Ratan, (508) 836-4200

Superconducting Wires for Alternating Current Magnet Applications - DOE Contact James Daley, (202) 586-1165; American Superconductor Corporation Contact Mr. Ramesh Ratan, (508) 836-4200

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

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

Gallium Phosphide Ultraviolet Diode Arrays - DOE Contact Michael O'Connell, (202) 586-9311; AstroPower, Inc. Contact Mr. Thomas J. Stiner, (302) 366-0400

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

A New Alloy for Refiner Plates in the Pulp and Paper Industry - DOE Contact Charles Sorrell, (202) 586-1514; Climax Research Services Contact Mr. James R. Lakin, (810) 489-0720

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

Slicing of Silicon Ingots with Reduced Kerf - DOE Contact Alec Bulawka, (202) 586-5633; Crystal Systems, Inc. Contact Dr. Chandra P. Khattak, (508) 745-0088

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

Development of Novel Iron-Chromium-Silicon Alloys for Use in Kraft Recovery Boilers - DOE Contact Charles Sorrell, (202) 586-1514; E. R. Johnson Associates, Inc. Contact Mr. L.H. Donaldson, (703) 359-9355

High Capacity Carbon Anodes for Lithium Ion Batteries - DOE Contact Robert Marianelli, (301) 903-5808; EIC Laboratories, Inc. Contact Dr. A. C. Makrides, (617) 769-9450

Refractory Coatings for Improved Papermaking - DOE Contact Charles Sorrell, (202) 586-1514; Eltron Research, Inc. Contact Ms. Eileen E. Sammells, (303) 440-8008

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

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

Pseudo-Porous Zirconium Carbide Fiber Coating for Environmentally Durable Silicon Carbide/Silicon Carbide Composites - DOE Contact Helen Kerch, (301) 903-2346; Hyper-Therm High-Temperature Composites, Inc. Contact Mr. Wayne S. Steffer, (714) 375-4085

A Resistive Fault Current Limiter Based on Highly Directional Superconductor Thick Film Conductors - DOE Contact James Daley, (202) 586-1165; Illinois Superconductor Corporation Contact Ms. Ora Smith, (708) 391-9400

A Low Cost, Windable Yttrium-Barium-Copper-Oxide Conductor by Continuous Ion Beam Assisted Deposition/Metal Organic Chemical Vapor Deposition on a Metallic Substrate Tape - DOE Contact James Daley, (202) 586-1165; Intermagnetics General Corporation Contact Mr. Carl H. Rosner, (518) 782-1122

In-Situ Removal and Recycling of Copper Indium Selenide from Thin-Film Solar Cells - DOE Contact Alec Bulawka, (202) 586-5633; Interphases Research Contact Mr. Leslie Affonso, (805) 492-9814

Conformal Source Ion Implantation - DOE Contact Cynthia Carter, (301) 903-5997; ISM Technologies, Inc. Contact Mr. Robert J. Stinner, (619) 530-2332

Synthesis and Application of a Novel Electrode Material for Use in Proton-Exchange-Membrane Fuel Cells Capable of Using Simple Organic Fuels and Fuel Reformate - DOE Contact Cynthia Carter, (301) 903-5997; Lynntech, Inc. Contact Dr. Oliver J. Murphy, (409) 693-0017

A Novel Tritium Collection Technology Using Fullerence Tritides - DOE Contact William Weaver, (301) 903-7038; Materials And Electrochemical Research Corporation Contact Dr. R. O. Loutfy, (602) 574-1980

A Steam-Resistant Hydrogen Selective Ceramic Membrane for Fuel Cell Applications - DOE Contact Cynthia Carter, (301) 903-5997; Media And Process Technology, Inc. Contact Dr. Paul K. T. Liu, (412) 826-3711

Low-Cost Durable Tooling for High Production Rate Structural Reaction Injection Molding/Resin Transfer Molding Processing - DOE Contact Sidney Diamond, (202) 586-8032; Metal Matrix Cast Composites, Inc. Contact Dr. James A. Cornie, (617) 893-4449

Silicon Hexaboride Reinforced Aluminum Ingot Material Development for the Transportation Industry - DOE Contact Cynthia Carter, (301) 903-5997; Millennium Materials, Inc. Contact Ms. Pamela S. Clabough, (615) 691-2170

An Advanced Scintillator for Medical Imaging - DOE Contact Prem Srivastava, (301) 903-4071; Mission Support, Inc. Contact Mr. David B. Merrill, (801) 773-7900

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

Nanostructured Thermal Barrier Coatings for Natural Gas-Fired Advanced Turbines - DOE Contact William J. Gwilliam, (304) 285-4401; Nanomaterials Research Corporation Contact Dr. Angelo Yializis, (602) 575-1354

Aggressive, Abrasion-Resistant Cutters for Hard Rock Drill Bits - DOE Contact William J. Gwilliam, (304) 285-4401; Novatek Contact Mr. David R. Hall, (801) 374-6000

An Integrated Catalyst/Substrate for Catalytic Combustion - DOE Contact Cynthia Carter, (301) 903-5997; Precision Combustion, Inc. Contact Mr. J. Kevin Burns, (203) 786-5215

Cesium Iodide Bromide and Cesium Iodide Chloride Scintillators for High-Rate Applications - DOE Contact Richard Rinkenberger, (301) 903-3613; Rais Enterprises, Inc. Contact Dr. Emmanuil Raiskin, (619) 452-0500

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

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

Bonding of Ceramic Composites for Structural Applications in Fusion Energy Systems - DOE Contact F. W. Wiffen, (301) 903-4963; Starfire Systems, Inc. Contact Dr. Walter J. Sherwood, 518-276-2112

An Energy Efficient Design for a Surface Treatment Process which Improves Wear Properties of Materials - DOE Contact Charles Sorrell, (202) 586-1514; Stirling Technologies Inc. Contact Mrs. Bobbie C. Stirling, (615) 483-0142

Fabrication of a Flexible Reacted Niobium Tin Cable for Applications in React and Wind Magnets - DOE Contact Marvin M. Cohen, (301) 903-4253; Supercon, Inc. Contact Ms. Elaine Drew, (508) 842-0174

Low Temperature Fabrication of Copper Swirl Tubes for the International Thermonuclear Experimental Reactor - DOE Contact Marvin M. Cohen, (301) 903-4253; Surmet Corporation Contact Dr. Suri A. Sastri, (617) 272-3250

Fabrication of Copper-Backed Dense Tungsten Plasma Facing Component Armor - DOE Contact Marvin M. Cohen, (301) 903-4253; Surmet Corporation Contact Dr. Suri A. Sastri, (617) 272-3250

A Novel Fabrication Process to Enable Joining of Ceramics and Intermetallics - DOE Contact William J. Gwilliam, (304) 285-4401; T/J Technologies, Inc. Contact Ms. Maria A. Thompson, (810) 347-0305

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

A Discontinuous Fiber Composite Interlayer for Increased Brazed Joint Reliability - DOE Contact Marvin M. Cohen, (301) 903-4253; Technical Research Associates Contact Mr. Charles D. Baker, (801) 485-4991

Controlled Shear Strength Oxidation-Resistant Interfacial Coatings - DOE Contact Helen Kerch, (301) 903-2346; Ultramet Contact Mr. Craig N. Ward, (818) 899-0236

PHASE II PROJECTS (FIRST YEAR)

A Ceramic Material and Process for Use in Monolithic CeramicCross-Flow Filters - DOE Contact Theodore McMahon, (304) 291-4865; Blasch Precision Ceramics, Inc. Contact Mr. David W. Bobrek, (518) 372-9416

Jet Vapor Deposition of Multilayer and Nanocluster Thick Films Targets for Radioactive Nuclear Beams and Medical Applications - DOE Contact Richard Rinkenberger, (301) 903-3613; Jet Process Corporation Contact Mr. Jerome J. Schmitt, (203) 786-5130

Design and Applications of Close-Spaced Thermionic Converters with Novel Isothermal Electrodes - DOE Contact Cynthia Carter, (301) 903-5997; Space Power, Inc. Contact Mr. Joseph A. Dodson, (408) 434-9500

A Multilayer Silicon Carbide Fiber Coating for Toughened, Neutron Radiation-Resistant Silicon Carbide/Silicon Carbide Composites - DOE Contact F. W. Wiffen, (301) 903-4963; Hyper-Therm, Inc. Contact Mr. Wayne S. Steffier, (714) 375-4085

Economical and Reliable Niobium-Tin Conductors via Innovations in Stabilizers - DOE Contact T.V. George, (301) 903-4957; IGC Advanced Superconductors, Inc. Contact Mr. B. A. Zeitlin, (203) 753-5215

Carbon-Carbon to Copper Joining for Fusion Reactor Applications - DOE Contact T.V. George, (301) 903-4957; Surmet Corporation Contact Dr. Suri A. Sastri, (617) 272-3250

PHASE II PROJECTS (SECOND YEAR)

Multi Layer, Quantum Well Layer Film Thermoelectrics - DOE Contact John Warren, (301) 903-6491; Hi-Z Technology, Inc. Contact Mr. Norbert B. Elsner, (619) 535-9343

Production of Carbon Materials from Biomass - DOE Contact David Boron, (202) 586-0080; Advanced Fuel Research, Inc. Contact Dr. David G. Hamblen, (203) 528-9806

Oxide Dispersion Strengthened Silver for Use in High-Temperature Superconductor Composite Wires - DOE Contact Cynthia Carter, (301) 903-5997; American Superconductor Corporation Contact Mr. Edward P. Hamilton, (617) 923-1122

Low Temperature Deposition of Titanium Nitride - DOE Contact Cynthia Carter, (301) 903-5997; ISM Technologies, Inc. Contact Mr. Robert J. Stinner, (619) 530-2332

Coated Micrograin Carbides for Wear Resistance - DOE Contact Cynthia Carter, (301) 903-5997; Ultramet Contact Mr. Craig N. Ward, (818) 899-0236

Composite Plasma-Polymer Membranes - DOE Contact Robert Marianelli, (301) 903-5804; Bend Research, Inc.Contact Dr. Walter C. Babcock, (503) 382-4100

Improved Coated-Metal Hydrogen Extraction Membranes - DOE Contact Robert Marianelli, (301) 903-5804; REB Research and Consulting Contact Dr. Robert E. Buxbaum, (517) 332-0243

Methods of Improving Internal-Tin Niobium-Tin for Fusion Applications - DOE Contact Warren Marton, (301) 903-4965; IGC Advanced Superconductors, Inc. Contact Mr. B. A. Zeitlin, (203) 753-5215

Advanced Nondestructive Evaluation for Quality Assurance of Divertor Plate Armor Tiles in Plasma Fusion Reactors - DOE Contact Warren Marton, (301) 903-4965; Karta Technology, Inc. Contact Dr. G. P. Singh, (210) 681-9102

Dense, High Conductivity, Copper/Aluminum/Beryllium Functionally Gradient Plasma Facing Components - DOE Contact Warren Marton, (301) 903-4965; Plasma Processes Contact Ms. Cheri M. McKechnie, (205) 881-7572

Flexible Electrochromic Window Materials Based on Poly (Diphenyl Amine) and Related Conducting Polymers - DOE Contact Sam Taylor (202) 586-9214; Ashwin-Ushas Corporation, Inc. Contact Dr. P. Chandrasekar, (908) 462-1270

Advanced Window Materials Based on Conducting Polymer/Sol-Gel Ceramic Composites - DOE Contact Sam Taylor, (202) 586-9214; Gumbs Associates, Inc. Contact Dr. Ronald W. Gumbs, (908) 257-9049

An Innovative Approach for the Formation of Silicon Carbide/Silicon Carbide Composites - DOE Contact F. W. Wiffen, (301) 903-4963; Lanxide Corporation Contact Mr. Robert J. Ferris, (302) 456-6216

Doping of Chemically Vapor infiltrated Silicon Carbide to Enhance Thermal Conductivity - DOE Contact F.W. Wiffen, (301) 903-4963; Materials and Electrochemical Research Corporation Contact Dr. J. C. Withers, (574) 674-1980

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

PHASE I PROJECTS

Low Cost, Novel Precursors to Beta Alumina Solid Electrolyte - DOE Contact Cynthia Carter, (301) 903-5997; TDA Research, Inc. Contact Mr. Michael E. Karpuk, (303) 940-2301

A Nanolayer Coating for Dry Machining - DOE Contact Cynthia Carter, (301) 903-5997; Technology Assessment & Transfer, Inc. Contact Mrs. Sharon Fehrenbacher, (301) 261-8373

Development of a Process Management Technology for the Manufacture of High Temperature Superconductors to Improve Conductor Quality - DOE Contact James Daley, (202) 586-1165; American Superconductor Corporation Contact Mr. Ramesh Ratan, (508) 836-4200

An In-Process Quality Monitoring System for High Temperature Superconducting Wire Manufacturing - DOE Contact James Daley, (202) 586-1165; Quality Engineering Associates, Inc. Contact Dr. Ming-Kai Tse, (617) 221-0080

Low Cost, High Conductivity Plasma Facing Components - DOE Contact Marvin M. Cohen, (301) 903-4253; Fiber Materials, Inc. Contact Mr. David R. Audie, (207) 282-5911

Structure-Property Relationships of Internal-Tin Niobium Tin - DOE Contact Marvin M. Cohen, (301) 903-4253; IGC Advanced Superconductors, Inc. Contact Mr. Bruce A. Zeitlin, (203) 753-5215

Nondestructive Characterization of Radiation Embrittlement in Fusion Structural Materials Using Laser Ultrasound - DOE Contact F. W. Wiffen, (301) 903-4963; Karta Technology, Inc. Contact Dr. G.P. Singh, (210) 681-9102

Silicides for Space Power and Waste Heat Applications - DOE Contact Bill Barnett, (301) 903-3097; Hi-Z Technology, Inc. Contact Mr. Norbert B. Elsner, (619) 535-9343

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

A Modular Inspection System for Complete In-Service Examination of a Nuclear Reactor Pressure Vessel, Including the Beltline Region - DOE Contact Dennis Harrison, (301) 903-2884; Quest Integrated, Inc. Contact Ms. Diana J. Suzuki, (206) 872-9500

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

A Modified Natural Clay Sorbent for Control of Mercury from Coal Fired Combustors - DOE Contact Sean Plasynski, (412) 892-4867; Energy And Environmental Research Corporation Contact Dr. Randall Seeker, (714) 859-8851

Improved Solid Oxide Fuel Cell Seals - DOE Contact Richard Johnson, (304) 291-4564; Technology Management, Inc. Contact Mr. Benson P. Lee, (216) 541-1000

A Cost Efficient Method for Producing Ceramic Composites for Coal-Fired Furnace Applications - DOE Contact William J. Gwilliam, (304) 285-4401; Advanced Refractory Technologies, Inc. Contact Mr. Keith A. Blakely, (716) 875-4091

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

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

PHASE II PROJECTS (FIRST YEAR)

An Apparatus for Structural Analysis of High Temperature Materials Using Synchrotron Radiation - DOE Contact Manfred Leiser, (301) 903-3426; Containerless Research, Inc. Contact Dr. Paul C. Nordine, (708) 467-2678

A Novel High Strength Ceria-Zirconia Toughened Alumina Ceramic with Superior High Temperature Corrosion and Erosion Resistance - DOE Contact Cynthia Carter, (301) 903-5997; Selee Corporation Contact Mr. Kenneth R. Butcher, (704) 697-2411

Improvement in the Characteristics of Ternary Niobium Titanium Tantalum Alloys - DOE Contact Jerry Peters, (301) 903-5228; IGC Advanced Superconductors, Inc. Contact Mr. B. A. Zeitlin, (203) 753-5215

X-Ray Absorption Spectroscopy for Trace Analysis of Chemical Phase and Composition - DOE Contact Manfred Leiser, (301) 903-3426; Advanced Fuel Research, Inc. Contact Dr. David G. Hamblen, (203) 528-9806

High Temperature Thermally Stable Multi-Layer Quantum Well Films - DOE Contact Bill Barnett, (301) 903-3097; Hi-Z Technology, Inc. Contact Mr. Norbert B. Elsner, (619) 535-9343

A Long Life Zinc-Oxide-Titanium-Oxide Sorbent - DOE Contact Ronald Staubly, (304) 291-4991; TDA Research, Inc. Contact Mr. Michael E. Karpuk, (303) 940-2301

PHASE II PROJECTS (SECOND YEAR)

A Testing Process to Define Electrode Current Wear Mechanisms and Develop Improved Electrodes - DOE Contact Sean Plasynski, (412) 892-4867; Montec Associates, Inc. Contact Mrs. Cynthia K. Farrar, (406) 494-2596

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

PHASE I PROJECTS

A Highly Efficient and Low Emission Catalytic Radiant Burner - DOE Contact Cynthia Carter, 301-903-5997; Selee Corporation Contact Mr. Kenneth Butcher, 704-697-2411

Light Emitting Devices Based on Germanium Quantum Crystals in a Direct Bandgap Matrix (Aluminum Nitride) - DOE Contact Cynthia Carter, (301) 903-5997; Structured Materials Industries, Inc. Contact Dr. Gary S. Tompa, 908-885-5909

A Two Dimensional Semiconductor Imaging Array for Scattered Cold Neutrons - DOE Contact Bill Oosterhuis, (301) 903-3426; Intraspec, Inc. Contact Mr. John Walter, (615) 483-1859

A Thermal Neutron Detector Based upon a Lanthanum Boron Germanate Scintillator - DOE Contact Bill Oosterhuis, (301) 903-3426; Mission Support, Inc. Contact Mr. David B. Merrill, (801) 773-7900

Advanced Silicon Carbide and Beryllium/Aluminum Alloy Integrally Cooled X-ray Synchrotron Mirrors - DOE Contact Bill Oosterhuis, (301) 903-3426; SSG, Inc. Contact Mr. Dexter Wang, (617) 890-0204

A New Type of Acoustical Sensor for Chemical Measurements - DOE Contact Robert Marianelli, (301) 903-5808; Analysis Consultants Contact Dr. B. G. Martin, (714) 830-1033

Chemically Resistant Gas Separation Perfluoromembranes - DOE Contact Robert Marianelli, (301) 903-5808; Compact Membrane Systems, Inc. Contact Dr. Stuart Nemser, (610) 499-8860

Advanced Chemiresistor Devices as Micron Size Sensors for the Rapid, On-Line Measurement of Chemical Vapors - DOE Contact Robert Marianelli, (301) 903-5808; Microsensor Systems, Inc. Contact Dr. Hank Wohltjen, (502) 745-0099

Interactive Particle Detector Teaching Aids Based on Plastic Scintillators - DOE Contact David Sutter, (301) 903-5228; Quantum Research Services, Inc. Contact Dr. William L. Dunn, (919) 544-4952

A Thermally Stable Iron Core Permanent Magnet Dipole Utilizing a Flux Shunt - DOE Contact Jerry Peters, (301) 903-5228; Field Effects, Inc. Contact Mr. Carl H. Rosner, (518) 782-1122

Enhanced Flux Pinning at High Fields in Niobium-Titanium-Tantalum by Magnetic Artificial Pinning Centers - DOE Contact Jerry Peters, (301) 903-5228; IGC Advanced Superconductors, Inc. Contact Mr. Bruce A. Zeitlin, (203) 753-5215

Development of Artificial Pinning Center Niobium-Titanium Superconductors with Very High Residual Resistivity Ratio Aluminum Stabilizers - DOE Contact Jerry Peters, (301) 903-5228; Supercon, Inc. Contact Ms. Elaine Drew, (508) 842-0174

A High Resolution Multi-hit Time to Digital Converter Integrated Circuit - DOE Contact Robert Woods, (301) 903-3367; Lecroy Corporation Contact Mr. Joseph Migliozzi, 914-578-6006

A Segmented Deep Depletion Depth Silicon Detector and Application Specific Integrated Circuits Signal Conditioning Systems for Physics Research - DOE Contact Richard Rinkenberger, (301) 903-3613; Intraspec, Inc. Contact Mr. John Walter, (615) 483-1859

Microporous Alumina Microchannel Plates - DOE Contact Richard Rinkenberger, (301) 903-3613; Nanosystems Inc. Contact Mr. Robert Boerstler, (203) 354-3668

Manufacturing Technologies, Improved Performance, and Cost Reduction of Superconducting Radiofrequency Resonant Niobium Cavities - DOE Contact Richard Rinkenberger, (301) 903-3613; Atlas Technologies, Inc. Contact Mr. Richard D. Bothell, (360) 385-3123

A High Brightness Cold Cathode Electron Beam Source - DOE Contact Richard Rinkenberger, (301) 903-3613; NZ Applied Technologies, Inc. Contact Dr. Peter E. Norris, (617) 935-2030

A High Conductance Thermal Interface - DOE Contact Marvin M. Cohen, (301) 903-4253; Energy Science Laboratories, Inc. Contact Dr. Timothy R. Knowles, (619) 552-2034

A Helium-Cooled Faraday Shield Using Porous Metal Cooling - DOE Contact T. V. George, (301) 903-4957; Thermacore, Inc. Contact Mr. Donald M. Ernst, (717) 569-6551

Low Cost Fabrication of Large Silicon Carbide/Silicon Carbide Composite Structures - DOE Contact F. W. Wiffen, (301) 903-4963; Lanxide Corporation Contact Dr. Christopher Kennedy, 302-456-6320

Accurate Broadband Detectors for Plasma Diagnostics - DOE Contact Charles Finfgeld, (301) 903-3423; Boulder Metric Contact Ms. Alice O. McDonald, (303) 494-9680

Bandgap-Engineered Thermophotovoltaic Devices for High Efficiency Radioisotope Power - DOE Contact Bill Barnett, (301) 903-3097; Edtek, Inc. Contact Mr. W. E. Horne, (206) 395-8084

Ion-Selective Ceramic Membranes for Separation of Radioactive Wastes - DOE Contact Joseph Paladino, (301) 903-7449; Materials And Systems Research, Inc. Contact Dr. Anil V. Virkar, (801) 466-1262

Removal and Concentration of Heavy Metals and Radionuclides from Polluted Groundwater - DOE Contact Kristine Bilenki, (301) 903-1687; Membrane Technology And Research, Inc. Contact Ms. E. G. Weiss, (415) 328-2228

Rugged, Tunable Infrared Laser Sources - DOE Contact Michael O'Connell, (202) 586-9311; Deacon Research Contact Dr. Olive Lee, (415) 493-6100

A Mid-Infrared Laser for Remote Sensing of Chemicals - DOE Contact Michael O'Connell, (202) 586-9311; INRAD, Inc. Contact Ms.Maria Murray, (201) 767-1910

A Membrane-Based Process for the Removal of Nitrogen from Natural Gas - DOE Contact William J. Gwilliam, (304) 285-4401; Bend Research, Inc. Contact Mr. Kelly L. Smith, (503) 382-4100

Electrochemical Activation of Natural Gas Constituents to Alcohols Using Bimetallic Anode Electrocatalysts - DOE Contact William J. Gwilliam, (304) 285-4401; Eltron Research, Inc. Contact Ms. Eileen E. Sammels, (303) 440-8008

An Innovative Membrane and Process for Removal and Recovery of Natural Gas Liquids - DOE Contact William J. Gwilliam, (304) 285-4401; Membrane Technology and Research, Inc. Contact Ms. E. G. Weiss, (415) 328-2228

A Tubular Intermediate Temperature Natural Gas Fuel Cell Incorporating a Perovskite Solid Electrolyte - DOE Contact William J. Gwilliam, (304) 285-4401; Eltron Research, Inc. Contact Ms. Eileen E. Sammells, (303) 440-8008

A Lower Cost Molten Carbonate Matrix - DOE Contact William J. Gwilliam, (304) 285-4401; M-C Power Corporation Contact Mr. Patrick F. McSweeney, (708) 986-8040

Fabrication of Multi-layer Molten Carbonate Fuel Cell Composites - DOE Contact William J. Gwilliam, (304) 285-4401; M-C Power Corporation Contact Mr. Patrick F. McSweeney, (708) 986-8040

Low Cost Molten Carbonate Fuel Cell Anodes - DOE Contact William J. Gwilliam, (304) 285-4401; M-C Power Corporation Contact Mr. Patrick F. Sweeney, (708) 986-8040

Abrasive-Waterjet Machining Techniques for Ceramic-Material Coal-Based Power System Components - DOE Contact William J. Gwilliam, (304) 285-4401; Quest Integrated, Inc. Contact Ms. Diana J. Suzuki, (206) 872-9500

Advanced Hot Gas Filter Development - DOE Contact William J. Gwilliam, (304) 285-4401; Ultramet Contact Mr. Craig N. Ward, (818) 899-0236

PHASE II PROJECTS (FIRST YEAR)

Economical Photochromic Films Based on Metal Oxides - DOE Contact Cynthia Carter, (301) 903-5997; EIC Laboratories, Inc. Contact Dr. A. C. Makrides, (617) 769-9450

A Continuous Cryopump/Pellet-Fabrication Apparatus for Fusion - DOE Contact T.V. George, (301) 903-4957; Cryogenic Applications F, Inc. Contact Dr. Christopher A. Foster, (615) 435-5433

Development of Expansive Cements Using Dry Flue Gas Desulfurization Solid Wastes - DOE Contact Mary Ashbaugh, (304) 291-4966; Praxis Engineers, Inc. Contact Ms. Suzanne C. Shea, (408) 945-4282

Highly Selective Membranes for the Separation of Organic Vapors Using Super-Glassy Polymers - DOE Contact Robert Marianelli, (301) 903-5804; Membrane Technology and Research, Inc. Contact Ms. E. G. Weiss, (415) 328-2228

A Long Life Perovskite Oxygen Electrode for Calcium and Lithium Oxide Processing in Nuclear Fuel Cycles - DOE Contact Eli Goodman, (301) 903-2966; Eltron Research, Inc. Contact Ms. Eileen E. Sammells, (303) 440-8008

Fullerene Based Catalysts for Heavy Oil Upgrading - DOE Contact Udaya Rao, (412) 892-4743; TDA Research, Inc. Contact Mr. Michael E. Karpuk, (303) 940-2301

A Low Emission Alkali Metal Thermal to Electric Converter Automotive Power System - DOE Contact Robert Astheimer, (301) 903-4410; Advanced Modular Power Systems, Inc. Contact Dr. Thomas K. Hunt, (313) 677-4260

An Acoustic Plate Mode Sensor for Aqueous Mercury - DOE Contact Paul Hart, (301) 903-7456; BIODE, Inc. Contact Dr. Douglas McAllister, (207) 883-1492

PHASE II PROJECTS (SECOND YEAR)

Glass-Ceramic Construction Tiles from Coal-Fired Boiler Flyash - DOE Contact Mary B. Ashbaugh, (304) 291-4966; Vortec Corporation Contact Dr, James G. Hnat, (215) 489-2255

A High Repetition-Rate High Power, All-Solid-State Pulsed Driver for Electrodeless Inductive Thrusters - DOE Contact John Warren, (301) 903-6491; Science Research Laboratory, Inc. Contact Dr. Jonah Jacob, (617) 547-1122

Demonstration of an Integrated Carbon Dioxide/Thermal Management System for Carbonate Fuel Cells - DOE Contact Clifford Carpenter, (304) 291-4041; Energy Research Corporation Contact Dr. Hans Maru, (203) 792-1460

Porous Aluminum Nitride Part Fabrication to Support Advanced Battery Development - DOE Contact Cynthia Carter, (301) 903-5997; Advanced Refractory Technologies, Inc. Contact Mr. Keith A. Blakely, (716) 875-4091

Capacitive Energy Storage Using High Surface Area Transition Metal Compounds - DOE Contact Cynthia Carter, (301) 903-5997; Chemat Technology, Inc. Contact Ms. Xin Qin, (818) 727-9786

Advanced Ceramic Fibers for a Carbonate Fuel Cell Matrix - DOE Contact Bruce Harrington, (304) 291-5427; Energy Research Corporation Contact Dr. Hans Maru, (203) 792-1460

An In-Situ Particle Sensor for Metal Forming Processes - DOE Contact Manfred Leiser, (301) 903-3426; Advanced Fuel Research, Inc. Contact Dr. David G. Hamblen, (203) 528-9806

Development of a High Spatial Resolution Neutron Detector - DOE Contact Manfred Leiser, (301) 903-3426; BioTraces, Inc. Contact Dr. A. K. Drukier, (301) 864-0816

A High Resolution Scintillator-Based Neutron Detector - DOE Contact Manfred Leiser, (301) 903-3426; Nanoptics, Inc. Contact Dr. Dr. James K. Walker, (904) 378-6620

On-Chip Infrared-Spectral Sensors by Superconducting Detector Arrays - DOE Contact Robert Marianelli, (301) 903-5804; Advanced Fuel Research, Inc. Contact Dr. David G. Hamblen, (203) 528-9806

Radiation Resistant Radio Frequency Feedthrough Insulators for Fusion Applications - DOE Contact Warren Marton, (301) 903-4965; Composite Technology Development, Inc. Contact Dr. Naseem A. Munshi, (303) 447-2226

Helium-Cooled Divertors with Low-Activation Materials and Simple Fabrication Techniques - DOE Contact Warren Marton, (301) 903-4965; Creare, Inc. Contact Mr. Robert A. Hicken, (603) 643-3800

Niobium-Tin Superconducting Wire with a Built-in Niobium Surface Coating to Limit Inter-Strand Eddy Currents in Cables - DOE Contact Warren Marton, (301) 903-4965; Supercon, Inc. Contact Ms. Elaine Drew, (508) 842-0174

Ceramic Filters for Ultrafine Particulate Separation in Combustion Gas Environments - DOE Contact Richard Tischer, (412) 892-4891; Materials and Electrochemical Research Corporation Contact Dr. J. C. Withers, (602) 574-1980

A Carbonate Fuel Call Monolith for Low-Cost and High Power Density Operation - DOE Contact Venkat Venkataraman, (304) 291-4105; Energy Research Corporation Contact Dr. Hans Maru, (203) 792-1460

SMALL BUSINESS TECHNOLOGY TRANSFER PROGRAM

The Small Business Technology Transfer (STTR) program, now completing its first year, was established as a three-year pilot program in compliance with the Small Business Research and Development Enhancement Act of 1992, Public Law 102-564. Grant applications are solicited from small science- and technology-based U.S. firms (with 500 employees or less) in collaboration with a non-profit research institution (e.g. National laboratories and universities). Awards are made competitively to the small business with the collaborating research institution serving as a subcontractor. STTR supports innovative R&D and encourages conversion of that R&D into commercial applications of economic benefit to the Nation. The STTR program is designed for implementation in three phases, with Phase I determining, insofar as possible, the scientific or technical merit and feasibility of ideas proposed for investigation. The period of performance in this initial phase is about nine months, and awards are limited to $100,000. Phase II is the principal research or R&D effort, and only Phase I awardees can compete for Phase II awards of up to $500,000 for work to be performed in a period of up to two years. In Phase III, commercial application of the research or R&D is pursued using non-Federal funding or, alternatively, it may involve follow-on non-STTR Federal contracts for products or services desired by the Government.

The materials-related projects, like all other projects in the STTR program and the SBIR program, were selected on the basis of scientific and technical merit, as judged against the specific criteria listed in the solicitation. Award selections were based on reviews performed by personnel in DOE laboratories, universities, private industry, and government.

As in the SBIR program, these projects represent high-risk research, but the potential benefits are also high if the objectives are met. Brief descriptions of all DOE STTR projects, not only those of interest in materials research, are given in Abstracts of Phase I Awards 1995 (DOE/ER-0652).

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

PHASE I PROJECTS

Laser Processing of Thermal Sprayed Beryllium Plasma Facing Components - DOE Contact T. V. George, (301) 903-4957; Plasma Processes, Inc. Contact Mr. Tim McKechnie, (205) 851-7653

Amorphous Silicon/Crystalline Silicon Heterojunctions for Nuclear Radiation Detector Applications - DOE Contact Richard Rinkenberger, (301) 903-3613; Quantrad Sensor, Inc. Contact Dr. Nicholas J. Szluk, (408) 727-7827

An Investigation to Determine the Commercial Feasibility of Vanadium-Hafnium-Zirconium Laves Phase C-15 Superconductor - DOE Contact Jerry Peters, (301) 903-5228; Supercon, Inc. Contact Ms. Elaine Drew, (508) 842-0174

Production of Jelly-Roll Process Niobium-Aluminum Superconducting Wire Using Low Oxygen Niobium Foils and Special Softening Techniques During Deformation - DOE Contact Jerry Peters, (301) 903-5228; Supercon, Inc. Contact Ms. Elaine Drew, (508) 842-0174

Catalysts for Heterogeneous Alkene Hydroformylation - DOE Contact William Millman, (906) 227-1059; TDA Research, Inc. Contact Mr. John D. Wright, (303) 422-7819

Low Loss Sapphire Windows for High Power Microwave Transmission - DOE Contact T. V. George, (301) 903-4957; Thoughtventions Unlimited Contact Dr. Stephen C. Bates, (203) 657-9014

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

PHASE I PROJECTS

An Advanced X-ray Detector and Detector Array - DOE Contact Richard Rinkenberger, (301) 903-3613; Astralux, Inc. Contact Dr. Ethel Pankove, (303) 494-0670

Environmentally Benign Manufacturing of Compact Disk Stampers - DOE Contact Helen Kerch, (301) 903-2346; Prism Company Contact Mr. Peter Ciriello, (508) 785-2511

Improved Strained-Layer Photocathodes for Spin-Polarized Electrons - DOE Contact Jerry Peters, (301) 903-5228; Spire Corporation Contact Mr. Richard S. Gregorio, (617) 275-6000

OFFICE OF ENVIRONMENTAL MANAGEMENT

	FY 1995
Office of Environmental Management - Grand Total	$30,489,600
Office of Waste Management	$ 7,563,600
High Level Waste Division	$ 7,563,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 5,667,000
Technical Support to West Valley Demonstration Project	1,300,000
Ceramic Final Forms	300,000
Microencapsulation in Final Forms	67,000
Final Waste Form Program	4,000,000
Materials Properties, Behavior, Characterization or Testing	$ 1,896,600
Materials Characterization Center Testing of West Valley Formulation Glass	396,600
Argonne National Laboratory High-Level Waste Borosilicate Glass Testing Program	1,500,000
Office of Science and Technology	$22,926,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$16,070,000
Polymer Encapsulation	1,764,000
Microwave Solidification	1,300,000
Fixed Hearth Plasma Treatment Process	3,455,000
Fixed Hearth Plasma Radioactive Waste Test	2,623,000
Phosphate-Bonded Ceramic Waste Forms	(carryover funding)
High Temperature Demonstrations on Actual Mixed Waste	909,000
Plasma Testing & Support	2,160,000
Stainless Steel Beneficial Reuse	1,931,000
Recycle of Depleted Uranium Studies	400,000
Demonstrate Contaminated Metal Recycle Integration and Optimization	649,000
Metal Recycle Technology Development	299,000
Surface Acoustic Wave Array Detectors	230,000
Versatile, Robust, Miniature Sized and Real-Time Radiation Detector	350,000
Materials Properties, Behavior, Characterization or Testing	$ 6,856,000
Vitrify to Delist to Dispose	736,000
Vitrification of Rocky Flats Waste	309,000
Plasma Hearth Process Radioactive Waste Test - Idaho	1,350,000
Vitreous Ceramic Compositional Envelope Study	200,000
Graphite DC Plasma Arc Melter	1,242,000
Vitreous Ceramic Formulation	200,000
Hot Cell Studies	400,000
Cesium Removal Demonstration	700,000
Tc and Ni Removal Ion Exchange	546,000
Crystalline Silicotitanate for Cs/Sr Removal	873,000
TUCS/Phosphate Immobilization of Actinides	300,000

OFFICE OF ENVIRONMENTAL MANAGEMENT

The Office of Environmental Management (EM) was established to effectively coordinate and manage the Department's activities to remediate the DOE Defense Complex and to properly manage waste generated by current operations. EM conducts materials research within four 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 technology developers 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 Environmental Restoration - The Office of Environmental Restoration directs the cleanup of inactive facilities and sites contaminated by waste generated from past nuclear operations. The mission of the Office is to ensure that risks to the environment and to human health and safety posed by inactive and surplus facilities and sites are either eliminated or reduced to prescribed, acceptable levels.

Office of Science and Technology - The Office of Science and Technology is responsible for managing the national program of environmental applied research and technology development. The Office manages and directs research, development, demonstration, testing, and evaluation programs and activities that are designed to provide complete innovative technologies and technology systems to address the major problems facing the Office of Environmental Management.

Office of Nuclear Materials and Facility Stabilization - One of the Office of Environmental Management's (EM) goals is to ensure that the risks to human health and safety and to the environment posed by inactive and surplus facilities are either eliminated or reduced to prescribed, acceptable levels. The Office of Facility Transition and Management was established within EM to develop and institutionalize a Departmental process for the timely and effective transfer of surplus facilities and to implement that process in transitioning surplus facilities to EM for final disposition.

Five 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:

Contaminant Plume Containment and Remediation - Uncontained hazardous and radioactive contaminants in soil and ground water exist throughout the DOE Complex. There is insufficient information at most sites on the contaminants' distribution and concentration. The migration of some contaminants threatens water resources and, in some cases, has already had an adverse impact on the off-site environment. Many current characterization, containment, and treatment technologies are ineffective or too costly. Improvements are needed in characterization and data interpretation methods, containment systems, and in situ treatment.

Landfill Stabilization - Numerous DOE landfills pose significant remediation challenges. Some existing landfills have contaminants that are migrating, thus requiring interim containment prior to final remediation. Materials buried in retrievable storage pose another problem. Retrieval systems must be developed to reduce worker exposure and secondary waste quantities. Another high-priority need is in situ methods for containment and treatment.

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 for 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.

Materials development work may be performed in any of these five Focus Areas. Focus Area-specific projects are identified as such. Other projects serving more than one Focus Area are supported by one of the three OST Crosscut Programs: the Characterization, Monitoring, and Sensor Program, the Robotics Program and the Efficient Separations and Processing Program. Funding levels are reported for the total project, which includes materials development and demonstration. For most projects, materials development accounts for less than 25 percent of the funds.

OFFICE OF WASTE MANAGEMENT

HIGH LEVEL WASTE DIVISION

The objective of the High Level Waste Division is to conduct waste management activities for ending interim storage of high-level waste and achieving permanent disposal of high-level waste at the Savannah River Site in South Carolina. Additionally, Congress directed the Department in 1980 to demonstrate the solidification of liquid high-level waste at West Valley (New York) which originated at the nation's only commercial plant to reprocess spent nuclear fuel. At both of these sites a program is in place to immobilize the high-level waste in preparation for geologic disposal.

At Savannah River and West Valley, high-level waste will be immobilized in a borosilicate glass prepared in a liquid-fed ceramic joule-heated melter. The Defense Waste Processing Facility at Savannah River is beginning non-radioactive operations in preparation for radioactive operation. West Valley is constructing the vitrification cell. For these two projects, materials research focuses on verifying the product consistency of the waste form based on a reference formulation chosen some time ago.

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

234. **TECHNICAL SUPPORT TO WEST VALLEY DEMONSTRATION PROJECT**
$1,300,000
DOE Contact: J. J. May, (716) 942-2161
PNNL Contact: M. Elliot, (509) 376-9858

The West Valley Support Project (WVSP) conducted by the Pacific Northwest National Laboratory (PNNL) is designed to meet the technology needs for the West Valley Demonstration Project (WVDP) and provide support to the subsequent site stabilization activities. The current objectives of the WVDP, as understood by PNNL, are: (1) to complete nonradioactive process testing, operational readiness reviews, and radioactive start-up of the vitrification facility; (2) to maintain safe storage of liquid high-level waste at the West Valley site; (3) to maintain a knowledgeable core of process support personnel to resolve current and future technical issues; (4) to resolve issues related to the site Environmental Impact Statement and other documents; and (5) to proceed with development of site stabilization activities particularly in the area of tank heel removal.

Keywords: Process Control, Storage, Technology

235. **CERAMIC FINAL FORMS**
$300,000
DOE Contact: Ronald D. Streit, (510) 422-7045
LLNL Contact: Robert Hoppert, (510) 423-2420

Operations of the Mixed Waste Management Facility (MWMF) will yield ash-like residues (oxides, nitrates, etc. containing RCRA metals and radioactive elements) from the organic components of low-level mixed waste. These residues will be stabilized as a durable and leach-resistant ceramic waste form produced by traditional high-temperature powder technologies. Formulations for various input waste streams are being optimized.

Keywords Ceramic, Final Waste Form, Ash

236. **MICROENCAPSULATION IN FINAL FORMS**
$67,000
DOE Contact: Ronald D. Streit, (510) 422-7045
LLNL Contact: Robert Hoppert, (510) 423-2420

Operations of the Mixed Waste Management Facility (MWMF) will yield salt residues from the destruction of organic components of low-level mixed waste. Salts will be cleaned to the extent possible for "direct" disposal. Salts containing RCRA metals and radioactive elements after processing will be stabilized by microencapsulation in polyethylene or in a thermosetting polymer. Volatile inorganic solids will be microencapsulated in sulfur polymer cement. Pending funding availability, these technologies are being optimized for MWMF operations.

Keywords Final Waste Form, Encapsulation, Polymer

237. **FINAL WASTE FORM PROGRAM**
$4,000,000
DOE Contact: Michael Torbert, (301) 903-7109

In support of the Oak Ridge Reservation (ORR) LDR Federal Facility Compliance Agreement as well as the Federal Facility Compliance Act, a program is underway to demonstrate, at the bench-scale level, applicable final waste forms for sludges, soils, other treatment residues, and secondary wastes. The primary focus of this activity is to demonstrate appropriate grout waste forms, glass waste forms, and thermoplastic waste forms. This work is being done on actual ORR wastes and supports the LDR FFCA. It will provide technology support to ORR privatization activities. This activity will support a joint CRADA with Savannah River Technical Center and SEG.

Keywords Final Waste Form, Grout, Glass, Thermoplastic, Bench-Scale

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

238. **MATERIALS CHARACTERIZATION CENTER TESTING OF WEST VALLEY FORMULATION GLASS**
$396,600
DOE Contact: J. J. May, (716) 942-2161
PNNL Contact: G. L. Smith, (509) 372-1957

Materials Characterization Center (MCC) is evaluating the chemical durability of glasses whose compositions are within the expected range of composition of the West Valley Demonstration Project borosilicate glass waste form. These include nonradioactive glass containing surrogate elements for radionuclides and radioactive glass doped with appropriate radionuclides. The MCC also is testing of a small sample of glass containing actual West Valley high-level waste.

Keywords Radioactive Waste Host

239. **ARGONNE NATIONAL LABORATORY HIGH-LEVEL WASTE BOROSILICATE GLASS TESTING PROGRAM**
$1,500,000
DOE Contact K. Picha, (301) 903-7199

Argonne National Laboratory (ANL) is continuing a series of tests of high-level waste borosilicate glass. These tests, which have been supported by the Office of Environmental Management since FY 1989, will provide a better understanding of the long-term borosilicate glass corrosion mechanisms and durability concerns. Included in these tests are: Defense Waste Processing Facility (DWPF)-based glass drip tests, DWPF sludge-based glass performance tests, long term drip testing on actinide-doped ATM-10 glass, and continued performance testing of West Valley Demonstration Project reference 6 glass.

Keywords Waste, Waste Form, Borosilicate Glass, Waste Acceptance Specifications

OFFICE OF SCIENCE AND TECHNOLOGY

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, testing and evaluation 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 the environment.

Certain areas of OST's Technology Development Program focus on materials research in order to provide better, faster, safer and more cost-effective approaches to identify, characterize and clean up DOE's waste problem. The Technology Development Program is investigating various types of cement and polymer technologies for stabilization and containment of wastes. The applicability of these substances is being demonstrated, tested, and evaluated for implementation at specific sites. Technology development and demonstrations into glasses and ceramics are being pursued to better understand high-temperature technologies, useful for containment of contaminated soils. Vitrification and plasma technologies are being developed for treating specific mixed waste streams. OST will continue to fund these materials research projects, as well as others, to provide the basis for other applied research in the Technology Development Program.

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH, OR FORMING

240. **POLYMER ENCAPSULATION**
$1,764,000
DOE Field Office Contact: Julie Conner, (208) 526-0648
DOE HQ Program Manager: Alison Johnson, (301) 903-7923 and Grace Ordaz, (301) 903-7440
EG&G Rocky Flats Contact: Andrea Faucette, (303) 966-6420
EM Focus Area: Mixed Waste

Polymer encapsulation of mixed wastes encloses waste products in thermoplastic materials using commercially available processing technologies. The configuration under development at the Rocky Flats Environmental Technology Site uses a twin-screw extruder to microencapsulate waste. The process aims at meeting applicable disposal site, EPA and DOT acceptance criteria for various wastes. Microencapsulation involves combining thermoplastic polymers (i.e. polyethylene) with dried waste; melting, mixing, and extruding the combination in a commercially-available extruder; and allowing the molten plastic to cool and solidify. Hazardous constituents are immobilized in the plastic matrix. Nitrate salts, bypass sludge, incinerator ash, and secondary wastes are the target streams. Microencapsulation tests of a variety of waste streams have been performed with the extruded waste forms meeting TCLP leach test performance limits.

Keywords: Alternative Final Waste Form, Polymer Encapsulation, Hydroxide Sludge, Polyethylene

241. **MICROWAVE SOLIDIFICATION**
$1,300,000
DOE Field Office Contact: Julie Conner, (208) 526-0648
DOE HQ Program Manager: Alison Johnson, (301) 903-7923 and Grace Ordaz, (301) 903-7440
EG&G Rocky Flats Contact: Greg Sprenger, (303) 966-3159
EM Focus Area: Mixed Waste

The microwave solidification project is developing a method to immobilize wastes for compliance with EPA disposal regulations and to minimize volume of wastes for storage and disposal. Microwave solidification uses 915 MHZ microwave energy to vitrify waste solids. Dried waste and glass formers are fed into drums and melt "in the drum" from applied microwave heating. This technology is being evaluated as a potential method to treat several mixed wastes, including process sludges, incinerator ash, and miscellaneous wastes, such as crucibles and foundry materials.

Keywords: Alternative Final Waste Form, Microwave Solidification, Vitrification, In Drum Melting

242. **FIXED HEARTH PLASMA TREATMENT PROCESS**
$3,455,000
DOE Field Office Contact: Julie Conner, (208) 526-0648
DOE HQ Program Manager: Alison Johnson, (301) 903-7923 and Grace Ordaz, (301) 903-7440
EG&G Idaho Contact: Ray Geimer, (208) 528-2144
EM Focus Area: Mixed Waste

This technology, the Plasma Hearth Process (PHP), converts entire drums of low-level mixed waste (LLMW) directly into an enhanced waste form without extensive pretreatment or characterization. Organics are destroyed while metals and inorganics are melted, creating a vitrified slag and molten metal. The process is characterized by high-efficiency destruction of organics, encapsulation of heavy metals and radionuclides in the vitrified final waste form, large volume reduction of waste to be disposed, possible recycling of metals, low off-gas flow rates, and the capability of processing many waste types in a single-step process. The non-radioactive proof-of-principle concept demonstration has been completed. The remaining work in this task focuses on design, fabrication, and demonstration of a near full-scale pilot system for non-radioactive operation.

Keywords: Plasma, Final Form, Low-Level Mixed Waste, Pilot-Scale

243. **FIXED HEARTH PLASMA RADIOACTIVE WASTE TEST**
$2,623,000
DOE Field Office Contact: Julie Conner, (208)-526-0648
DOE HQ Program Manager: Alison Johnson, (301) 903-7923 and Grace Ordaz, (301) 903-7440
ANL-W Field Contact: Carla Dwight, (208) 533-7651
EM Focus Area: Mixed Waste

This project involves the design and construction of the facility modifications to house the bench-scale Plasma Hearth Process to be tested in the Plasma Hearth Process Radioactive Waste Test - Idaho. It also includes tasks to develop the mechanisms by which actual waste can be repackaged for testing in the bench-scale system, the radioactive waste forms produced by the process can be sampled and analyzed, and the pertinent analysis to be made to ensure safe operation of the plasma system in the

ANL-W TREAT facility. Waste operations and sampling and analysis during the bench-scale demonstration are covered in the task.

Keywords: Plasma, Final Form, Low-Level Mixed Waste, Bench-Scale

244. **PHOSPHATE-BONDED CERAMIC WASTE FORMS**
(Carryover funds)
DOE Field Office Contact: Julie Conner, (208) 526-0648
DOE HQ Program Manager:
Alison Johnson, (301) 903-7923 and
Grace Ordaz, (301) 903-7440
ANLC Contact: Arun Wagh, (708) 252-4295
EM Focus Area: Mixed Waste

Chemically-bonded ceramics (CBCs) are being investigated as an alternative final waste form for streams that cannot be handled by other established methods. Phosphate bonded ceramics are a subclass of CBCs and have several advantages over other systems for stabilization and encapsulation of LLMW. These include insolubility in water, high-temperature stability, and the ability to cure at room temperatures. Studies are underway to stabilize waste streams containing liquid mercury, mercury-contaminated aqueous liquids, toxic and heavy metal containing materials, salt cakes, beryllium wastes, and pyrophorics by encapsulating them in phosphate-bonded ceramics. (Effort was conducted during FY95 using carryover funds.)

Keywords: Alternate Final Waste Form, Ceramics, Phosphate

245. **HIGH TEMPERATURE DEMONSTRATIONS ON ACTUAL MIXED WASTE**
$909,000
DOE Field Office Contact: Julie Conner, (208) 526-0648
DOE HQ Program Manager:
Alison Johnson, (301) 903-7923 and
Grace Ordaz, (301) 903-7440
Savannah River Contact: Ray Schumacher, (803) 725-3803
EM Focus Area: Mixed Waste

This project investigated innovative methods of vitrification that provide higher temperature processing capabilities. High temperature processing is desirable where there are insufficient fluxing agents available within the wastes. Higher temperatures however, can also increase volatilization, which is undesirable. Methods of vitrification under consideration include induction, plasma, and high temperature joule heating.

Keywords: Vitrification, High Temperature

246. **PLASMA TESTING & SUPPORT**
$2,160,000
DOE Field Office Contact: Gary Staats (412) 892-6741
DOE HQ Program Manager:
Alison Johnson, (301) 903-7923 and
Grace Ordaz, (301) 903-7440
MSE Contact: Jeff Ruffner (406) 494-7412
EM Focus Area: Mixed Waste

This project included the testing of several high-metals content feeds in the Plasma Centrifugal Furnace and general engineering/technical support in high temperature processing areas for a future Minimum Additive Waste Stabilization (MAWS) demonstration. A small-scale plasma unit was purchased for expedited testing on a variety of wastes in support of slag waste form compositional envelope development. This was required before full-scale testing in the larger PACT 6 plasma unit.

Keywords: Plasma, Centrifugal Furnace, MAWS

247. **STAINLESS STEEL BENEFICIAL REUSE**
$1,931,000
DOE Field Office Program Manager: Paul Hart, (304) 285-4358
DOE HQ Program Manager: Jerry M. Hyde, (301) 903-7914
WSRC, SRS Principle Investigator: Bill Boettinger, (803) 725-4833
EM Focus Area: Decontamination & Decommissioning

The *Stainless Steel Beneficial Reuse* project involves participation of private industry to melt 304 stainless steel radioactive scrap metal (RMS), and then to fabricate the recycled metal into storage containers. The containers will include 100 cubic foot boxes, 55 gallon drums, 85 gallon overpacks, and other specialized items. The metal to be recycled primarily resides at the Savannah River Site (SRS), but it is the intent to include other sites' RMS in the future. The SRS metals originate from process water heat exchanger components, primary piping, handling equipment, and duct work. All metals selected will meet the Department of Transportation requirement of low-specific activity (LSA) for transportation to the selected subcontractors. Two subcontractors, Manufacturing Sciences Corporation and Carolina Metals, Inc., have participated in a full scale demonstration in and delivered the first complete products, 100 cubic foot boxes, in August. The SRS has already implemented the boxes for temporary storage of waste.

Keywords: Stainless Steel, Recycle, Storage, Containers

248. **RECYCLE OF DEPLETED URANIUM STUDIES**
$400,000
DOE Field Office Program Manager: Paul Hart, (304) 285-4358
DOE HQ Program Manager: Carl R. Cooley, (301) 903-7276
INEL Principle Investigator: W. J. Quapp, (208) 526-9443
EM Focus Area: Decontamination & Decommissioning

The primary objective of this project is to perform an initial assessment of the feasibility and economic incentives of alternative management options for storing, recycling, and/or disposing of the large depleted uranium (DU) reserves within the DOE Complex. As an alternative to disposal, a concept for converting depleted uranium into concrete shielding material has been developed. Laboratory work continues to improve pellet densities, and preparation for fabrication of depleted uranium DUROCK samples using UO_3 from SRS was initiated, and leach testing of DUCRETE samples was also initiated.

Keywords: Depleted Uranium, DUROCK, DUCRETE, Shielding

249. **DEMONSTRATE CONTAMINATED METAL RECYCLE INTEGRATION AND OPTIMIZATION**
$649,000
DOE Field Program Manager: Paul Hart, (304) 285-4358
DOE HQ Program Manager: Jerry Hyde, (301) 903-7914
DOE Field Project Manager: Melvin Shupe, (406) 494-7205
MSE/PETC Principle Investigator: Bob Balhiser, (406) 494-7282
EM Focus Area: Decontamination & Decommissioning

The objective of this project is to prove the technical and economic feasibility of building and operating a regional radioactive scrap steel (RSS) recycling facility in the western United States. This includes the development of a facility conceptual design based on state-of-the-art commercial steelmaking processes. Activities during FY95 include selecting and collaborating with an industrial team partner to assist MSE in evaluating the feasibility of such a facility. Anticipated activities for FY 1996 include completing a conceptual design of the facility, evaluating alternative sites and developing recommendations, and completing the analysis of regional RSS availability.

Keywords: Radioactive Scrap Steel, Regional Recycling Facility

250. **METAL RECYCLE TECHNOLOGY DEVELOPMENT**
$299,000
DOE Field Program Manager: Paul Hart, (304) 285-4358
DOE HQ Program Manager: Jerry Hyde, (301) 903-7914
ORNL Principle Investigator: H. Wayne Hayden, (615) 574-6936
EM Focus Area: Decontamination & Decommissioning

The objective of this project is the development of effective technologies for the decontamination, recycle, and reuse of radiologically contaminated scrap metal (RSM) from various sites in the DOE complex and the stimulation of the expansion of a commercial RSM recycle industry for processing such scrap. This task evaluates the use of existing DOE equipment and development of improved recycling technologies for RSM. Activities include a contract to Bliss-Salem, Inc. to evaluate the rolling of products from RSM, a proposed CRADA with SEG, Inc. to increase the effectiveness of removal of radiological contaminants and development of prerelease technologies that would result in the product form that could be released for wide use, and the testing of a technology for the removal of radiological contaminants for nickel scrap.

Keywords: Radiological Scrap Metal, Nickel, Recycle

251. **SURFACE ACOUSTIC WAVE ARRAY DETECTORS**
$230,000
DOE Field Contact: Roger Christensen, (509) 372-4606
DOE HQ PM: Caroline Purdy (301) 903-7672
PNNL Contact: Jay W. Grate (509) 375-4547
EM Crosscut Program Characterization, Monitoring, and Sensor Technology

The purpose of this task is to design, develop and demonstrate array sensor systems for sensing volatile organic compounds (VOCs), including chlorinated hydrocarbons and other vapors of interest with regard to environmental cleanup and occupational safety. These sensor arrays will be based on polymer-coated surface acoustic wave (SAW) vapor sensors and data processing using pattern recognition and chemometric techniques. The advantages of the SAW vapor sensor technology include the rugged planar design of the devices; the suitability of polymer-coated devices for use in arrays with pattern recognition; the fast response times (seconds); rapidly reversible responses-the selective material is not altered by the vapor; the high vapor sensitivities (ppm to ppb detection limits depending on the particular vapor); and the flexibility of the array approach to be adapted to many detection problems. The analyte or analytes to be detected can be changed merely by the selection of the polymer coating and the pattern recognition algorithm used. The combination of the information from the sensor array with modern chemometric data processing techniques creates an intelligent sensor system. The sensor array approach provides greatly increased selectivity and reliability in field environments over a single sensor. Single sensors cannot determine if an interfering species is present that might invalidate the measurement. SAW sensors are more sensitive than other microsensors such as fiber optic devices.

Keywords: Array Sensor, Volatile Organic Compounds, Surface Acoustic Wave

252. **VERSATILE, ROBUST, MINIATURE SIZED AND REAL-TIME RADIATION DETECTOR**
$350,000
DOE Field Contact: Steve Webster (708) 252-2822
DOE HQ PM: Caroline Purdy (301) 903-7672
BNL Contact: Eng-Kie Souw (516) 282-5407
EM Crosscut Program Characterization, Monitoring, and
Sensor Technology

The objective for this project is to develop a miniature, real-time solid-state sensor capable of detecting alpha particles, beta particles and gamma rays. The project has applicability for rapidly scanning surface soils, waste processing streams and facility walls, floors and equipment for decontamination and decommissioning. Although diamond is an ideal detector due to its physical hardness and chemical inertness, its low stopping power makes it suitable for detecting alphas, low energy betas and x-rays. For higher energy betas and gamma rays, stacked layers of cadmium telluride will be developed for the detector. For FY95 the objective is to design, develop and test carbon vapor deposited (CVD) diamond films for use on p-type intrinsic metal diamond nuclear detectors. The project is joint with Northrup-Grumman Corp. and the New Jersey Institute of Technology.

Keywords: Sensor, Alpha Particles, Beta Particles, Gamma Rays

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

253. **VITRIFY TO DELIST TO DISPOSE**
$736,000
DOE Field Office Contact: Julie Conner, (208) 526-0648
DOE HQ Program Manager:
Alison Johnson, (301) 903-7923 and
Grace Ordaz, (301) 903-7440
Savannah River Site Contact: Denny Bickford, (803) 725-3737
EM Focus Area: Mixed Waste

Vitrification involves converting wastes, which are primarily inorganic in nature, into a durable, leach-resistant glass. Emphasis has been placed on broadening the number of waste streams applicable to vitrification by establishing the processing envelopes for specific representative waste streams. Surrogates of radioactive waste streams have been vitrified in pilot-scale demonstrations conducted at Clemson University in FY95. In addition, a pilot-scale radioactive demonstration on actual Savannah River Site M-area sludge was conducted at Catholic University. A major effort was initiated in FY95 to identify an actual mixed waste stream and procure the equipment to assemble a transportable field-scale vitrification unit. The waste stream, Oak Ridge WETF (an inorganic wastewater treatment residue) sludge, was successfully vitrified at the bench-scale at Oak Ridge. A field-scale radioactive demonstration using the transportable vitrification system is underway at the Oak Ridge K-25 Site.

Keywords: Vitrification, Low-Level Mixed Waste, Joule Heated Glass Melter

254. **VITRIFICATION OF ROCKY FLATS WASTE**
$309,000
DOE Field Office Contact: Julie Conner, (208) 526-0648
DOE HQ Program Manager:
Alison Johnson, (301) 903-7923 and
Grace Ordaz, (301) 903-7440
PNNL Contact: Richard Peters (509) 376-3903
EM Focus Area: Mixed Waste

This project determined the vitrification process envelope for three actual waste streams. The process envelopes were defined in terms of waste stream compositional variability, glass forming additives, and the limits of incorporation of troublesome species. The process envelopes were determined by a combination of crucible tests, pilot-scale melter runs and vitrification processing modeling. Leaching tests show that the mixed waste glasses are generally as durable or more durable than high-level waste glasses.

Keywords: Vitrification, Low-Level Mixed Waste, Joule Heated Glass Melter

255. **PLASMA HEARTH PROCESS RADIOACTIVE WASTE TEST - IDAHO**
$1,350,000
DOE Field Office Contact: Julie Conner, (208) 526-0648
DOE HQ Program Manager:
Alison Johnson, (301) 903-7923 and
Grace Ordaz, (301) 903-7440
EG&G Idaho Contact: Bob Gillans, (208) 528-2114
EM Focus Area: Mixed Waste

This project involved the design, construction, testing, and evaluation of a bench-scale Plasma Hearth Process (PHP). The primary goal of this work was to assess the performance of the PHP on actual radioactive wastes and to determine the fate of the radionuclides contaminating the waste upon treatment. The successful conclusion of this project will ensure that the PHP can be employed in radioactive service. In addition data collected in this work will improve the simulation of radionuclides in pilot-scale systems by surrogates.

Keywords: Plasma, Final Form, Low-Level Mixed Waste, Bench-Scale

256. **VITREOUS CERAMIC COMPOSITIONAL ENVELOPE STUDY**
$200,000
DOE Field Contact: James Brown (803) 725-2760
DOE HQ PM: Skip Chamberlain (301) 903-7248
ANL Contact: Dave Wronkiewicz (708) 252-7263
EM Focus Area: Landfill Stabilization

The objective of this program is to utilize tailored slag waste forms to expand the range of waste streams that can be treated using the MAWS approach. Compositional ranges appropriate to the production of tailored slag waste forms will be identified for these waste streams. These studies will complement the composition envelopes being studied for glass waste forms.

Keywords: Composition, Characterization, MAWS

257. **GRAPHITE DC PLASMA ARC MELTER**
$1,242,000
DOE Field Contact: James Brown (803) 725-2760
DOE HQ PM: Skip Chamberlain (301) 903-7248
UMIT Contact: Jeff Surma (509) 376-4905
EM Focus Area: Landfill Stabilization

The objective of this program is to demonstrate the applicability of the Graphite DC Plasma Arc Melter for treating mixed wastes and contaminated soils and for providing an extremely durable waste form for disposal. An engineering scale, radioactive capable furnace system was to be installed and tested at PNNL. This furnace includes analytical instruments for making spatially resolved measurements of furnace and glass temperatures and for the on-line measurements of exhaust emissions, both in the furnace chamber and the off-gas. The capacity of the system will be optimized through the use of process diagnostics.

Keywords: Graphite, DC, Plasma, Arc, Melter

258. **VITREOUS CERAMIC FORMULATION**
$200,000
DOE Field Contact: James Brown (803) 725-2760
DOE HQ PM: Skip Chamberlain (301) 903-7248
UMIT Contact: Xiangdong Feng (509) 373-7284
EM Focus Area: Landfill Stabilization

The object of this program is to use vitreous ceramic waste forms to expand the range of waste streams that can be treated and to develop vitreous ceramics into desirable final waste forms for treating low-level waste and mixed waste. The work is aimed at those waste streams not amenable to producing glass waste forms with high waste loading. The compositional envelopes will serve as guides for remediation of a wider variety of waste streams and reduction of overall disposal costs.

Keywords: Ceramics, Vitrification, Waste forms

259. **HOT CELL STUDIES**
$400,000
DOE Field Office Contact: J. O. Moore, (423) 576-3536
DOE HQ Program Manager: Dave Geiser, (301) 903-7688
ORNL Contact: Rodney Hunt, (505) 667-0088
EM Focus Area: Radioactive Tank Waste Remediation

The U.S. Department of Energy is faced with safely treating and disposing millions of gallons of Liquid Radioactive

Waste stored in High Level Waste tanks across the United States. Only a small amount of radioactive material contributes to the millions of gallons of High Level waste. By removing the radioactive components from the waste, a large volume reduction of waste to be solidified is achieved. A separations program has been established to accomplish this task. Various sorbents are being developed and tested to evaluate their effectiveness to remove cesium (Cs) from these waste streams. The removal (concentration) of cesium is important to reduce the volume of High Level Waste processed for glass formulation.

Keywords: Separations, Cesium, Hot Cells, High Level Waste

260. **CESIUM REMOVAL DEMONSTRATION**
$700,000
DOE Field Office Contact: J. O. Moore, (423) 576-3536
DOE HQ Program Manager: Dave Geiser, (301) 903-7688
ORNL Contact: Rodney Hunt, (505) 667-0088
EM Focus Area: Radioactive Tank Waste Remediation

The U.S. Department of Energy is faced with safely treating and disposing millions of gallons of Liquid Radioactive Waste stored in High Level Waste tanks across the United States. Only a small amount of radioactive material contributes to the millions of gallons of High Level waste. By removing the radioactive components from the waste, a large volume reduction of waste to be solidified is achieved. A separations program has been established to accomplish this task. Various sorbents are being developed and tested to evaluate their effectiveness to remove cesium (Cs) from these waste streams. This project chooses sorbents studied in the ORNL hot cell tests to treat 25,000 gallons of Melton Valley Storage Tank Waste at ORNL. The removal (concentration) of cesium is important to reduce the volume of High Level Waste processed for glass formulation.

Keywords: Separations, Cesium, High Level Waste

261. **Tc AND Ni REMOVAL USING ION EXCHANGE**
$546,000
DOE Field Office Contact: Dennis Alona, (505) 845-4296
DOE HQ Program Manager Kurt Gerdes, (301) 903-7289
LANL Contact: Moses Attrep, (505) 667-0088
EM Crosscut Program: Efficient Separations and Processing

The U.S. Department of Energy is faced with safely treating and disposing millions of gallons of Liquid Radioactive Waste stored in High Level Waste tanks across the United States. Only a small amount of radioactive material contributes to the millions of gallons of High Level waste. By removing the radioactive components from the waste, a large volume reduction of waste to be solidified is achieved. A separations program has been established to accomplish this task. Anion exchangers are being developed and tested to evaluate their effectiveness to remove Technetium (Tc) and Nickel (Ni) from these waste streams. Removal of these materials is important for efficient processing of High Level Waste into glass.

Keywords: Anion, Separations, High Level Waste

262. **CRYSTALLINE SILICOTITANATE FOR Cs/Sr REMOVAL**
$873,000
DOE Field Office Contact: Dennis Alona, (505) 845-4296
DOE HQ Program Manager: Kurt Gerdes, (301) 903-7289
LANL Contact: Norman Brown, (505) 845-8180
EM Crosscut Program: Efficient Separations and Processing

The U.S. Department of Energy is faced with safely treating and disposing millions of gallons of Liquid Radioactive Waste stored in High Level Waste tanks across the United States. Only a small amount of radioactive material contributes to the millions of gallons of High Level waste. By removing the radioactive components from the waste, a large volume reduction of waste to be solidified is achieved. A separations program has been established to accomplish this task. Ion exchange resins are being developed and tested to evaluate their effectiveness to remove Cesium (Cs) and Strontium (Sr) from these waste streams. Removal of these materials is important for efficient processing of High Level Waste into glass. Hot cell studies are being performed for this material with anticipation of performing pilot scale processing.

Keywords: Ion Exchange, Separations, High Level Waste

263. **TUCS/PHOSPHATE IMMOBILIZATION OF ACTINIDES**
$300,000
DOE Field Office Contact: S Webster, (708) 252-3653
DOE HQ Program Manager:
Kurt Gerdes, (301) 903-7289
Argonne Contact: K. Nash, (708) 252-3581
EM Crosscut Program: Efficient Separations and Processing

The U.S. Department of Energy facilities face the challenge of restoring facilities following years of radioactive materials processing. Various DOE sites have contaminated soil that needs remediation. The Thermally Unstable Complexants (TUCS) technology (used to sequester and immobilize actinides in soil by phosphate mineralization), is being developed and evaluated. This process will enhance DOE's ability to restore sites contaminated with radioactive constituents.

Keywords: Plumes, Soil, Immobilization, Restoration

OFFICE OF NUCLEAR ENERGY, SCIENCE AND TECHNOLOGY

	FY 1995
Office of Nuclear Energy, Science and Technology - Grand Total	$48,165,000
Office of Engineering and Technology Development	$ 2,165,000
Space and National Security Programs	$ 2,165,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 1,435,000
Development of an Improved Process for the Manufacture of DOP-26 Iridium Alloy Blanks, Product Characterization and Exploratory Alloy Improvement Studies	965,000
Carbon-Bonded Carbon Fiber Insulation Production Maintenance, Manufacturing Process Development and Product Characterization	470,000
Materials Properties, Behavior, Characterization or Testing	$ 730,000
Development of an Improved Carbon-Carbon Composite Graphite Impact Shell Replacement Material	370,000
Development of Materials for Advanced Radioisotope Power Systems	360,000
Office of Naval Reactors	$46,000,000*

*This excludes $44 million for the cost of irradiation testing in the Advanced Test Reactor (ATR).

OFFICE OF NUCLEAR ENERGY, SCIENCE AND TECHNOLOGY

OFFICE OF ENGINEERING AND TECHNOLOGY DEVELOPMENT

SPACE AND NATIONAL SECURITY PROGRAMS

Space and National Security Programs include the development and production of radioisotope power systems for both space and terrestrial applications and the technical direction, planning, demonstration and delivery of nuclear reactor power and propulsion systems for military and civilian space missions and for special military terrestrial applications. During FY1995, nuclear reactor power system activities were phased out. Essentially all materials programs were designed to support the production of General Purpose Heat Source-Radioisotope Thermoelectric Generators for the NASA Cassini Mission and preliminary scoping studies for support of the future Pluto Express NASA mission. This applied materials research programs are supported in the areas of thermoelectric materials and devices, advanced energy conversion systems, high temperature heat source materials, materials systems compatibility and safety related materials characterization and testing.

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

264. **DEVELOPMENT OF AN IMPROVED PROCESS FOR THE MANUFACTURE OF DOP-26 IRIDIUM ALLOY BLANKS, PRODUCT CHARACTERIZATION, AND EXPLORATORY ALLOY IMPROVEMENT STUDIES**
$965,000
DOE Contact: W. Barnett, (301) 903-3097
RNL Contacts: E. P. George, (615) 574-5085 and
E. K. Ohriner, (615), 574-8519

An iridium alloy, DOP-26 (i.e., Ir-0.3 wt.% W with Th and Al dopant additions), serves as the fuel clad or capsule material for isotope heat sources employed in recent and contemporary space power systems for NASA deep space missions. This program is aimed at the optimization of the new improved process route previously selected for the production of DOP-26 iridium alloy sheet, namely a consumable vacuum arc cast/extrusion/"warm" rolling route. The effectiveness of this production process was further demonstrated in the FY 1995 production of DOP-26 alloy blanks, foil and clad vent sets for the Cassini Mission. Production yields have continued to exceed our goals.

Significant progress was made in the preparation for introducing bare rolling into the sheet production process. Crowned carbide rolls are being procured to evaluate possible improvements in sheet shape control. A suitable die/lubrication system for bare forming of clad vent set cups was identified.

Studies of bare rolling of blank stock and bare forming of cups was continued.

Continued product characterization studies, particularly for simulated service conditions, continued to show behaviors equivalent or superior to the prior process product.

Studies of alternate iridium alloy doping agents were continued. The objective is to maintain or exceed the properties of the DOP-26 alloy at a significantly lower thorium dopant level. An iridium alloy containing 0.3 wt.%W with dopant additions of 40 appm cerium and 15 appm thorium was selected for scale-up. A nominal six kilogram consumable arc melted ingot was preferred, extruded and sheet preparation was initiated.

Keywords: Consumable Arc Melt, Extrusion, Noble Metal

265. **CARBON-BONDED CARBON FIBER INSULATION PRODUCTION MAINTENANCE, MANUFACTURING PROCESS DEVELOPMENT AND PRODUCT CHARACTERIZATION**
$470,000
DOE Contact: W. Barnett, (301) 903-3097
ORNL Contacts: C. E. Weaver and R. Dunwiddie,
(615) 574-9978

Carbon-bonded carbon fiber (CBCF) type thermal insulation material is employed in Isotopic General Purpose Heat Source (GPHS) Module assemblies for use in current GPHS-RTG (radioisotope thermoelectric generator). This material was originally employed in GPHS-R7Gs for the Galileo/NASA (1989 launch) and Ulysses/NASA-ESA (1990 launch) Missions. Material produced for the Cassini Mission (1997 launch) was made with a replacement carbon fiber (new vendor, former source not available) utilizing an optimized process and process controls. The FY 1995 program encompassed (1) maintenance of capability for both tube and plate billet production through the year, and (2) characterization of Cassini CBCF insulation thermal conductivity.

Particular attention was focused on evaluation of the effects of short-term very high temperature short-time exposures on thermal conductivity. Equations were developed which express thermal conductivity as a function of temperature and peak exposure temperature and time.

Keywords: Insulators/Thermal, High Temperature Service, Fibers

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

266. DEVELOPMENT OF AN IMPROVED CARBON-CARBON COMPOSITE GRAPHITE IMPACT SHELL REPLACEMENT MATERIAL
$370,000
DOE Contact: W. Barnett, (301) 903-3097
Oak Ridge National Laboratory Contact:
G. R. Romanowski, (616) 574-4838

The Graphite Impact Shell (GIS), a component of the General Purpose Heat Source isotopic heat source module is a closed end/capped tubular shape machined from AVCO 3D-CC fine weave pierced fabric material. It is anticipated that a change in the fiber reinforcement architecture from the current orthogonal structure to a cylindrical type structure will enhance energy absorption in high velocity impact. The current program is a feasibility study of commercially available and experimental materials.

During FY 1995 impact tests were conducted on all 38 candidate materials representing at least two levels of densification for each architectural variant. Impact testing was performed at 55 m/s using a copper mass simulant to match the typical mass of a GPHS fueled clad. Force versus time was measured at the impact face. While significant improvement in hoop strength was attained, only minor enhancement in energy absorption was achieved.

Keywords: Composites, Carbon-Carbon

267. DEVELOPMENT OF MATERIALS FOR ADVANCED RADIOISOTOPE POWER SYSTEMS
$360,000
DOE Contact: W. Barnett, (301) 903-3097
Iowa State University, Ames Laboratory Contact:
B. Cook, (515) 294-9673

The objectives of this activity are: (1) evaluate the potential of new thermoelectric materials, (2) develop and characterize rare earth based selective emitters for potential thermophotovoltaic systems application, provide support in the areas of materials compatibility and transport.

Keywords: Radioisotope Power, Thermoelectrics, Thermophotovoltaics

OFFICE OF NAVAL REACTORS

The materials program supports the development and operation of improved and longer life reactors and pressurized water reactor plants for naval nuclear propulsion.

The objective of the materials program is to develop and apply, in operating service, materials capable of use under the high power density and long life conditions required of naval ship propulsion systems. This work includes irradiation testing of reactor fuel, poison, and cladding materials in the Advanced Test Reactor at the Idaho National Engineering Laboratory. This testing and associated examination and design analysis demonstrates the performance characteristics of existing materials as well as defining the operating limits for new materials.

Corrosion, mechanical property, and wear testing is also conducted on reactor plant structural materials under both primary reactor and secondary steam plant conditions to confirm the acceptability of these materials for the ship life. This testing is conducted primarily at two Government laboratories-Bettis Atomic Power Laboratory in Pittsburgh and Knolls Atomic Power Laboratory in Schenectady, New York.

One result of the work on reactor plant structural material is the issuance of specifications defining the processing and final product requirements for materials used in naval propulsion plants. These specifications also cover the areas of welding and nondestructive testing.

Funding for this materials program is incorporated in naval projects jointly funded by the Department of Defense and the Department of Energy. This funding amounts to approximately $90 million in FY1995 including approximately $44 million as the cost for irradiation testing in the Advanced Test Reactor. The Naval Reactors contact is David I. Curtis, (703) 603-5565.

OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT

	FY 1995
Office of Civilian Radioactive Waste Management - Grand Total	$9,700,000
Materials Properties, Behavior, Characterization or Testing	$9,700,000
Waste Packages	$9,700,000

OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT

Materials research is ongoing in the Office of Civilian Radioactive Waste Management in the development of waste packages for eventual geologic disposal.

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

268.WASTE PACKAGES

$9,700,000
DOE Contact: David Haught, (702) 794-5474
M&O Contacts: Hugh Benton, (702) 794-1891 and David Stahl, (702) 794-7778

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. Progress on the advanced conceptual design of the waste package and the supporting materials studies has been recently documented in the Waste Package Conceptual Design Report.

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, and DOE-owned spent nuclear fuel. The analytical effort that is underway to support these designs includes thermal, structural, and neutronic analyses. Also included are materials selection and engineering development.

The waste package materials effort includes the testing and modeling of materials being considered for inclusion in the waste package and the engineered barrier system. The testing includes general aqueous and atmospheric testing, localized attack such as pitting and crevice corrosion, microbiologically influenced corrosion, and stress corrosion cracking. The corrosion test facility will start the long-term (at least five-year) test program in FY 1996. Waste form materials are also being evaluated for oxidation and leaching under repository-relevant conditions. Chemical simulations have recently been performed to evaluate the potential performance of additives to backfill. These latter efforts support both design and performance assessment.

Keywords: Yucca Mountain, Repository, Waste Package, Engineered Barrier System

OFFICE OF DEFENSE PROGRAMS

	FY 1995
Office of Defense Programs - Grand Total	$90,355,000
The Weapons Research, Development and Test Program	$90,355,000
Sandia National Laboratories	$42,452,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$14,587,000
Environmentally Conscious Manufacturing Technologies	767,000
Microelectronics & Photonics Materials	731,000
Micromechanical Technology	1,822,000
Chemical Processing Science	506,000
Polymer Synthesis, Process & Reliability	1,049,000
Porous & Microporous Materials	1,439,000
Metal Joining Technologies	1,388,000
Smart Processing Of Materials	1,607,000
Materials Science Research Support	276,000
Template-Mediated Ontogenesis: A Novel Approach to Mesomorphic Materials	350,000
Dynamics of Nucleation in Chemical Vapor Deposition	367,000
Atomic-Scale Measurement of Liquid Metal Wetting and Flow	364,000
Atomic Layer Epitaxial Growth of Diamond Using Halogenated Gases	397,000
Development of a Scaleable, Flat-Flame Technology for the Synthesis of Diamond Films	384,000
Synthesis and Processing of High Strength SiC Foams: A Radically New Approach to Ceramic-Ceramic Composite Materials	365,000
Molecular Adhesion Including Chemical Reactions at Polymer-Solid Interfaces	380,000
Synthesis of Ceramics Using Supercritical Fluids	365,000
Carbon Nanotube Reinforced Composites	396,000
Advanced Materials for Biomedical and Aerospace Applications	217,000
Chemical Functional of Oligosilanes: Economically Attractive Routes to New Photoresponsive Materials	393,000
Polyphosphaacetylenes: New Conducting Hybrid Organic-Inorganic Materials	300,000
New Adhesive Systems Based On Functionalized Block Copolymers	228,000
Engineered Monodisperse Porous Materials	321,000
Low-Dielectric and High-temperature Films for Multichip Modules	175,000
Materials Structure and Composition	$ 1,811,000
Advanced Analytical Methods For Materials Research	1,272,000
Adaptive Scanning Probe Microscopies	417,000
Characterization and Correlation of Physical Properties of Ceramics Through Orientation Imaging Microscopy	122,000

OFFICE OF DEFENSE PROGRAMS (Continued)

	FY 1995
The Weapons Research, Development and Test Program (continued)	
Sandia National Laboratories (continued)	
Materials Properties, Behavior, Characterization or Testing	$19,762,000
Energetic Material Center	106,000
Computational Solid Dynamics	2,716,000
Applied Materials & Mechanics Collaborations	635,000
Development Of More Efficient Power Sources	1,044,000
Basic Science Of Materials Stability	1,829,000
Advanced Materials Characterization Science	1,006,000
Photonics Technology	1,206,000
Electronic Ceramics	899,000
Ultrahard Materials Research	594,000
Impurity Effects On Interfaces	997,000
Materials Aging & Reliability	1,155,000
Engineering Sciences Research	6,157,000
Gas Separation of Fullerene Membranes	300,000
PbO-free Composites for Low Temperature Packaging	359,000
Demonstration of Molecular-Based Transistors	317,000
Nanocomposite Materials Based on Hydrocarbon-Bridged Siloxanes	442,000
Device or Component Fabrication, Behavior or Testing	$ 5,589,000
MC4300 Neutron Tube	329,000
Smartweld II	1,985,000
Manufacturing Technology	1,859,000
Electronic & Microelectromechanical Systems (MEMS) Components	1,416,000
Instrumentation and Facilities	$ 703,000
Materials Processes for Manufacturing	703,000
Lawrence Livermore National Laboratory	$20,876,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 5,245,000
Engineered Nanostructure Laminates	1,800,000
Sol Gel Coatings	335,000
KDP Growth Development	900,000
ICF Capsule Ablators via Plasma Polymerization	500,000
Vicarious Nucleophilic Substitution Chemistry	400,000*
CHEETAH Thermochemical Code	190,000*
Hard Target Penetrator Explosive	900,000*
Injection Moldable Explosives	220,000*

*This activity is jointly funded (50:50) by DOE DP and the DoD.

OFFICE OF DEFENSE PROGRAMS (Continued)

	FY 1995
The Weapons Research, Development and Test Program (continued)	
Lawrence Livermore National Laboratory (continued)	
Materials Properties, Behavior, Characterization or Testing	$ 1,260,000
Interfaces, Adhesion, and Bonding	460,000
Laser Damage: Modeling and Characterization	400,000
KDP Characterization	400,000
Instrumentation and Facilities	$14,371,000
Scanning Tunneling Microscopy (STM) and Atomic Force Microscopy (AFM)	250,000
Treatment of Waste and Water with Carbon Aerogel Electrodes	425,000
Trilayer Josephson Junctions (Technology Transfer Initiative)	375,000
Lithium Cell Development	200,000
Environmentally Safe Disposal of Explosive Wastes: SERDP Project	800,000
Laminated Metal Composites for Aerospace Applications	700,000
Fatigue of Metal Matrix Composites	500,000
Novel Materials for Optoelectronics and Photonics	600,000
Novel Materials Studies at High Pressures and Temperatures	400,000
Materials Produced with Dynamic High Pressure	400,000
Properties of Hydrogen at High Shock Pressures and Temperatures	300,000
Low Density Foam Shells for Cryogenic ICF Experiments	600,000
Atomic Level Explosive Calculations	400,000
Explosive Equation of State	700,000
Metastable Solid-Phase High Energy Density Materials	236,000
Metastable Solid-Phase High Energy Density Materials	535,000
AFM Investigations of Crystal Growth	210,000
Superplastic Forming of Stainless Steel Automotive Components	150,000
Formability and Joining Analysis for Superplastic Panel Design	360,000
Microstructural Evolution in Welds	330,000
Uranium Casting Program	1,000,000
Uranium Spin Forming	1,500,000
Plutonium Near Net Shape Casting	2,500,000
Electron Beam Cold Hearth Melting of Uranium	900,000
Los Alamos National Laboratory	$27,027,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 5,055,000
Actinide Processing Development	1,350,000
Plutonium Oxide Reduction	150,000
Low Density Microcellular Plastic Foams	200,000
Physical Vapor Deposition and Surface Analysis	300,000
Chemical Vapor Deposition (CVD) Coatings	150,000
Polymers and Adhesives	430,000
Tritiated Materials	175,000
Salt Fabrication	800,000
Slip Casting of Ceramics	300,000

OFFICE OF DEFENSE PROGRAMS (Continued)

	FY 1995
Los Alamos National Laboratory (continued)	
Materials Preparation, Synthesis, Deposition, Growth or Forming (continued)	
Plasma-Flame Spraying Technology	300,000
Rapid Solidification Technology	500,000
Bulk Ceramic Processing	250,000
Synthesis of Ceramic Coatings	150,000
Materials Structure or Composition	$ 1,237,000
Actinide Surface Properties	700,000
Neutron Diffraction of Pu and Pu Alloys and Other Actinides	237,000
Surface, Material and Analytical Studies	300,000
Materials Properties, Behavior, Characterization or Testing	$ 2,500,000
Mechanical Properties of Plutonium and Its Alloys	450,000
Phase Transformations in Pu and Pu Alloys	450,000
Plutonium Shock Deformation	350,000
Non-Destructive Evaluation	550,000
Powder Characterization	50,000
Shock Deformation in Actinide Materials	300,000
Dynamic Mechanical Properties of Weapons Materials	350,000
Device or Component Fabrication, Behavior or Testing	$ 3,900,000
Target Fabrication	1,500,000
Filament Winder	100,000
High Energy Density Welding in Hazardous Environments	800,000
Uranium Scrap Conversion and Recovery	1,500,000
Laboratory Directed Research and Development	$10,802,000
Electronically Correlated Materials at Ambient and Extreme Conditions	328,000
Organometallic Chemical Vapor Deposition	248,000
Polymer Sorbents for Hazardous Metal Uptake	164,000
Microscopic Materials Modeling: Textures and Dynamics	109,000
Surface Modification of Materials	315,000
Integration of Fundamental Knowledge in Plasticity and Textures to Provide Technical Tools for Microscopic Applications	290,000
High Resolution Electron Microscopy of Materials	350,000
Nano-Fabrication	255,000
Thin Film Micro-Electrochemical Sensor Development	210,000
Liquid Crystal Thermosets	200,000
Neutron and Resonant X-ray Scattering by Materials	350,000
Structural and Electronic Competitions in Low-Dimensional Materials	360,000
Fundamental Aspects of Photoelectron Spectroscopy in Highly Correlated Electronic Systems	300,000

OFFICE OF DEFENSE PROGRAMS (Continued)

	FY 1994
Los Alamos National Laboratory (continued)	
Laboratory Directed Research and Development (continued)	
Development of High Strength High Conductivity Materials for High Magnetic Field Devices	100,000
Low Temperature STM for Structural and Spectroscopic Studies of High Temperature Superconductors and Other Electronic Materials	50,000
Materials with Fine Microstructures	365,000
Ion Beam Materials Research	330,000
Texture Studies of Highly Deformed Composite Materials	192,000
Pressure Dependency of the Structure of High Explosives: Nitromethane	192,000
Neutron Reflection Studies of Thin Film and Multilayer Structures	300,000
Neutron Reflectivity Studies of In Situ Corrosion of Metal Surfaces	145,000
The Dynamics of Amorphous Materials	330,000
Advanced Material Science Algorithms for Supercomputer Architectures	75,000
Metal Vapor Synthesis in Organometallic Chemistry	235,000
Separation Chemistry of Toxic Metals	250,000
Polymers for Integrated Optical Interconnects	266,000
High Temperature Materials Synthesis Without Heat:Oxide Layer Growth on Electronic Materials Using High Kinetic Energy Atomic Species	164,000
Dynamic Deformation of Advanced Materials	855,000
Strain Measurements in Individual Phases of Multi-Phase Materials	130,000
Artificially Structured Nonlinear Optic and Electro-Optic Materials	465,000
Structural Phase Transitions in Non-Stoichiometric Oxides	275,000
Strongly Correlated Electronic Materials	495,000
Plasma Immersion Ion Implantation for Semiconductor Film Growth	261,000
Analysis of Structure and Orientation of Adsorbed Polymer in Solution Subject to Dynamic Shear Stress	172,000
Development of Pair Distribution Function Analysis of Mesostructural Details in Single Crystal Perovskites and Nanocrystalline Materials	170,000
Neutron Scattering as a Probe of the Structure of Liquid Crystal Polymer-Reinforced Composite Materials	180,000
Strain Measurements in Individual Phases of Multi-Phased Materials During Thermomechanical Loading: LANSCE Neutron Scattering Experiment Support	318,000
A New Approach to Texture Measurements: ODF Determination by Rietveld Refinement	73,000
Applications of Fullerenes in Nuclear Technology	360,000
Ceramic Oxide Foams for Separation	400,000
Materials Modeling Project	125,000
Synthesis and Optical Characterization of Novel Fullerene-Based Composites	50,000
Technology Transfer Initiative	$ 3,533,000
A Pilot Program: Chemical Vapor Deposition of Diamond in a Fluidized-Bed for Cutting Tool and Tribological Applications	250,000
Advanced Beryllium Processing	632,000
Automated Pulsed Laser Deposition System	130,000
Plasma Source Ion Implantation for the Automotive Industry	1,326,000
Processing Modeling and Control for U.S. Steel Industry	1,195,000

OFFICE OF DEFENSE PROGRAMS

Summaries of materials activities which were selected to present the diversity of materials research, development and application projects conducted for the Office of the Assistant Secretary for Defense Programs are included in this section. Activities are organized in groupings that indicate the Defense Program Laboratory at which the specific project was performed. Funds for FY95 materials activities within Defense Programs were provided by the Weapons Research, Development and Test program including the Core Research and Development program and the Technology Transfer Initiative program and by the Inertial Confinement Fusion program, the Production and Surveillance program, and Laboratory Research and Development program. Projects with proprietary, patentable, or classified information were not reported.

THE WEAPONS RESEARCH, DEVELOPMENT AND TEST PROGRAM

SANDIA NATIONAL LABORATORIES

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

269. **ENVIRONMENTALLY CONSCIOUS MANUFACTURING TECHNOLOGIES**
$767,000
DOE Contact: R. Staffin, (202) 586-7590
SNL Contact: D. L. Lindner (510) 294-3306

This project develops environmentally conscious manufacturing, ECM, technologies required for the manufacture of nuclear weapons components.

Keywords: Environmental

270. **MICROELECTRONICS & PHOTONICS MATERIALS**
$731,000
DOE Contact: R. Staffin, (202) 586-7590
SNL Contact: A. D. Romig, (505) 844-8358

This project involves exploratory investigations into new semiconductor materials and heterostructures for photonic and microelectronic devices and systems. These investigations are expected to be foundational to the development of photonic and microelectronic technologies that will replace present day optical, electronic, electro-mechanical, and mechanical components and systems and offer more effective, efficient, compact, rugged, radiation hard, and electromagnetic pulse (EMP), resistant components for future generation systems.

Keywords: Semiconductors, Heterostructures

271. **MICROMECHANICAL TECHNOLOGY**
$1,822,000
DOE Contact: R. Staffin, (202) 586-7590
SNL Contact: A. D. Romig, (505) 844-8358

Sandia presently has both an established surface micro mechanical technology and bulk micromechanical technology. Extensive internal and external customers exist for novel sensors and devices fabricated using these technologies. Most of these applications benefit from the integration of on-chip control and sense electronics, which lower costs, improve performance, decrease system size and increase manufacturability. These activities focus on the integration of Sandia's established digital/analog Complimentary Metal-Oxide Semiconductor (CMOS) technology with the existing micromechanical technologies.

Keywords: Micromechanical

272. **CHEMICAL PROCESSING SCIENCE**
$506,000
DOE Contact: R. Staffin, (202) 586-7590
SNL Contact: A. D. Romig, (505) 844-8358

This project will advance the technology base that will enable: (1) intelligent design of chemical processes and reactors, (2) scientifically based optimization of processes and (3) in situ process monitors and sensors for real time control. We shall develop and maintain expertise in chemical vapor deposition (CVD) processes of importance to Microelectronics Development Laboratory (MDL) and Compound Semiconductor Research Laboratory (CSRL) in the fabrication of microelectronic and photonic devices. We shall develop and employ the scientific techniques of optical spectroscopies, chemical kinetics, surface science, and numerical modeling to address Si and III-V chemistry issues.

Keywords: Chemical Vapor Deposition, Modeling

273. **POLYMER SYNTHESIS, PROCESS & RELIABILITY**
$1,049,000
DOE Contact: R. Staffin, (202) 586-7590
SNL Contact: H. J. Saxton, (505) 845-8739

The goal of this project is to expand our organic materials support capabilities through a science base in the following technology areas: (1) materials reliability and lifetime prediction; (2) optical and electronic materials, (3) molecular engineering of structural materials, (4) blends and interfaces, and (5) explosives aging.

Keywords: Polymers, Reliability

274. **POROUS & MICROPOROUS MATERIALS**
$1,439,000
DOE Contact: R. Staffin, (202) 586-7590
SNL Contact: H. J. Saxton, (505) 845-8739

The purpose of this project is to develop a fundamental understanding of the synthesis, processing, characterization, and performance of porous and microporous materials for weapons and other applications. Specific applications include aging of polymeric materials for use in components such as neutron generators and explosively actuated power supplies, porous carbon electrode technology for use in rechargeable lithium batteries, and low dielectric polymers for electronics packaging.

Keywords: Polymers, Porous

275. **METAL JOINING TECHNOLOGIES**
$1,388,000
DOE Contact: R. Staffin, (202) 586-7590
SNL Contact: H. J. Saxton, (505) 845-8739

This project develops technologies required for the joining of metal hardware for Defense Programs. Specific applications include development of metal joining processes for environmentally conscious manufacturing and agile manufacturing. The subprojects encompass welding, soldering and brazing.

Keywords: Welding, Soldering, Brazing

276. **SMART PROCESSING OF MATERIALS**
$1,607,000
DOE Contact: R. Staffin, (202) 586-7590
SNL Contact: H. J. Saxton, (505) 845-8739

The SMART processing project is formulated to provide synergy in the area of intelligent processing across a broad range of materials and processes. Research in this case is designed to dove-tail with the more applied SMART programs being supported under Defense Program (DP) capabilities. The products of the research are predictive scientific models or materials/processing knowledge which can be integrated or packaged for use in Model-based design systems. The funding for this project is divided among metals, ceramics, and polymers. In metals, three areas of process understanding are targeted: (1) characterization of the heat transfer process during welding; (2) microstructural evolution models for solidification of castings and welds; and (3) materials response models for predicting mechanical property/microstructural changes during large scale deformation processes such as forming/forging/welding. In the area of ceramics, the focus is in identifying the critical process parameters required to obtain homogenous properties in compacted ceramics as a function of particle size, shape, rheology and processing parameters. In the area of polymers, the focus is on developing the experimental data and process response maps needed to generate predictive models for mold filling and property evolution during curing or solidification of structural polymers.

Keywords: Processing, Welding, Powders, Polymers

277. **MATERIALS SCIENCE RESEARCH SUPPORT**
$276,000
DOE Contact: R. Staffin, (202) 586-7590
SNL Contact: H. J. Saxton, (505) 845-8739

The purpose of this project is to provide program management support to research projects in the Engineered Materials & Processes portfolio at Sandia. One goal is to start new projects to meet strategic plan objectives, e.g., the electrochromic organic materials project, and SmartForge project.

Keywords: Forging, Electrochromic

278. **TEMPLATE-MEDIATED ONTOGENESIS: A NOVEL APPROACH TO MESOMORPHIC MATERIALS**
$350,000
DOE Contact: M. J. Katz, (202) 586-5799
SNL Contact: J. E. Martin, (505) 844-9125

Mesomorphic materials have properties that are fundamentally different from those of their microscopic constituents. This frequently leads to greater utility, but producing mesoheterogeneous materials is often difficult since the only constraint imposed during synthesis is macroscopic-the reaction path itself. In this project, we use surfactant templates to produce novel mesoheterogeneous materials whose unique properties address specific materials goals. These include Chemically Selective

Filters, Size-Exclusion Chromatography Media; and an Optical Switch.

Keywords: Templates, Processing

279. **DYNAMICS OF NUCLEATION IN CHEMICAL VAPOR DEPOSITION**
$367,000
DOE Contact: M. J. Katz, (202) 586-5799
SNL Contact: T. A. Michalske, (505) 844-5829

The structure and properties of a thin film are highly dependent on the conditions employed during growth. In particular, nucleation is known to be an important rate limiting step, and responsible for the evolution of the macroscopic structure for many materials. We have initiated a program to investigate nucleation in chemical vapor deposition of metals on silicon substrates for the purpose of understanding both the microscopic dynamics of growth processes and the relationship of these to the structure of the resulting film. We examine nucleation of Fe and Al on single crystal Si surfaces by thermal dissociation of suitable precursors in ultra high vacuum. We employ variable temperature scanning tunneling microscopy (STM) to directly image nucleation sites, structure of nuclei, and number and size distribution of nuclei in real time. These measurements will be complemented by global measures of structure, composition, and growth kinetics, including x-ray reflectivity (XRR), x-ray photoelectron spectroscopy (XPS), and reflection infrared spectroscopy (IR). We will also employ simulation and theoretical modeling of nucleation to test the sensitivity of structure to different dynamic processes and to examine the evolution of microstructure of the film.

Keywords: Nucleation, Chemical Vapor Deposition, Surfaces

280. **ATOMIC-SCALE MEASUREMENT OF LIQUID METAL WETTING AND FLOW**
$364,000
DOE Contact: M. J. Katz, (202) 586-5799
SNL Contact: T. A. Michalske, (505) 844-5829

The wetting and flow of liquid metals plays an important role in materials synthesis and joining technologies. For example, soldering, brazing and welding require a liquid metal to wet the interface between two solids, and the fabrication of light-weight, metal-matrix structural composites involves the infiltration of a liquid metal into a porous ceramic preform. Despite the pervasive presence of liquid metal interfaces in materials problems, solutions are almost always the result of trial and error, rather than an atomic-scale scientific understanding. Just as microscopic flow processes determine the stability of atomically-thin grain boundary films, the wetting and flow of a macroscopic liquid are controlled by atomic motions at the leading edge of the spreading droplet. Current continuum models of spreading do not address atomic-scale flow mechanisms and fail to predict correctly wetting, flow, and stability of interfacial liquid metals. In this project we will (1) develop a new Acoustic Wave Damping experimental technique that can measure the atomic-scale flow behavior of liquid metals on solid substrates, and (2) use this technique to make the first viscoelastic measurements of well-characterized liquid metal layers. This project will have significant impact on scientific issues common to a wide variety of materials problems by providing new atomic level understanding that can be used to develop improved predictive engineering models for liquid flow and spreading phenomena.

Keywords: Wetting, Solder

281. **ATOMIC LAYER EPITAXIAL GROWTH OF DIAMOND USING HALOGENATED GASES**
$397,000
DOE Contact: M. J. Katz, (202) 586-5799
SNL Contact: W. A. Hsu, (510) 294-2379

Atomic layer epitaxy (ALE) is a technique which has been exploited successfully in the area of compound semiconductors, such as the II-VI and III-V materials. The concept is to sequentially expose a substrate to alternating gaseous reagent species to build up, in an atomic layer-by-layer manner, the desired repeating compound layer structure. The reagent pairs that we are investigating in this technique include the CF_4/H_2 and CH_4/F_2 the systems. Our objectives are: (1) Deposit diamond at close to room temperature, (2) develop a process that is scalable to large area deposition, (3) control the deposition process so that it can potentially result in single crystal epitaxial growth.

Keywords: Diamond, Epitaxy

282. **DEVELOPMENT OF A SCALEABLE, FLAT-FLAME TECHNOLOGY FOR THE SYNTHESIS OF DIAMOND FILMS**
$384,000
DOE Contact: M. J. Katz, (202) 586-5799
SNL Contact: K. F. McCarty, (510) 294-2067

We are developing a combustion technology that can be scaled to manufacture diamond films of arbitrary size. Flat-flames based on inherently scaleable stagnation flows give rapid and uniform diamond growth. A novel flow manifold, called a trumpet bell, is used to produce all the ideal properties of an infinite stagnation flow, but on a finite scale that maximizes the use of reagent gas. Computational modeling is used to understand and optimize the deposition process and to investigate potentially advantageous but high risk processes.

Keywords: Diamond, Processing

283. **SYNTHESIS AND PROCESSING OF HIGH STRENGTH SiC FOAMS: A RADICALLY NEW APPROACH TO CERAMIC-CERAMIC COMPOSITE MATERIALS**
$365,000
DOE Contact: M. J. Katz, (202) 586-5799
SNL Contact: J. M. Hruby (510) 294-2596

Prohibitively high processing costs due to restricted fiber preform connectivity have kept silicon carbide, SiC, composites from entering mass commercial markets in spite of their favorable strength to weight ratio and oxidative stability. Our novel approach will bypass expensive fiber processing steps by providing a 3D interconnected network of struts having open connectivity to all pores. We propose several routes to synthesize and process the SiC foams. We will explore whether stressing the foams during pyrolysis can induce polymer chain alignment resulting in increased strength in the resulting SiC preform. This project will be the first sol gel entry into SiC materials, using designed precursor materials with the intent of preparing well defined foams. A variety of characterization techniques, including x-ray microtomography, x-ray diffraction, surface area, pore size distribution, and SEM, will be performed on the resulting new and unique materials. Many applications have been identified in an already large and growing area that would greatly benefit from near net shape processing, high strength, non-fiber processing, and energy savings.

Keywords: Ceramics, Porosity, SiC

284. **MOLECULAR ADHESION INCLUDING CHEMICAL REACTIONS AT POLYMER-SOLID INTERFACES**
$380,000
DOE Contact: M. J. Katz, (202) 586-5799
SNL Contact: W. D. Wilson, (510) 294-2264

The goal of this project is to investigate mechanisms of adhesion of polymers to ionic, covalent, and metallic substrates. The program involves the development of a consistent model of surface atoms and polymeric functional groups which includes electrostatic, polarization and covalent effects. The embedded atom method of determining an atom's energy as a function of the total charge density at its center due to both molecules and solid atoms in its vicinity provides the underlying, unifying formalism.

Keywords: Adhesives, Polymers

285. **SYNTHESIS OF CERAMICS USING SUPERCRITICAL FLUIDS**
$365,000
DOE Contact: M. J. Katz, (202) 586-5799
SNL Contact: C. L. Adkins, (505) 845-9119

Supercritical fluids such as H_2O, CO_2, NH_3, etc., have unique solvation properties that make them appealing for the synthesis of materials that cannot be made by conventional means. If a solute-laden supercritical fluid is rapidly expanded through a nozzle, a powder is produced as the fluid expands. The rapid expansion of the fluid can lead to the production of unusual, nonequilibrium phases of the solute that might prove to be more readily sinterable. This technique combines the benefits of gas-phase powder synthesis with the high throughputs possible using spray technology. Waste minimization is automatic since the working fluid can be recycled. We will explore the use of supercritical fluids to synthesize novel (e.g., ultrafine, more reactive) ceramic powders.

Keywords: Supercritical, Powders

286. **CARBON NANOTUBE REINFORCED COMPOSITES**
$396,000
DOE Contact: M. J. Katz, (202) 586-5799
SNL Contact: P. A. Cahill, (505) 844-5754

Carbon fiber composites are important advanced materials for applications from rocket casings to golf clubs because of their high strength to weight ratios. We propose to investigate carbon fiber composites in which the reinforcing carbon fibers are 1000 times smaller than the currently used micron-sized PAN or pitch derived fibers. This revolutionary decrease in the size of the fibers can be expected to lead to materials with greatly enhanced strength, stiffness, and durability. These improvements in physical properties are qualitatively predicted to be derived from: (1) the size of the fiber (because stress transfer from the matrix to the fiber becomes more efficient as the size of the fiber decreases and as the fiber surface area to weight ratio increases), and (2) the direct chemical reaction of the fiber with the matrix, which is generally not possible with micron sized carbon fibers, should lead to an extremely strong fiber-matrix interface. We propose to isolate pure 1-nanometer diameter carbon nanotubes from inexpensive, commercially-available, nanotube/soot mixtures, add solubilizing and reactive groups (as needed) to the side of the tubes, and fabricate fiber reinforced composite materials. Both the mechanical and dielectric (or conducting) properties of the composites will be fully characterized.

Keywords: Carbon, Composites

287. **ADVANCED MATERIALS FOR BIOMEDICAL AND AEROSPACE APPLICATIONS**
$217,000
DOE Contact: M. J. Katz, (202) 586-5799
SNL Contact: J. T. McCord, (505) 844-5157

We have developed new materials and processes for hermetic glass-to-titanium seals that can be used in a variety of aerospace and biomedical electronic components. In particular, we have developed a new family of lanthanoborate sealing glasses that have the requisite thermal and chemical properties to form reliable seals. We have used these new glasses to produce prototype seals. We have characterized the interfacial reactions that lead to good chemical bonding between these glasses and titanium. We have also characterized biocompatible glasses in the Fe_2O_3- and TiO_2-CaO-P_2Os systems that also possess the thermal/chemical properties for titanium sealing.

Keywords: Glass, Seals, Biocompatible

288. **CHEMICAL FUNCTIONAL OF OLIGOSILANES: ECONOMICALLY ATTRACTIVE ROUTES TO NEW PHOTORESPONSIVE MATERIALS**
$393,000
DOE Contact: M. J. Katz, (202) 586-5799
SNL Contact: C. L. Renschler, (505) 844-0324

Polysilanes, [Si(R)(R')]n, are saturated macromolecules whose unusual electronic absorption behavior closely resembles those of conjugated polyenes. With synthetic routes previously available, they are not commercially viable as photointeractive materials, as current production (restricted to Japan) involves a very hazardous and unreliable synthetic approach. Low molecular weight oligosilanes can be formed under mild conditions, with reactive silane (Si-H) residues. We propose to utilize these oligo(hydrido)silanes as versatile precursors to a wide variety of new photoconductor materials with xerography and LED applications. Computer aided molecular design (CAMD) will be employed to select rational synthetic targets for oligosilane elaboration. Chemical modification at the Si-H bond will access numerous new oligosilanes and permit development of a wide variety of hybrid polymeric systems with novel polymer architectures; applications may include photoactive elastomers, thermoplastics and sensor materials, graft/block copolymers, LED display devices and controlled porosity thin films, fibers and monolithic bodies.

Keywords: Polymers, Displays, Photosensitive

289. **POLYPHOSPHAACETYLENES: NEW CONDUCTING HYBRID ORGANIC-INORGANIC MATERIALS**
$300,000
DOE Contact: M. J. Katz, (202) 586-5799
SNL Contact: C. L. Renschler, (505) 844-0324

The purpose of this project has been to develop linear polyphosphaacetylenes, [P=C(R)]n, as a new class of conducting hybrid organic-inorganic polymer. Thermal, photochemical and transition metal-mediated metathesis polymerization of phosphaacetylene monomers are viewed as viable routes to the generation of formable polymeric materials with metal-like electrical conductivities. Expertise in computer aided molecular design has provided theoretical evidence that high electrical conductivities are achievable, as the organophosphorus polymeric backbones are predicted to be highly coplanar. Such materials should show conductivities superior to other conducting polymers reported to date. Synthetic efforts have established an efficient methodology to monomer fabrication, and design and synthesis of metathesis catalysts is underway.

Keywords: Polymer, Conductive, Synthesis

290. **NEW ADHESIVE SYSTEMS BASED ON FUNCTIONALIZED BLOCK COPOLYMERS**
$228,000
DOE Contact: M. J. Katz, (202) 586-5799
SNL Contact: J. H. Aubert, (505) 844-4481

The need to control and optimize the properties of polymer/solid interfaces is critical in a host of technologies. Often the adhesive strength of the interface, the resistance to moisture, and the ability to transfer stress through the interface are critical to the overall performance of the product. A few specific examples include layers of conducting metals and polymer dielectrics in electronic packaging, filled rubber systems such as are used in the manufacture of tires, and structural adhesives. Recent evidence indicates that the adhesive failure in these interfaces often occurs a very short distance into the polymer matrix, typically 10-100 nm. This interphase region has proved difficult to design from first principles. Primer formulations involving small molecule coupling agents often must be tailored by a time consuming and inefficient trial and error process with very little underlying strategy. For many problems, adhesion is currently achieved by roughening surfaces in order to develop mechanical interlocking. This often involves the use of harsh chemicals which are hazardous to the environment. We propose to design and test new adhesive systems based on block copolymers, where one block (A) attaches to the surface while the second block (B) is compatible with and bonds to the polymeric matrix. An important advantage of block copolymers is that the B block can easily be made long enough to span the weak region of 10-100 nm and form a strong interlock with the matrix. We believe that these systems will lead to improved adhesion, more systematic design of the interphase region, and a decreased dependence on mechanical roughness and the environmentally unfriendly processes which are currently required.

Keywords: Adhesive, Polymer

291. **ENGINEERED MONODISPERSE POROUS MATERIALS**
$321,000
DOE Contact: M. J. Katz, (202) 586-5799
SNL Contact: J. H. Aubert, (505) 844-4481

Porous materials are available with pore sizes ranging from 1's of Å to 100's of microns and beyond. Beyond 15Å it becomes difficult to obtain complete control over pore size, size-distribution, and ordering. We propose to use the novel properties of block copolymers to create monodisperse, controllable, ordered porous materials spanning the mesoporous range (20-500Å). Block copolymers consist of homopolymers chemically attached at their ends. These polymers want to phase separate from each other but are limited by the chemical attachment. The result is well-ordered, monodisperse, meso-size domains of one polymer surrounded by the other. We plan to make block copolymers where one phase can be crosslinked and the other phase can be chemically or thermally removed. This would give the desired controllable mesoporous materials. Block copolymer phase separation also gives a variety of architectures, including spherical, cylindrical, tetrahedral, and lamellar. These would lead to unique mesoporous architectures. In conjunction with the synthesis of these materials, we will be modeling our block copolymers using density functional theory, which can predict architecture based on the chemical and physical aspects of the block copolymer. This modeling will be useful in saving time and material. The synthetic technique we will use is called Ring Opening Metathesis Polymerization, and allows us to have tremendous control over polymer chain length, block ratios, and chemical composition. This control leads directly to control of the pore size and architecture. We will be analyzing our block copolymer materials to determine domain size, distribution, ordering, and architecture, both before and after pore formation. Both the modeling and synthesis of these well ordered, mesoporous, monodisperse materials is a novel approach to mesoporous material formation. These types of materials will have impact on several technology areas, including polymer separations, gas separations, remote sensor and bio-sensor materials, and catalyst supports.

Keywords: Polymer, Porous

292. **LOW-DIELECTRIC AND HIGH-TEMPERATURE FILMS FOR MULTICHIP MODULES**
$175,000
DOE Contact: M. J. Katz, (202) 586-5799
SNL Contact: J. H. Aubert, (505) 844-4481

Thin low-dielectric and high-temperature films are used to separate multiple layers of patterned conductors in multichip module packaging. Significant improvements in processing speed could be obtained from the use of lower dielectric materials. We propose to obtain lower dielectric materials by preparing porous polymer films. Since the dielectric constant of air is close to that of vacuum, and much lower than any polymer, the porosity will lower the average dielectric constant of the film. To be able to prepare thin (<100 □m) films requires the use of very small-celled foams. We have substantial experience in this area, and have previously demonstrated the ability to prepare polymer films with cell sizes under 0.1 μm. In addition, porosities as high as 90 percent are attainable even with this small cell size. Conceivably, the dielectric constant of such a film will be reduced by as much as 90 percent of the difference between that of the bulk polymer and that of air. We propose to develop microcellular polyimide foams for this application. Polyimide is a high-temperature polymer used frequently for thin film dielectrics. In addition, we propose to develop the required processing techniques to allow us to concurrently prepare the foam and process it into its final form. This will involve the development of a process to spin-coat microcellular foams.

Keywords: Polymer, Dielectric, Thin Film

MATERIALS STRUCTURE AND COMPOSITION

293. **ADVANCED ANALYTICAL METHODS FOR MATERIALS RESEARCH**
$1,272,000
DOE Contact: R. Staffin, (202) 586-7590
SNL Contact: H. J. Saxton, (505) 845-8739

This project consists of several tasks, each of which is a relatively independent analytical methods development activity including: advanced microanalysis development; chemometrics; surface polymer contamination characterization; by x-ray diffraction in thin films; metal impurity characterization on semiconductor surfaces; sensor development and x-ray and ion beam tomography.

Keywords: Analysis, Diffraction, Tomography

294. **ADAPTIVE SCANNING PROBE MICROSCOPIES**
$417,000
DOE Contact: M. J. Katz, (202) 586-5799
SNL Contact: T. A. Michalske, (505) 844-5829

In the short time that Scanning Probe Microscopies (SPM) have been on the scene, they have demonstrated great potential to contribute to fundamental materials science problems, process science studies and new approaches to production quality control. However, the simple data acquisition and analysis procedures that are currently used severely restrict our ability to extract quantitative information regarding, for example, atomic scale rate processes or local chemical compositions. In this project we will develop a new paradigm for operating SPMs whereby the microscope adapts its data acquisition to focus on the most important features of the structure under examination. Currently, SPMs scan a region of material by devoting an equal amount of time to all areas of the image. However, for most materials problems, only the data that are associated with specific features such as defects or possibly nucleation centers are used to analyze the state of the material. An adaptive scanning approach could be used to locate, track and image features of interest without the overhead of acquiring data over the entire sample region. By using this approach, the time required to collect information will be decreased by several orders of magnitude, which will enable us to study kinetic processes with unprecedented microscopic-real-space resolution. In addition, current SPMs do not make use of the range of electronic data they can locally generate, so that chemical information on an atomic scale is usually not acquired. Pattern recognition techniques will be applied to these local data to distinguish and recognize features based on local electronic properties of the surface. The ability of the instrument to recognize specific features will greatly increase the operators ability to examine and analyze complex materials structures. This new capability will place us in a strong position to apply SPMs to a wider range of technologically important problems such as catalysis, corrosion, lubrication and biological processes.

Keywords: Scanning Probe Microscopy, Surfaces

295. **CHARACTERIZATION AND CORRELATION OF PHYSICAL PROPERTIES OF CERAMICS THROUGH ORIENTATION IMAGING MICROSCOPY**
$122,000
DOE Contact: M. J. Katz, (202) 586-5799
SNL Contact: P. F. Green, (505) 845-8929

This program is intended to be the proof-of-principle of an innovative approach to characterizing polycrystalline materials through orientation imaging microscopy. We propose to explore the use of the backscattered electron Kikuchi pattern (BEKP) technique for performing orientation imaging microscopy. This technique provides the crystallographic misorientation between adjoining grains, which should allow us to develop a more complete understanding of the relationship between grain boundary structure and properties, and the overall properties of a polycrystalline body. We are specifically interested in the relationship between the crystallographic misorientation and the fracture behavior of materials; however, crystallographic misorientation data are potentially as important for other properties and behavior.

Keywords: Microscopy, Microstructure

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

296. **ENERGETIC MATERIAL CENTER**
$106,000
DOE Contact: R. Staffin, (202) 586-7590
SNL Contact: D. J. Allen, (505) 845-9624

This project provides funds to perform collaborative program formulations with Lawrence Livermore National Laboratory in energetic materials, high explosives, pyrotechnics, and rocket fuels to fulfill the common mission goals of Science Based Stockpile Stewardship and Product Realization.

Keywords: Energetic Materials

297. **COMPUTATIONAL SOLID DYNAMICS**
$2,716,000
DOE Contact: R. Staffin, (202) 586-7590
SNL Contact: E. H. Barsis, (505) 845-8938

The purpose of this project is to develop and validate computational models for the response of materials to a spectrum of dynamic and quasi-static loading conditions that are required in the design of nuclear components and systems.

Keywords: Models, Stress

298. **APPLIED MATERIALS & MECHANICS COLLABORATIONS**
$635,000
DOE Contact: R. Staffin, (202) 586-7590
SNL Contact: D. L. Lindner (510) 294-3306

This project supports thirty-one separate projects in which Sandia staff collaborate with graduate students. Projects include work on low flux/low residue solders, development of hard tribological materials for stronglink application, sensor development, modeling of materials response in mixed environments, development of corrosion-resistant glasses for hermetic seals, modeling of composite materials, and development of advanced polymeric materials.

Keywords: Solders, Tribological, Corrosion

299. **DEVELOPMENT OF MORE EFFICIENT POWER SOURCES**
$1,044,000
DOE Contact: R. Staffin, (202) 586-7590
SNL Contact: D. L. Mangan, (505) 845-9538

The purpose of this project is to: (1) develop a state-of-the-art carbon anode for lithium ion rechargeable batteries and demonstrate its performance by building a prototype that demonstrates performance and manufacturability; (2) develop materials, device design and a working prototype of an advanced double layer capacitor; and (3) evaluate self-discharge kinetics to permit precise lifetime projections for Lithium/Titanium Carbide, Li/TC, Batteries. The project involves collaboration with domestic Lithium/Titanium Carbide producers to transfer our fundamental understanding of this system, enabling them to enter the growing market for high reliability, long life Lithium/Titanium Carbide batteries.

Keywords: Batteries, Carbon, Reliability

300. **BASIC SCIENCE OF MATERIALS STABILITY**
$1,829,000
DOE Contact: R. Staffin, (202) 586-7590
SNL Contact: P. L. Mattern, (505) 845-9490

The purpose of this project is to: (1) develop and apply atomic- and molecular-level microscopies, spectroscopies, and theoretical models in order to examine fundamental materials processes that control phenomena including: interfacial adhesion, lubrication, wear, thermal stability, thin-film and surface kinetics, radiation effects, corrosion, hydrogen effects, curing, fracture, and chemical and physical vapor deposition processes; (2) develop scientific basis for design, manufacture and application of small smart products; (3) transfer degradation resistant/stable materials technology to DOE defense program applications and to U.S. advanced materials industries and develop new models for predicting useful lifetimes for currently used materials and structure.

Keywords: Surfaces, Microscopy

301. **ADVANCED MATERIALS CHARACTERIZATION SCIENCE**
$1,006,000
DOE Contact: R. Staffin, (202) 586-7590
SNL Contact: P. L. Mattern, (505) 845-9490

The purpose of this project is to: (1) maintain, utilize and develop new state-of-the-art materials analysis/characterization techniques of general applicability to microelectronics photonics, materials research, energy, advanced testing, and weapons programs; (2) develop new approaches to test, quantify and understand/predict the performance of materials/components used in advanced weapon systems under normal or extreme conditions; (3) develop ultra-high resolution accelerator microbeam methods and utilize for submicron radiation exposure /imaging of integrated circuits (ICs) and components to be used in radiation environments (e.g., space, fission/fusion reactors, nuclear battlefield, etc.); (4) invent/perfect advanced atomic-level in situ and ex situ diagnostics based on x-ray diffraction and atom-force microscopy; (5) initiate new programs utilizing advanced characterization techniques and/or transfer technology to other Defense Program (DP) lab/industry; (6) publish/patent new techniques and communicate results to Defense Program.

Keywords: Microbeams, Radiation, Diffraction

302. **PHOTONICS TECHNOLOGY**
$1,206,000
DOE Contact: R. Staffin, (202) 586-7590
SNL Contact: A. D. Romig, (505) 844-8358

This project establishes exploratory investigations into new concepts for photonic structures, devices, and systems. These investigations are foundational to the development of photonic technologies that will replace present day optical, electronic, electro-mechanical, and mechanical components and systems and will offer more effective, efficient, compact, rugged, radiation hard, and electro-magnetic (EMP) resistant components.

Keywords: Photonics

303. **ELECTRONIC CERAMICS**
$899,000
DOE Contact: R. Staffin, (202) 586-7590
SNL Contact: H. J. Saxton, (505) 845-8739

The purpose of this project is to advance the chemistry and physics basis for the fabrication and use of electrically and optically active ceramics. One goal of this project is to investigate the basic chemistry of sol-gel processes in order to develop an intelligent and versatile approach to thin-film fabrication. Specific goals are to: (1) develop processing methods for producing optimized microstructures for ferroelectric thin films; (2) determine microstructures that enhance or suppress 90 degree domain switching in ferroelectric films; (3) investigate effects of thin-film stresses and microstructure on piezoelectric activity; (4) determine the relative contributions of various cations to ferroelectricity in perovskites; (5) determine defects that lead to intrinsic luminescence in zinc oxide phosphors; (6) investigate dopants to enhance red, green and blue luminescence in zinc oxide; (7) investigate degradation mechanisms in perovskite thin films.

Keywords: Ceramics, Ferroelectric, Piezoelectric

304. **ULTRAHARD MATERIALS RESEARCH**
$594,000
DOE Contact: R. Staffin, (202) 586-7590
SNL Contact: H. J. Saxton, (505) 845-8739

The purpose of this project is to develop and enhance research capabilities in the synthesis, characterization, and materials development that relate to nitrides, carbides, diamond, and diamond-like carbon. Specific tasks include: (1) investigate the mechanisms of film growth; (2) characterize the mechanical, electrical, and atomic structure of these materials; and (3) explore weapons and dual-use applications for these materials.

Keywords: Nitrides, Diamond

305. **IMPURITY EFFECTS ON INTERFACES**
$997,000
DOE Contact: R. Staffin, (202) 586-7590
SNL Contact: H. J. Saxton, (505) 845-8739

The major objective of this project is to quantify the permeation and trapping of impurities in metals, alloys, and inorganic materials and to relate these phenomena to embrittlement of grain boundaries, bi-crystals, coatings, and engineering materials. Theoretical models are developed to describe adhesion of metal films on ceramic oxide surfaces.

Keywords: Interfaces, Reliability, Films

306. **MATERIALS AGING & RELIABILITY**
$1,155,000
DOE Contact: R. Staffin, (202) 586-7590
SNL Contact: H. J. Saxton, (505) 845-8739

This project provides significant advances in the science-based stockpile stewardship of non-nuclear components by combining the interdisciplinary capabilities of materials science, high performance computing, integrated sensors, and advanced engineering simulation. The focus of the project is to advance the understanding of microstructural mechanisms which control the reliability and performance of materials. This understanding is translated into a mathematical description to allow improved predictive capabilities based on the development/deployment of integrated sensors and/or advanced simulations. An important goal is to support materials science work that is combined into projects that draw support and leverage from research. The combination of material (mathematical) modeling, and high performance computing and advanced engineering simulation transfers materials understanding into practical predictor tools that can be applied to the stockpile, as well as to commercial products and applications. Specific sensor development can then be based on the fundamental understanding of the materials behavior of the sensor as well as the signature of the specific event/degradation being sensed.

Keywords: Prediction, Models, Reliability

307. **ENGINEERING SCIENCES RESEARCH**
$6,157,000
DOE Contact: R. Staffin, (202) 586-7590
SNL Contact: P. J. Hommert, (505) 844-3449

The project is divided into four main elements that constitute the work areas within engineering sciences. These elements are Computational Methods for Engineering Analysis, Material Mechanics, Experimental Mechanics, and Manufacturing and Material Processes. Under each of these main program elements there are specific research tasks that are intended to further the engineering science capabilities available to apply to the laboratories applications. Specific projects include: (1) develop computational methods and models of energetic materials to predict multiphase effects; (2) develop new techniques for the prediction of lifecycle reliability using material response models for the prediction of aging and fatigue; (3) develop new models of polymer response for analysis of curing and shrinkage of seals and other components to enable improved design; (4) develop new material response models that bridge microscopic to macroscopic descriptions; (5) develop and apply experimental methods to validate advanced material response models; (6) implement advanced material response characterization into models of welding, stamping, material removal and coatings for advanced manufacturing processes; (7) improve the capability for finite element analysis of large deformations and material non-linearities through contact algorithms, shell elements and adaptivity; (8) develop gridless solver technology for application to component design and performance analysis; (9) develop the capability to implement non-deterministic and optimization simulation concepts in finite element analysis; (10) develop advanced fluid mechanics capabilities for the description of turbulent eddies for describing fire propation; (11) develop the capability to predict the response of cellular foams and distended materials for crash applications; and (12) develop models of energetic materials for predicting deflagration to detonation.

Keywords: Models, Mechanics, Processing

308. **GAS SEPARATION OF FULLERENE MEMBRANES**
$300,000
DOE Contact: M. J. Katz, (202) 586-5799
SNL Contact: J. E. Schirber, (505) 844-8134

Industrially important gas separation processes such as the removal of nitrogen from natural gas and separation of nitrogen and oxygen consume enormous amounts of energy. Most membrane separation processes are based on amorphous polymeric films which contain a broad distribution of pore sizes through which gas molecules diffuse at different rates. We have discovered that the lattice of fullerene C_{60} can function as a permeation barrier. Since the diffusion pathway is precisely defined by the channels between interstitial sites, we expect that the lattice will exhibit large separation factors for appropriate gas pairs and that the permeation rate can be made very high for thin films. In this study we propose to characterize the permeation process, model the separation process, prepare membranes by the sublimation of thin fullerene films on suitable substrates, measure the resulting separation factors and permeation rates, and address engineering aspects of preparing a functional membrane system.

Keywords: Separation, Membrane, Fullerene

309. **PbO-FREE COMPOSITES FOR LOW TEMPERATURE PACKAGING**
$359,000
DOE Contact: M. J. Katz, (202) 586-5799
SNL Contact: P. F. Green, (505) 845-8929

We will develop a new class of inorganic materials that will have the requisite thermal and chemical properties to replace PbO-solder glasses currently used in a variety of low temperature packaging applications. These new materials will be composites of low temperature, chemically stable glasses and low expansion, chemically compatible ceramics. Composites will be designed with thermal contraction coefficients between 70 and 100 x 10^{-7}/°C and seal temperatures below 450°C so that they can replace PbO-solder glasses used to seal flat panel displays, alumina sensor packages, and other hermetic packages.

Keywords: Solder, Lead-free, Packaging

310. **DEMONSTRATION OF MOLECULAR-BASED TRANSISTORS**
$317,000
DOE Contact: M. J. Katz, (202) 586-5799
SNL Contact: R. F. Clough, (505) 844-3492

Photonics and electronics technologies continue toward miniaturization, but these technologies are based largely on main-group semiconductors. An alternative approach lies in using macromolecular building blocks to build very small circuits. Research in the area of conducting polymers represents one of the first forays of chemists into this arena. A crucial element in any logic circuit is a transistor, in which a base current regulates the current between collector and emitter. We propose to develop optically-gated organic transistors based on photochromic organic conducting polymers. The operation of such a device would parallel that of a normal transistor, but the current switching would depend on both the electronic and structural changes in the polymer induced by photoreactions instead of a base current. Such a device represents a new method for integration of electronic and photonic processing. Intensive research on conducting polymers has narrowed the field of candidates viable for device applications. Polythiophene is an environmentally stable conducting polymer for which very high conductivities have been reported. In addition, many different routes are available to synthesize the required monomers and polymers. These features combine to make polythiophene an excellent candidate for device applications, and thus polythiophene derivatives will be the initial focus of our efforts. A photochromic compound is one that isomerizes from an initial form A to a different form B when irradiated with light of wavelength 1, and B in turn isomerizes to A when irradiated with light of wavelength 2. The conformational and electronic differences between such photoisomers will provide the mechanism for switching conductivity on and off in the proposed polymers. The overall goals of this project are (1) to provide examples of photoswitched conductivity in organic molecules and (2) to use this ability to fabricate microscale photoswitches and demonstrate their use in binary arrays (memory devices).

Keywords: Polymers, Transistors, Molecular

311. **NANOCOMPOSITE MATERIALS BASED ON HYDROCARBON-BRIDGED SILOXANES**
$442,000
DOE Contact: M. J. Katz, (202) 586-5799
SNL Contact: T. A. Ulibarri, (505) 844-5279

Silicones [polydimethylsiloxane (PDMS) polymers] are environmentally safe, nonflammable, weather resistant, thermally stable, low Tg materials that are attractive for general elastomer applications because of their safety and performance over a wide temperature range. However, PDMS is inherently weak due to its low glass transition temperature (Tg) and lack of stress crystallization. Fortunately, reinforced materials with suitable properties can be generated by mechanically blending PDMS polymers with pyrogenic silicas. While the U.S. is still the major producer of silicones, foreign competitors are gaining market share due to their improved technology and product quality as they duplicate and modify U.S. technology. Since silicone elastomers are used in numerous military and civilian applications, it is critical that significantly new manufacturing technologies be developed in the U.S. Recent work has indicated that two other ways to enhance elastomer strength are the use of bimodal polymer distributions and the introduction of hydrocarbon fragments into the polymer matrix. However, the origin of the improved properties cannot be fully understood and investigated in the systems presently available. We have devised a method which, for the first time, will allow us to completely control the length and identity of the short chain molecule and the hydrocarbon linkage. PDMS-based composite materials containing a variety of alkylene-and arylene-bridged polysilsesquioxanes will be synthesized in order to probe short chain and linkage effects in bimodal polymer networks. Monte Carlo simulations will be performed as a function of chain length to predict the optimal chain lengths required for maximum reinforcement. PRISM calculations will be performed on the PDMS/silsesquioxane blends as a function of molecular weight in order to understand the phase separation characteristics of the system. The silsesquioxane-PDMS networks will be synthesized and evaluated both as unfilled materials and as sol-gel generated silica-filled materials. Analysis of the mechanical properties of the materials will be coupled with molecular and structural analysis in order to determine structure/property relationships.

Keywords: Composite, Polymer

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

312. **MC4300 NEUTRON TUBE**
$329,000
DOE Contact: R. Staffin, (202) 586-7590
SNL Contact: D. J. Bohrer, (510) 294-3111

This project provides funds to design and develop in a timely and cost effective manner, a universal neutron tube satisfying the requirements of all stockpile weapons by the year 2002; specifically to evolve a design which minimizes fabrication parts and processing through studies to advance technologies such as diffusion bonding, ion optics, and cermets.

Keywords: Processing, Joining, Cermets

313. **SMARTWELD II**
$1,985,000
DOE Contact: R. Staffin, (202) 586-7590
SNL Contact: D. L. Lindner (510) 294-3306

This project continues the development of SMARTWELD. SMARTWELD is a concurrent engineering system which integrates product design and processing decisions within an electronic desktop engineering environment. It is being developed to provide the designer with transparent access to people, information, tools and past experience. Empirical understanding, along with process models, are synthesized within a knowledge-based system to identify the most optimal fabrication procedures based on cost, schedule, performance or environmental impact. Integration of the process simulation tools with design tools will enable the designer to assess a number of design and process options on the computer rather than on the manufacturing floor. Task models and generic process models are being embedded within user friendly Graphics User Interfaces, GUIs, to more readily enable the customer to use the SMARTWELD system without extensive training. The integrated system architecture under development will provide interactive communications and shared application capabilities across a variety of workstation and PC-type platforms either locally or at remote sites.

Keywords: Welding, Models

314. **MANUFACTURING TECHNOLOGY**
$1,859,000
DOE Contact: R. Staffin, (202) 586-7590
SNL Contact: D. L. Lindner (510) 294-3306

This project consists of three major efforts: (1) IMPReS which includes the integrated modeling and processing of resin-based structures and the extension of the SmartWeld paradigm 12 to polymer-based materials and structures; and (2) Advanced Process Controllers, which includes the development of controller hardware for brilliant real-time model-based control of manufacturing processes; and (3) Assembly Scripting which involves development of automatic assembly planning and scripting algorithms and systems.

Keywords: Polymers

315. **ELECTRONIC AND MICROELECTROMECHANICAL SYSTEMS (MEMS) COMPONENTS**
$1,416,000
DOE Contact: R. Staffin, (202) 586-7590
SNL Contact: W. R. Reynolds, (505) 844-3087

This project provides funds to: (1) develop stronglinks in several steps starting with use of micromachining technology to develop parts, then integrate parts to make stonglink; (2) develop all-quartz and integrated silicon-quartz resonators for small clocks and sensors for DOE, military and commercial applications; and (3) develop and characterize low temperature weaklink capacitor and coil and develop/characterize fiber optic sensors.

Keywords: Micromachining, Capacitors, Sensors

INSTRUMENTATION AND FACILITIES

316. **MATERIALS PROCESSES FOR MANUFACTURING**
$703,000
DOE Contact: R. Staffin, (202) 586-7590
SNL Contact: D. L. Lindner (510) 294-3306

This project will consist of two areas to enhance manufacturing capabilities: Virtual Reality and Development Plating Facility. *Virtual Reality* - This project will build on recent developments at Sandia. Free-form rapid prototyping, robotics, on-machine inspection coupled with sophisticated solid models and process models are rapidly emerging areas that will be evaluated and improved. *Development Plating Facility* - Finalize design and complete construction of new Development Plating Facility in the Advanced Manufacturing Process Center (AMPL).

Keywords: Prototyping, Models, Plating

LAWRENCE LIVERMORE NATIONAL LABORATORY

317. **ENGINEERED NANOSTRUCTURE LAMINATES**
$1,800,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LLNL Contact: Troy W. Barbee, Jr., (510) 423-7796

Multilayers are man-made materials in which composition and structure are varied in a controlled manner in one dimension during synthesis. Individual layers are formed using atom by atom processes (physical vapor deposition) and may have thicknesses of from one monolayer (0.2 nm) to hundreds of monolayers (>100 nm). At this time more than 75 of the 92 naturally occurring elements have been incorporated in multilayers in elemental form or as components of alloys or compounds. In this work deposits containing up to 225,000 layers of each of two materials to form up to 500□m thick samples have been synthesized for mechanical property studies of multilayer structures.

These unique man-made materials have demonstrated extremely high mechanical performance as a result of the inherent ability to control both composition and structure at the near atomic level. Also, mechanically active flaws that often limit mechanical performance are controllable so that the full potential of the structural control available with multilayer materials is accessible. Systematic studies of a few multilayer structures have resulted in free-standing foils with strengths approaching those of whiskers, approximately 70 percent of theory. Also, new mechanisms for mechanically strengthening materials are accessible with nanostructure laminates.

Applications now under development include: coatings for aircraft gas turbine engines; EUV, soft X-ray and X-ray optics spectroscopy and imaging; high performance capacitors for energy storage; capacitor structures for industrial applications; high performance tribological coatings; strength materials; integrated circuit interconnects; machine tool coatings; projection x-ray lithography optics.

Keywords: Thin Films, Multilayer Technology

318. **SOL GEL COATINGS**
$335,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LLNL Contact: I. M. Thomas, (510) 423-4430 and J. Britten, (510) 423-7653

We continue to investigate the preparation of multilayer sol-gel high reflection (HR) coatings using colloidal SiO_2 with either HfO_2 or ZrO_2. We have found that the incorporation of an organic polymer binder such as polyvinyl alcohol or polyvinyl pyrolidinone into the high index component has resulted in an increase in the damage threshold and a decrease in the number of layer pairs required for high reflection.

A laboratory size meniscus coater was evaluated and found to produce mirrors of high optical performance and adequate damage threshold. This is now the preferred method of application, and a large machine capable of producing Beamlet and NIF size mirrors is to be delivered in early FY 1994.

Keywords: Sol Gel Coatings, Meniscus Coater, HR Coatings

319. **KDP GROWTH DEVELOPMENT**
$900,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LLNL Contact: J. J. DeYoreo, (510) 423-4240

Potassium dihydrogen phosphate (KDP) and its deuterated analog (DKDP) are important nonlinear crystals used both for frequency conversion as well as for a large Pockels cell. These crystals are very expensive, due in part to the very long times required to grow large boules (2-3 years) and the cost of D_2O for growing DKDP. We are developing alternative growth techniques to dramatically increase the growth rate of these crystals.

We recently adopted a new growth technique with which we are growing both KDP and DKDP at 10 to 20 times the rates achieved with conventional methods. We have grown crystals up to almost 20cm on a side and have shown that crystals grown by this method are of exceptionally high quality. We are now working with crystallizers that are large enough to grow $50x50x50cm^3$ crystals. We will continue to grow crystals at the 10-15cm scale in order to determine optimum hydrodynamic and regeneration conditions, and to understand the effects of impurities and stresses in seed crystals on the stability of the growing crystal face.

Keywords: KDP, Nonlinear Crystals, Crystallization

320. **ICF CAPSULE ABLATORS VIA PLASMA POLYMERIZATION**
$500,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LLNL Contacts: R. Brusasco, (510) 422-3111, R. Cook, (510) 422-3117 and S. Letts, (510) 422-0937

Our group uses plasma polymerization to prepare conformal coatings of organic polymer for use as ICF capsule ablators. These coatings have some unique and stringent requirements, such as a surface roughness of the order of 10 nm or less at a coating thickness of several tens of micrometers and the strength to hold fuel pressures of from 50 to 100 atmospheres. The project supports development of methods to incorporate high Z dopants (e.g., germanium) into the polymer structure. The project also supports basic studies to understand the mechanism of roughness evolution during deposition and methods to enhance rate without seriously affecting roughness. The incorporation of beryllium into the ablator is also a focal point for exploratory research. A coating system with a computer interface aids the optimization of the coating process.

Keywords: Plasma, Polymer, Germanium, Beryllium, Fusion, Roughness

321. **VICARIOUS NUCLEOPHILIC SUBSTITUTION CHEMISTRY**
$400,000*
DOE Contact: G. J. D'Alessio, (301) 903-6688
LLNL Contact: R. L. Simpson, (510) 423-0379

Vicarious nucleophilic substitution chemistry is being used to synthesize energetic materials. New explosive molecules are being synthesized. Alternate routes to existing molecules, such as TATB, have been developed.

Keywords: Examination, Explosive, Energetic, TATB

322. **CHEETAH THERMOCHEMICAL CODE**
$190,000*
DOE Contact: G. J. D'Alessio, (301) 903-6688
LLNL Contact: R. L. Simpson, (510) 423-0379

A thermochemical code for the prediction of detonation performance is being developed. In addition to detonation performance, thermochemical calculations of impetus and specific impulse for propellant applications may also be made.

Keywords: Examination, Explosive, Energetic, TATB

323. **HARD TARGET PENETRATOR EXPLOSIVE**
$900,000*
DOE Contact: G. J. D'Alessio, (301) 903-6688
LLNL Contact: R. L. Simpson, (510) 423-0379

New explosives are being developed for hard target penetrators. The goals include insensitivity to shock loading and significantly higher energy density than that of currently available materials

Keywords: Explosive

324. **INJECTION MOLDABLE EXPLOSIVES**
$220,000*

Precision explosive materials that may be injection molded are being developed for precision applications.

Keywords: Explosive

*General energetic materials-related input. This activity is jointly funded (50:50) by DOE DP and the DoD.

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

325. **INTERFACES, ADHESION, AND BONDING**
$460,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LLNL Contact: Wayne E. King, (510) 423-6547

Our experimental effort is producing results that are directly comparable with theoretical calculations. We are investigating planar metal/metal interfaces and metal/ceramic interfaces (in anticipation of improvements in the theory) of well defined misorientations. In order to span the entire range of length scales described above, macroscopic bicrystals a few millimeters thick, with interfacial areas on the order of a square centimeter, will be required. In order to obtain such bicrystals, we plan to employ the diffusion bonding approach. An ultra-high-vacuum diffusion bonding machine has been developed in parallel with this research project.

Keywords: Interfaces, Bonding, Electronic Structure

326. **LASER DAMAGE: MODELING AND CHARACTERIZATION**
$400,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LLNL Contact: M. R. Kozlowski, (510) 424-5637

We have been working to understand the damage mechanism in thin film coatings used on Nova and other ICF lasers, with the ultimate goal of improving the damage threshold in coatings for future laser systems. We have utilized atomic force microscopy (AFM) and focused ion-beam (FIB) cross sectioning to characterize laser damage as well as the laser conditioning process which allows coatings to sustain higher laser fluences. We have shown that pre-existing nodular defects are the initiation points for most laser damage. The laser conditioning process is associated with the gentle ejection of these nodules to produce benign pits.

We have modeled the laser induced electromagnetic fields at "typical" nodular defects in a simple quarter-wave dielectric mirror coating. The model results demonstrated that large field enhancements are produced by these defects, which are composed of the same dielectric material as the coating materials. We are not calculating the thermal-mechanical response of these defects. Work to date has only looked at the normal incidence illumination case. With recent electromagnetics code advancements, we will now be able to model the more interesting non-normal incidence case.

Keywords: Coatings, Atomic Force Microscopy, Laser Damage

327. **KDP CHARACTERIZATION**
$400,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LLNL Contact: J. J. DeYoreo, (510) 423-4240

We require very large, high quality crystals of potassium dihydrogen phosphate (KDP) and its deuterated analogue (DKDP) for present and advanced high power lasers in the ICF Program. The performance of these crystals is limited by strain which induces anomalous birefringence and wavefront distortion and by defects which result in laser-induced damage at low laser fluence. The level of internal strain and the laser damage threshold are the most important factors in determining the yield of useable plates from an "as-grown" boule. Our goal has been to identify the defects which are the source of strain and damage in KDP and DKDP, understand how these defects are generated, and how to avoid them during the growth process.

We are using optical scatterometry, spectroscopy, x-ray typography, crystal growth and chemical analysis to determine the distribution of defects in crystals and their relationship to the growth process. We have been able to relate strain to specific defects using these methods and are now investigating, *in situ*, the process of laser damage as well as laser and thermal annealing.

Keywords: KDP, Strain, Crystal

INSTRUMENTATION AND FACILITIES

328. **SCANNING TUNNELING MICROSCOPY (STM) AND ATOMIC FORCE MICROSCOPY (AFM)**
$250,00
DOE Contact: G. J. D'Alessio, (301) 903-6688
LLNL Contact: W. Siekhaus, (510) 422-6884

A small building standing separate from noise-generating machinery and hence having a low natural vibration background is used to house all scanning probe instrumentation. The 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 non-contact AFM and STM, and an ultra-high vacuum instrument that can perform non contact AFM and STM measurements and STM spectroscopy (STS) have been used for the following studies in FY 95.

- Uranium Hydriding - Understanding the early stages of uranium hydriding is of paramount importance in science based stockpile stewardship. The UHV STM/AFM has been used to determine the initial stages of uranium hydriding by exposing a clean uranium surface to hydrogen and monitoring by AFM the change in surface morphology induced by hydriding. We have in this way identified with nm resolution the sites at which hydriding starts and monitored the growth of hydride at these sites as a function of time.

- Light-emission from Nanoscale Silicon Particles - Nm-scale clusters of Si have been deposited by laser ablation and by evaporation in a noble gas atmosphere onto the basal plane of graphite, and analyzed by STM to determine their size distribution and by optical spectroscopy to study the physical basis for light-emission from Si clusters and from oxidized Si.

- Dissolution Rate of Uranium Oxide - The transport of radioactive material from a long-term storage site into ground water is of concern in designing long-term storage facilities for nuclear waste material. The dissolution of uranium oxide by ground-water is a rate limiting step in this process. This dissolution rate has been determined by AFM on single crystal uranium oxide by monitoring the rate of recession of the UO_2 surface with reference to a gold marker. Moreover, the nm-scale morphology of the dissolution attack has been identified, showing that some crystallographic directions are preferentially attacked.

Keywords: NDE, Chemical Reaction, Uranium Hydriding, Stockpile Stewardship, Uranium Oxide Dissolution, Nuclear Waste Disposal, Etching, Si Light Emission

329. **TREATMENT OF WASTE AND WATER WITH CARBON AEROGEL ELECTRODES**
$425,000
DOE Contact: Douglas Gish, DP 42, (202) 586-1741
LLNL Contact: J. C. Farmer, (510) 423-6574

Carbon aerogel capacitive deionization (CDI) has been developed as a non-polluting, energy-effecient, cost-effective alternative to ion exchange, reverse osmosis, electrodialysis, and evaporation. This process is believed to offer dramatic advantages in terms of both waste minimization and processing cost to DOD and DOE. The benefits of this project include the elimination of secondary wastes associated with the chemical regeneration of ion exchange columns; the avoidance of flow through porous media as required by reverse osmosis (RO); the elimination of expensive and troublesome high-pressure pumps associated with RO; and the reduction of the required energy consumption to process water. This process could help facilitate low-cost desalination of brackish waste water for reclamation. This SERDP project has been recognized with a 1995 R&D100 Award.

Keywords: Capacitive Deionization

330. **TRILAYER JOSEPHSON JUNCTIONS (TECHNOLOGY TRANSFER INITIATIVE)**
$375,000
DOE Contact: W. T. Chernock, (301) 586-7590
LLNL Contact: R. H. Howell, (510) 422-1977

In this TTI Lawrence Livermore National Laboratory is working with Varian Associates to lay the groundwork for the routine, reproducible fabrication of high-temperature superconducting trilayer structures. The project was completed at the end of FY 1995. Project goals were to: (1) identify high temperature superconducting materials, metallic and insulating barrier materials and associated substrate and electrode materials for engineered trilayer structures that can provide Josephson Junction devices with desired characteristics for sensor or electronic circuit use; (2) identify and test potentially useful analysis techniques and to provide data appropriate for the validation and analysis of the input materials, trilayer structures and completed JJ devices; and (3) to integrate the analysis results with the existing Varian data base to optimize the growth and fabrication process to obtain more reproducible devices across each chip and from chip to chip. All milestones were met. The timing of the milestones was revised midway through the CRADA term to allow a longer time to pursue the objectives at no additional cost to either partner.

Varian Associates used their unique capabilities to fabricate high temperature superconducting thin films layered with other non-superconducting materials and to evaluate them for their suitability for fabrication into electronic devices. These films were made in several configurations using a variety of materials in the superconducting films. Films were then ananlyzed by LLNL using a suite of techniques including Rutherford Backscattering Spectroscopy, Secondary Ion Mass Spectroscopy, Electron Microprobe Analysis, Auger Microprobe Analysis, Ion Microprobe Spectroscopy, Scanning Tunneling Microscopy, Atomic Force Microscopy, Scanning Electron Microscopy and High Resolution Transmission Electron Microscopy. These techniques were first evaluated for their utility in providing useful information regarding either general film quality or the details of defects sometimes found after deposition. Some were then chosen for routine use in subsequent analysis.

Varian Associates have refined their fabrication process as a better understanding of the results of the film deposition grew from the analyses performed at LLNL. These activities constituted the program's main deliverables and were performed at the expected level. Varian Associates are now making the highest quality films of high temperature superconducting layered structures available in the world and are the only growers capable of supplying sufficient uniformity across a film to fabricate multiple electronic devices in an array. Additional development at Varian Associates is required to bring these films to their full commercial potential.

Keywords: Superconductors, High Transition Temperature, Josephson Junction, Tri-layers, Heteroepitaxy

331. **LITHIUM CELL DEVELOPMENT**
$200,000
DOE Contact: Andre Cygleman, (202) 586-8814
LLNL Contact: John R. Kolb, (510) 422-6424

We completed work on the development of a replacement electrolytic cell for the manufacture of lithium metal in support of the DOE Y-12 facility. Our development incorporates the introduction of a bipolar cell methodology where a bipolar electrode is one that is shared by two cells connected in electrical series. In the process developed, lithium is electrodeposited in an aqueous cell at ~30°C and then anodically removed and recovered as pure lithium at a molten lithium cathode. Lithium-depleted amalgam is returned to the aqueous cell after transferring heat counter-current to the incoming lithium-rich stream. The process eliminates high temperature electrolysis of LiCl and multiple unit processes to produce the anhydrous LiCl feedstock at Y-12. Computer control was rendered operational, but not fully employed. System auxiliaries (hot lithium transfer, vapor condensers, various diagnostics) were fabricated and installed but not fully tested. We established process feasibility by operating an integrated system consisting of aqueous cell, molten salt cell, thermal controls and amalgam circulation subsystems. Finally, we showed experimentally, that process energy efficiencies of 70% could be achieved at practical parameters.

Keywords: Lithium, Bipolar, Electrolytic Cell Development

332. **ENVIRONMENTALLY SAFE DISPOSAL OF EXPLOSIVE WASTES: SERDP PROJECT**
$800,000
DOE Contact: Andre Cygleman, (202) 586-8814
LLNL Contact: John R. Kolb, (510) 422-6424

In collaboration with researchers at Los Alamos National Laboratory and the Pantex Plant, we are exploring options to support the Department of Energy and the Department of Defense in their quest to develop environmentally sound techniques for the destruction of residual high explosive remnants after dismantlement and demilitarization occur. We intend to pursue and have demonstrated positively during this year, the capacity to minimize the amount of high explosive materials to be treated as waste and subsequently destroyed. We have chosen to manage the returning, surplus energetic material as an asset to be sold or given away in lieu of destruction. Through minimization of the amount of HE waste, we believe we can reduce, by an order of magnitude, the amount of material for which environmentally sound disposition techniques must be generated. We have focused on molten salt destruction, base hydrolysis and bioremediation as techniques to be investigated this year. We have also supported a study on the desirability of recycling and reusing insensitive high explosives with a minimum of waste generation or cleanup. No downselection among techniques was possible based on the final results of the study as reported. The effort ended in FY95 and combinations of the three techniques may be used for plant design.

Keywords: SERDP, Environmentally Benign High Explosive Waste Destruction

333. **LAMINATED METAL COMPOSITES FOR AEROSPACE APPLICATIONS**
$700,000
DOE Contact: Warren Chernock, (202) 586-7590
LLNL Contact: Donald Lesuer, (510) 422-9633

Laminated metal composites are materials in which two or more metal containing layers are deformation bonded. Previous work at LLNL has shown that these materials can have properties (such as fracture toughness, fatigue, damping capacity and impact behavior) that are superior to properties currently available in lightweight materials.

These materials also offer the possibility to tailor properties to a prescribed application through the choice of component materials, relative volume fraction of the components, interface strength, etc. This project is funded through the Technology Transfer Initiative and is exploring the application of these materials to fan containment systems for commercial jet engines and to airframe structural components.

Keywords: Materials Properties, Behavior, Characterization or Testing

396. **FATIGUE OF METAL MATRIX COMPOSITES**
$500,000
DOE Contact: Warren Chernock, (202) 586-7590
LLNL Contact: Donald Lesuer, (510) 422-9633

This project involves Lawrence Livermore National Laboratory, Oak Ridge National Laboratory and General Motors. The project is studying the mechanisms of high cycle fatigue in squeeze cast metal matrix composites. The life limiting microstructural features are being determined and the processing-structure-property correlations are being established. Models that can predict lifetimes will be developed.

Keywords: Materials Properties, Behavior, Characterization or Testing

334. **NOVEL MATERIALS FOR OPTOELECTRONICS AND PHOTONICS**
$600,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LLNL Contact: Howard W. H. Lee, (510) 423-5877

This program seeks to develop and implement promising new materials for optoelectronics and photonics that will substantially improve device and system performance and enable new and innovative technologies. Representative materials include nanocrystals, organics (conjugated polymers and small molecules), aerogels, and novel nonlinear optical (NLO) materials such as fullerenes. Our studies on the nonlinear optical properties of fullerenes showed their figure of merit to be very competitive with optical fibers for all-optical switching and have demonstrated the first fullerene-based all-optical switch. Thin films of NLO materials such as fullerenes permit an integrated optics approach which greatly minimizes the latency problem inherent with fiber optics. Other thin film NLO materials were also pursued for these applications. We have developed a type of nanocrystalline silicon (fabricated synthetically and from porous silicon) that photoluminesces throughout the visible. This nanocrystalline silicon is particularly easy to fabricate and can potentially serve as an efficient and inexpensive phosphor or as the luminescent center for flat panel displays and other light emitting applications. Nanocrystals of other materials were also studied. We have also fabricated arrays of miniature junction diodes from porous and nanocrystalline silicon that emit in the visible and near infrared. Silicon-based emitters are desirable because they integrate well with standard silicon-based microelectronics. Finally, we are developing doped aerogels and electroluminescent organic materials (conjugated polymers and small molecules) for light emissive applications such as light emitting devices, flat panel and three-dimensional displays.

Keywords: Optoelectronics, Photonics, Nanocrystals, Porous Silicon, Fullerenes, Polymers, Aerogels, Electroluminescence, Flat Panel Displays, All-Optical Switching

335. **NOVEL MATERIALS STUDIES AT HIGH PRESSURES AND TEMPERATURES**
$400,000
DOE Contact: Maurice Katz, (202) 586-5799
LLNL Contact: Choong-Shik Yoo, (510) 422-5848

The objective of this project is to study the direct elementary energetic reactions among particularly the 1st and 2nd row elements and diatomic molecules, by using a diamond-anvil cell laser-heating technique combined with synchrotron x-ray diffraction and micro-Raman spectroscopy. The feasibility of this experimental approach has well been demonstrated in our recent melting and phase transition studies of iron and actinides performed in an extended region of pressure to 1.3 Mb and temperature to 4000 K. In addition, this technique is also applicable to various energetic materials studies, including synthesis of a new class of energetic materials, electronic structures and metalization, hot spot initiation and laser combustion, at high pressures and temperatures.

Because the reactivity of materials increases substantially at high pressures and temperatures, we have been able to study highly energetic, elementary reactions between simple diatomic molecules (nitrogen, oxygen, and hydrogen) and light elements (B, Al, C, Si, etc.) or transition metals (Mg, Fe, U, etc.) at high pressures and temperatures. These reactions yield various technologically important oxides, nitrides, and hydrides, whose crystal structures can be modified by the P,T- conditions. We have also found that many of these reactions proceed extremely exothermically and can be used for metal combustion applications and/or for potential high explosives. For example, the oxidation reaction of uranium at 1 Mb and 2000 K releases extremely high transient energy which increases the temperature high enough to melt diamond (probably above 7000 K). The direct nitration reactions of boron and carbon proceed highly exothermically and yield novel materials like c-BN and various hard carbon nitrides. These kinds of energetic reactions could be of interest to DoE and DoD.

Keywords: Novel Materials Applications; Energetic Metastable Materials; Nitrides, Hydrides, Oxides and Ceramics; X-ray Laser Heating Experiments; High Pressures and Temperatures

336. **MATERIALS PRODUCED WITH DYNAMIC HIGH PRESSURE**
$400,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LLNL Contact: William Nellis, (510) 422-7200

This project produces novel materials (crystal structures, microstructures, and properties) using high shock pressures. The terms dynamic and shock are used synonymously in this context. Tuneable shock pressure pulses are produced by the impact of a projectile launched from a small two-stage light-gas gun. Shock pressures range from 0.01-1 Mbar, temperatures range from 50 up to a few 1000°C, strain rates on loading range above 10^8/s and quench rates on release of pressure are 10^{12} bar/s and 10^9 K/s in specimens which are recovered intact for investigation. A gas gun is used to achieve these high shock pressures. Specimens range from 1 micron to 3 mm thick and from 3 to 23 mm in diameter. The observed material structures are correlated with computational simulations to enhance understanding of the effects produced. For example, a computational model of the dynamic compaction of nanocrystalline Al particles was shown to be in good agreement with the structure of compacts produced experimentally. A wide variety of materials characterization measurements are made both before and after application of high dynamic pressures, including x-ray diffraction, TEM, SEM, magnetization, NMR, and neutron scattering. In the past year we have dynamically compacted nanocrystalline Al, ceramic, and magnetic powders, produced unusual glass in bulk and nanocrystalline Si in grain boundaries by shock compressing quartz single crystals, and investigated impacts in nature by studying structural effects in shocked minerals. This shock method can be used to produce nanocrystalline particles of many materials contained initially in single crystals.

Keywords: Shock Pressures, Gas Gun, Materials Characterization, Ceramics, Magnets, Nanocrystalline Si, Glass

337. **PROPERTIES OF HYDROGEN AT HIGH SHOCK PRESSURES AND TEMPERATURES**
$300,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LLNL Contacts: William Nellis, (510) 422-7200 and Neil Holmes, (510) 422-7213

The properies of hydrogen at high pressures and temperatures are a "Holy Grail" issue for laser fusion, condensed matter physics, and planetary physics. Hydrogen in the form of deuterium-tritium is the fuel in laser fusion targets; the metallization of hydrogen by electronic bandgap closure has been a key goal of condensed matter physics since the early part of this century: and Jupiter with its 300 Earth masses is 90 percent hydrogen at high pressures and temperatures. This project measures temperatures and electrical conductivities of cryogenic liquid hydrogen and deuterium shock-compressed to pressures up to 2 Mbar ($2x10^6$ bar) and temperatures up to 5000 K with a two-stage light-gas gun. These conditions are achieved by impact of projectiles accelerated to velocities up to 8 km/s. Shock temperatures up to 5000 K at 1 Mbar were measured by a fast optical spectrometer and show that hydrogen undergoes a continuous dissociative phase transition above 200 kbar. This continuous dissociation absorbs energy, which causes lower temperatures and higher densities in the Mbar shock pressure range than was thought previously.

Electrical conductivities were measured using metal electrodes at pressures in the range 1 to 2 Mbar at calculated temperatures of 2000 to 4000 K. A novel technique was used to produce just enough shock heating to excite just enough electronic carriers to be able to measure the electrical conductivity of hydrogen at Mbar pressures in the short time duration of the experiment. Ours are the only electrical conductivity measurements on condensed hydrogen at any pressure. We have, for the first time, metallized hydrogen at 1.4 Mbar and 3000 K in the fluid and determined the density dependence of the electronic bandgap in the molecular fluid phase. Our observed metallization pressure in the fluid is about one-half what was predicted for the solid at 0 K. Both molecular dissociation and electronic excitation (ionization) affect the hydrogen equation of state to make hydrogen more compressible than believed previously and, thus, facilitate laser fusion. We are the first to metallize hydrogen. Our improved hydrogen equation of state has produced an improved picture of the interior structure of Jupiter and we can now determine the electrical conductivity of hydrogen throughout the interior of Jupiter. The electrical conductivity determines the large magnetic field, which is about fifteen times larger than the Earth's.

Keywords: Shock Pressures, Shock Temperatures, Electrical Conductivities, Gas Gun, Hydrogen, Cryogenics, Equation of State, Dissociation, Metallization

338. **LOW DENSITY FOAM SHELLS FOR CRYOGENIC ICF EXPERIMENTS**
$600,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LLNL Contacts: R. Cook, (510) 422-3117

This program has as its goal the development of foam shells, from 1 to 2 mm in diameter with 100 μm foam walls whose density is 50 to 75 mg/cc and whose cell size is less than 1 μm. These shells must also have a 5 to 10 μm thick full density overcoat, and the outer surface finish must be better than 0.1 μm. Foam and overcoat must be composed of atoms with Z less than 9. These foam shells will be used to enhance the surface smoothness of solid DT layers in ICF experiments. The shells are formed using microencapsulation techniques. The foam material is based on a resorcinol-formaldehyde (R/F) foam chemistry. Optically transparant shells with 2 mm diameters and 100 μm thick walls have been prepared.

Keywords: Polymers, Laser Fusion Targets, Low Density Foam

339. **ATOMIC LEVEL EXPLOSIVE CALCULATIONS**
$400,000
DOE Contact: Maurice Katz, (202) 586-5799
LLNL Contacts: Larry Fried, (510) 422-7796

A package of atomic-level calculations has been assembled that will allow design of new explosive molecules. The package includes calculations of solid density, heat of formation, chemical stability and sensitivity. This package is being tried on various new postulated compositions in concert with feedback from three organic and inorganic synthesis chemists. The intent is to couple Molecular Design with actual synthesis routes at the start so that the final selected design will be something with a good chance of being made in the lab. The target is to provide 10 to 15 percent more detonation energy than CL-20 with no decrease in sensitivity.

Keywords: Energetic Materials, High Explosives, Molecular Design, Detonation

340. **EXPLOSIVE EQUATION OF STATE**
$700,000
DOE Contact: Maurice Katz, (202) 586-5799
LLNL Contacts: Clark Souers, (510)-423-4217

Detonation Equation of State research is proceeding on a broad front. Reaction zones and detonation front curvatures have been correlated and a certain capacity for prediction created. The Bigplate design provides an Equation of State with a continuous set of angles of incidence on copper that vary from 0° to about 70°. A JWL system method has been constructed that allows direct comparison between different explosives. It also provides a method for recalculating JWL's at slightly different densities. The failure of the JWL system indicates that the measurement is inside the reaction zone of the explosive. On-going efforts continue to seek a simple way to use Ignition & Growth for prompt detonation.

Keywords: Energetic Materials, High Explosives, Detonation, Equation of State

341. **METASTABLE SOLID-PHASE HIGH ENERGY DENSITY MATERIALS**
$236,000
DOE Contact: Maurice Katz, (202) 586-5799
LLNL Contacts: Andrew McMahan, (510) 422-7198 and Albert Holt, (510) 423-4126

Ab-initio theoretical methods are being used to predict and characterize novel high energy density materials. The class of metastable solid phases being explored is characterized by extended and continuous networks of covalent or metallic bonds, without the weak van der Waals links of familiar chemical fuels, propellants, and explosives. One of the most promising candidates investigated previously in this project is a phosphorus-like or polymeric form of nitrogen which should have a stored specific energy per unit volume about three times that of the HMX explosive. More recent work has considered boron hydrides, and in particular suggests that a boron equivalent of the observed aluminum trihydride should be metastable at atmospheric pressure with a hydrogen storage capacity per volume about two and a half times larger than cryogenic liquid hydrogen. All of these new phases are predicted to be high pressure stable, suggesting a natural synthesis route, which is being explored at LLNL by H. E. Lorenzana and collaborators.

Keywords: Energetic Materials, High Energy Density Materials, Atomic-level Materials Modeling, *Ab-initio* Electronic Structure Methods

342. **METASTABLE SOLID-PHASE HIGH ENERGY DENSITY MATERIALS**
$535,000
DOE Contact: Maurice Katz, (202) 586-5799
LLNL Contacts: H. Lorenzana, (510) 422-8982 and M. Finger, (510) 422-6370

Current conventional energetic compounds rely on strong covalent bonds within individual molecules for energy storage. These molecular liquids or solids are characterized by *large equilibrium volumes* resulting from weak van der Waals interactions between neighboring molecules. Our goal is to demonstrate proof-of-principle synthesis of new compounds that achieve an unprecedented enhancement in energy density by completely replacing these weak van der Waals interactions with highly energetic covalent bonds. Recent theoretical studies at LLNL and elsewhere indicate that solid-state phases having uniform and continuously bonded networks (*extended solids*) offer entirely new and unexplored opportunities as novel energetic materials. These novel systems represent the analog of infinite, energetic molecules. Specifically, a parallel theory effort at LLNL has predicted that nitrogen can be stabilized under ambient conditions in a three-dimensional, continuously bonded configuration characterized by a stored energy per unit volume of 34 KJ/cm^3, about *three times* that of typical monofuels such as hydrazine as well as fuel mixtures such as gasoline/liquid O_2. The recent adaptation of laser heating methods to the diamond-anvil-cell (DAC) offers the most promising synthesis route for proof-of-existence demonstration of these novel high-pressure phases, given the technique's diagnostic versatility and controlled access to extremes of pressure and temperature. Our preliminary experimental results at high pressures indicate substantial weakening of the N_2 triple bond, a necessary condition to synthesizing the polymeric nitrogen phase. On another front, we have begun studies on carbon monoxide, a compound that is isoelectronic with nitrogen and exhibits very similar high pressure phase transformations. Carbon monoxide polymerizes under pressure into a solid that can be recovered and may be energetic. The class of materials proposed here represent a radically different approach to energy storage that remains unexplored.

Keywords: Energetic Materials, High Energy Density Materials

343. **AFM INVESTIGATIONS OF CRYSTAL GROWTH**
$210,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LLNL Contact: J. J. DeYoreo, (510) 423-4240

The nanometer-scale morphology of crystalline surfaces exerts a strong control on materials properties and performance. While many researchers have studied vapor deposited metal and semiconductor surfaces grown far from equilibrium, few studies have given attention to the morphology of crystal surfaces grown from melts or solutions near equilibrium despite the fact that most bulk crystals are grown in this regime. Understanding the mechanisms of growth and the origin of defects in such crystals can impact materials performance in a number of fields including optics, electronics, molecular biology, and structural biology. We are using atomic force microscopy (AFM) to investigate the growth of single crystal surfaces from solution in order to determine the mechanism of growth, the kinetics of step advancement, the effect of impurities, and the origin of defects.

In 1995 we performed both *ex situ* and *in situ* AFM measurements on three systems, the ionic crystal KH_2PO_4 (KDP), the canonical solution grown crystal, and the protein crystal Canavalin, a prototypical macromolecular biological crystal and crystals of the Sattelite Tobacco Mosaic Virus (STMV). Our results have provided insight into the mechanisms of growth step kinetics and defect incorporation in these systems. In 1996 we will investigate the effect of impurities on step dynamics in these systems and begin to explore the process of biomineralization.

Keywords: Morphology, Crystal Surfaces, Atomic Force Microscopy

344. **SUPERPLASTIC FORMING OF STAINLESS STEEL AUTOMOTIVE COMPONENTS**
$150,000
DOE Contact: M. Michaelis, (202) 586-4105
LLNL Contact: J. W. Elmer, (510) 422-6543

Superplastic forming of automotive exhaust components is being investigated as a possible method for fabrication of low emission exhaust systems. Development of a superplastic stainless steels alloy that will meet the required fabrication and performance criteria is being performed. This alloy must be laser welded and superplastically formed to yield a component that maintains a high resistance to exhaust gas degradation during operation. To date welding and superplastic forming of a baseline stainless steel alloy has been demonstrated. New work will focus on continued development of superplastic stainless steel alloys, and testing of laser welded and superplastically formed exhaust system segments.

Keywords: Superplastic Forming, Stainless Steel Alloys, Laser Welding

345. FORMABILITY AND JOINING ANALYSIS FOR SUPERPLASTIC PANEL DESIGN
$360,000
DOE Contact: J. Van Fleet, (202) 586-5782
LLNL Contact: J. W. Elmer, (510) 422-6543 and
D. J. Trummer, (510) 423-8848

The fabrication of internally stiffened aerospace panel components is being investigated. These panels are fabricated by welding and superplastic forming. Numerical modeling of the forming behavior of titanium and aluminum alloy panels is being performed to predict superplastic pressure schedules and to optimize weld placement. The numerical models developed here will be used as a design tool to help reduce the cost and lead time required to fabricate these panels by conventional trial and error methods.

Keywords: Superplastic Forming, Numerical Modeling, NIKE-3D, Laser Welding, Titanium Alloys, Aluminum Alloys

346. MICROSTRUCTURAL EVOLUTION IN WELDS
$330,000
DOE Contact: Bharat Agrawal, (301) 903-2057
LLNL Contact: J. W. Elmer, (510) 422-6543 and
Joe Wong, (510) 423-6385

Although welding is an established technology used in many industrial settings, it is least understood in terms of the phases that actually exist, the variation of their spatial disposition with time, and the rate of transformation from one phase to another at various thermal coordinates in the vicinity of the weld. With the availability of high flux and, more recently, high brightness synchrotron x-radiation sources, this work develops *spatially resolved x-ray diffraction (SRXRD)* for in-situ investigations of phase transformations in the heat affected zone (HAZ) of fusion welds. In this investigation, SRXRD will be used as a direct method for monitoring the phases present during welding of titanium in order to track the time-temperature history of welding-induced phase transformations. Results of these experiments will be used to aid in the numerical modeling of the kinetics of phase transformations under the highly non-isothermal conditions that exist in the HAZ of welds.

Keywords: Synchrotron Radiation, X-ray Diffraction, In-Situ Experiments, Phase Mapping, Arc Welding, Titanium, Non-isothermal, Phase Transformation Kinetics

347. URANIUM CASTING PROGRAM
$1,000,000
DOE Contact: Marshall Sluyter, (301) 903-5491
LLNL Contact: Steve Root, (510) 423-5216

The uranium casting program is addressing the use of permanent molds for near net shape castings, controlled cooling for segregation and microstructure control and the effect of alloy additions and subsequent heat treatment on microstructure. Process modeling has played a key role in producing high quality castings in uranium and uranium alloys.

Keywords: Uranium Casting

348. URANIUM SPIN FORMING
$1,500,000
DOE Contact: Marshall Sluyter, (301) 903-5491
LLNL Contact: Steve Root, (510) 423-5216

Spin forming is being explored as a method to produce near net shape wrought uranium components. Process modeling has been useful in predicting stress/strain distribution and spring back. Near net shape components have been produced

Keywords: Spin Forming

349. PLUTONIUM NEAR NET SHAPE CASTING
$2,500,000
DOE Contact: Marshall Sluyter, (301) 903-5491
LLNL Contact: Steve Root, (510) 423-5216

Near net shape casting is being explored using permanent molds. High quality castings have been produced. Process modeling has played a significant role in defining conditions needed for solidification control.

Keywords: Shape Casting

350. ELECTRON BEAM COLD HEARTH MELTING OF URANIUM
$900,000
DOE Contact: Marshall Sluyter, (301) 903-5491
LLNL Contact: Steve Root, (510) 423-5216

An existing electron beam evaporation chamber has been modified to produce controlled solidification uranium alloy ingots. Scrap feeders of various types are being evaluated. High quality ingots which meet the applicable uranium alloy specification have been produced.

Keywords: Electron Beam Melting, Uranium

LOS ALAMOS NATIONAL LABORATORY

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

351. **ACTINIDE PROCESSING DEVELOPMENT**
$1,350,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LANL (Contract No. W-7405-ENG-36) Contact:
R. L. Gutierrez, (505) 665-3919

The aim of this project is the development and characterization of fabrication processes and the study of new processing technologies for plutonium. Research involves casting, thermomechanical working, and stability studies. Measurements of resistivity, thermal expansion, magnetic susceptibility, and formability are made to evaluate fabrication processes and alloy stability.

Keywords: Radioactive Materials, Plutonium Alloys, Ductility, Thermal Expansion, Electrical Resistivity, Stability

352. **PLUTONIUM OXIDE REDUCTION**
$150,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LANL (Contract No. W-7405-ENG-36) Contact: K. Axler,
(505) 667-4045

The thermodynamics of interactions among the components used in the pyrochemical processing of plutonium are determined along with the relevant phase relations.

Keywords: Radioactive Materials, Plutonium, Thermodynamics, Phase Diagrams, Direct Oxide Reduction, Electrorefining, Molten Salt Extraction

353. **LOW DENSITY MICROCELLULAR PLASTIC FOAMS**
$200,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LANL (Contract No. W-7405-ENG-36) Contact: P. Apen,
(505) 667-6887

Microstructural polyolefin foams with densities between 0.01 g/cc and 0.2 g/cc are manufactured by a nonconventional foaming process. Foams are both open and closed celled and have large surface areas. This process is being expanded to other polymeric materials for a wide variety of applications. Foams have cell sizes from 25μm down to the 1μm range, depending on the process. Composite foams are being produced with submicron cell sizes while maintaining structural properties.

Keywords: Foams, Polyolefins, Polyurethanes, Silicones, Polyesters

354. **PHYSICAL VAPOR DEPOSITION AND SURFACE ANALYSIS**
$300,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LANL (Contract No. W-7405-ENG-36) Contact:
M. Scott, (505) 667-7557

Physical vapor deposition, one electron beam sputtering, and dual ion beam sputtering are employed to produce materials for structural applications, corrosion resistance, optical properties, and thin film transducers. Materials being developed include doped, *in situ* laminates of aluminum and Al_xO_y having high strength and smooth surface finish. Also included are ion assisted deposition and ion sputtering onto various substrates for corrosion resistance to gases and liquid plutonium, reflective and anti-reflective coatings for infrared, visible, ultraviolet and X-ray wavelengths. Novel photocathodes are being made and evaluated by these processes.

Keywords: Coatings and Films, Physical Vapor Deposition, Sputtering, Ion Plating, Corrosion, Nondestructive Evaluation

355. **CHEMICAL VAPOR DEPOSITION (CVD) COATINGS**
$150,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LANL (Contract No. W-7405-ENG-36) Contacts:
J. R. Laia and M. Trkula, (505) 667-0591

Chemical vapor deposition (CVD) techniques are used to deposit thin-film and bulk coatings of a wide variety of elements and compounds. Coatings are deposited by the following techniques: conventional flow-by, fluidized-bed, plasma-assisted, and chemical vapor infiltration. To support and enhance our basic CVD program, efforts are underway to study the fundamental nature of the CVD process, including *in situ* diagnostics in the gas phase just above the substrate and modeling efforts to predict gas flows, reactor design, and chemical behavior within the CVD systems. Another collaborative effort at Los Alamos is attempting to synthesize organometallic precursors to deposit coatings at temperatures <300°C. Substrates coated by the CVD technique range from particles 2.0 μm diameter to infiltrations of fabrics a square meter in area.

Applications include nuclear and conventional weapons, space nuclear reactor systems (fuels and structural components), inertial confinement fusion program, high temperature engine and structural components for advanced high-performance aircraft, hard/wear resistant coatings (tribological), corrosion resistant coatings, coatings of complex geometries, near-net-shape fabrication, heat-pipe structures, precision CVD of ultra-thin, freestanding shapes.

Keywords: Chemical Vapor Deposition, Coatings (metal and ceramic)

356. **POLYMERS AND ADHESIVES**
$430,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LANL (Contract No. W-7405-ENG-36) Contact:
D. A. Hemphill, (505) 667-8335

The objective of this project is to identify potential weapons engineering and physics applications for plastic and composite materials, select or develop appropriate materials, develop low cost fabrication techniques compatible with Integrated Contractor production capabilities, and characterize promising materials on a timely basis to provide optimum material choices for new weapons designs. Material or process development projects include: highly filled polymers, composite structural and spring components, cushioning materials, and high-explosive compatible adhesives, potting materials. This work will be compatible with all current and future ES&H guidelines.

Keywords: Adhesives, Composites, Plastics, Polymers, Weapons Design, Weapons Engineering, Integrated Contractors

357. **TRITIATED MATERIALS**
$175,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LANL (Contract No. W-7405-ENG-36) Contact:
J. R. Bartlit, (505) 667-5419

Advanced research and development efforts are focused on tritiated materials for tritium storage. New methods for preparing, fabricating, and containing such compounds are under investigation. We are also using laser-Raman techniques for *in situ* measurements of hydrogen-deuterium-tritium gas mixtures.

Keywords: Tritium, Tritiated Materials, Radioactive Materials

358. **SALT FABRICATION**
$800,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LANL (Contract No. W-7405-ENG-36) Contact:
D. Carstens, (505) 667-5849

Development and evaluation of new fabrication and containment processes for LiH and LiD. This includes preparation of device parts for WTS tests. Research topics include development of hot pressing, machining techniques for salt compacts.

Keywords: Tritium, Hydrides, Machining, Radioactive Materials, Near-Net-Shape Processing

359. **SLIP CASTING OF CERAMICS**
$300,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LANL (Contract No. W-7405-ENG-36) Contact:
D. S. Phillips, (505) 667-5128

We are slip casting many ceramics including alumina, zirconia-toughened alumina (ZTA), and magnesia. The technology uses colloidal chemistry and powder characterization techniques, along with materials engineering. Considerable progress was made in the development of ZTA ceramic alloys with a superior microstructure and improved thermal shock resistance. The scope of work has expanded to include frits and insulation materials, as well as dense crucibles.

Keywords: Ceramics, Microstructure, Strength, Transformation Toughened Ceramics, Thermal Shock

360. **PLASMA-FLAME SPRAYING TECHNOLOGY**
$300,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LANL (Contract No. W-7405-ENG-36) Contact:
R. Castro, (505) 667-5191

Free-standing shapes and metallic and ceramic coatings are fabricated by plasma spraying. Materials examined recently include Be, ^{238}U, $MoSi_2$ and ZrO_2. Applications include: radiochemical detectors; temperature-, oxidation-, and corrosion-resistant coatings; and electrically insulating coatings.

Keywords: Coatings, Metals, Ceramics, Plasma-Flame Spraying, High Temperature Service, Surface Characterization and Treatment

361. **RAPID SOLIDIFICATION TECHNOLOGY**
$500,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LANL (Contract No. W-7405-ENG-36) Contact:
P. Stanek, (505) 667-6914

RSR technologies such as melt spinning, splat cooling, and rapid solidification plasma spraying, are being developed to evaluate a range of RSR alloys, intermetallics and composites for defense and energy applications. Activities include alloy development, microstructural analysis, mechanical and physical properties testing, process development and modeling.

Keywords: Rapid Solidification, Low Pressure Plasma, Alloy Development, Composites, Intermetallics

362. **BULK CERAMIC PROCESSING**
$250,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LANL (Contract No. W-7405-ENG-36) Contact:
J. D. Katz, (505) 665-1424

Cold pressing and cold isostatic pressing, followed by sintering, are used to produce ceramic and metal components for various physics experiments and for plutonium processing. Materials fabricated include alumina, magnesia and boron.

In addition, a collaborative effort was established with the University of New Mexico Center for Micro-Engineered Ceramics to investigate the effect of 2.45 GHz microwave energy on the diffusion of cations in ceramic oxides. This research consists of both a theoretical and experimental component. The results have shown that although microwave enhanced diffusion of chromium in alumina does not exist, microwave sintering has been found to be a very effective engineering tool for densifying even large alumina ceramics.

Finally, considerable effort was devoted to developing methods for sintering, rather than hot pressing, boron carbide to achieve high density. This work involves a collaboration with the A.W.E. in the United Kingdom.

Keywords: Ceramics, Sintering, Microwave Sintering, Cold Pressing

363. **SYNTHESIS OF CERAMIC COATINGS**
$150,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LANL (Contract No. W-7405-ENG-36) Contact:
C. P. Scherer, (505) 665-3202

The objective of this effort is to synthesize ceramic films for liquid metal containment. One approach entails the use of organic and aqueous solvents to deposit erbia films, which are subsequently heat treated to densification. The second approach involves the *in situ* conversion of a metal surface to a nitride by precise heating in a nitrogen environment.

Keywords: Ceramic Coatings, Sol Gel, Nitration

MATERIALS STRUCTURE OR COMPOSITION

364. **ACTINIDE SURFACE PROPERTIES**
$700,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LANL (Contract No. W-7405-ENG-36) Contact:
J. M. Haschke, (505) 665-3342

Characterization of actinide metal, alloy and compound surfaces using the techniques of X-ray photoelectron spectroscopy, Auger analysis, ellipsometry and Fourier-transform infrared spectroscopy. Surface reactions, chemisorption, attack by hydrogen, and the nature of associated catalytic processes are being studied.

Keywords: Actinides, Hydrides, Surface Characterization and Treatment, Hydrogen Effects, Radioactive Materials

365. **NEUTRON DIFFRACTION OF PU AND PU ALLOYS AND OTHER ACTINIDES**
$237,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LANL (Contract No. W-7405-ENG-36) Contact:
A. C. Lawson, (505) 667-8844

Physical structure and properties of plutonium are being studied by pulsed neutron diffraction at the Manuel Lujan, Jr., Neutron Scattering Center (Los Alamos) and the Intense Pulsed Neutron Source (Argonne). A time-of-flight technique is used to measure diffraction at cryogenic and elevated temperatures.

Keywords: Alloys, Radioactive Materials, Transformation, Microstructure

366. **SURFACE, MATERIAL AND ANALYTICAL STUDIES**
$300,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LANL (Contract No. W-7405-ENG-36) Contact:
W. C. Danen, (505) 667-4686

Studies are underway in four key areas: surface and interfacial structures and properties, explosives dynamics, laser-based isotopic analysis, and metastable energetic materials. Current investigations in surface and interfacial studies include: surface modification, HTSC composition and structure, and the use of MeV ion beams. In explosives chemistry, we are using real-time optical- and mass-spectral methods to probe the early-time dynamics of detonation. Analytical studies have centered on the use of resonance ionization mass spectrometry to eliminate isobaric interferences in the measurement of high-dynamic range isotope ratio measurements. We continue to study the synthesis and characterization of a new class of high energy density materials consisting of atomically-thin multilayered composite materials.

Keywords: Surface, Explosives, Interfaces, Composite Materials

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

367. **MECHANICAL PROPERTIES OF PLUTONIUM AND ITS ALLOYS**
$450,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LANL (Contract No. W-7405-ENG-36) Contact:
R. L. Gutierrez, (505) 665-3919

The mechanical properties of plutonium and its alloys are related to the pre-test and post-test microstructures of the materials using optical and electron microscopy and X-ray, electron and neutron diffraction.

Keywords: Alloys, Radioactive Materials, Microstructures, Strength, Transformation

368. **PHASE TRANSFORMATIONS IN PU AND PU ALLOYS**
$450,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LANL (Contract No. W-7405-ENG-36) Contact:
R. L. Gutierrez, (505) 665-3919

Mechanisms and crystallography of thermally and mechanically induced allotropic transformations are studied with differential scanning calorimetry, optical and electron microscopy and electron and X-ray diffraction.

Keywords: Alloys, Radioactive Materials, Microstructure, Transformations

369. **PLUTONIUM SHOCK DEFORMATION**
$350,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LANL (Contract No. W-7405-ENG-36) Contact:
M. J. Reisfeld, (505) 667-8485

Plutonium and actinide alloys are subjected to shock deformation, recovered without further damage and examined to determine how the shock affected their microstructures and mechanical properties.

Keywords: Radioactive Materials, Plutonium Alloys, Microstructure, Strength

370. **NON-DESTRUCTIVE EVALUATION**
$550,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LANL (Contract No. W-7405-ENG-36) Contact:
Thomas Claytor, (505) 667-1973

Development of Nondestructive Evaluation Technology that produces quantitative estimates of material properties. Use of tomographic techniques to enhance radiographic inspection. Flash, cine-radiography, high speed video recorded optical and X-ray diagnostics of dynamic and ultra-fast events. Real-time radiography. Image enhancement of output results from all techniques. Development of ultrasonic inspection techniques.

Keywords: Nondestructive Evaluation, Radiography, Ultrasonic Microscopy, Tomography, Cine Radiography, Bonding Processes, Real-Time Radiography, Image Enhancement

371. **POWDER CHARACTERIZATION**
$50,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LANL (Contract No. W-7405-ENG-36) Contact:
G. J. Vogt, (505) 667-5813

Synthesis and processing of ceramic or metal powders depends critically on the physical characterization of the starting powders being used. Typical starting powders include commercial powders of thoria, magnesia, alumina, tungsten, copper, tungsten carbide, and boron carbide. In the past year, considerable effort has been expended on characterizing palladium alloy powders. Physical properties of interest include particle size and distribution, surface area, bulk and packed densities, morphology, pore size and distribution, and zeta potential. The crystalline-phase composition of the starting powders and processed powders can be determined by X-ray diffraction.

Keywords: Ceramic Powder, Metal Powder, Particle Size, Superconducting Powder, X-ray Diffraction, Surface Area

372. **SHOCK DEFORMATION IN ACTINIDE MATERIALS**
$300,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LANL (Contract No. W-7405-ENG-36) Contact:
R. L. Gutierrez, (505) 665-3919

Measurement of shock-wave profiles in uranium, plutonium, and plutonium alloys. Use of soft-shock recovery test to examine the microstructural changes occurring during shock deformation. Measurement of spall strength in actinide materials and examination of fracture surfaces.

Keywords: Actinides, Shock Deformation, Microstructure, Spall Strength

373. **DYNAMIC MECHANICAL PROPERTIES OF WEAPONS MATERIALS**
$350,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LANL (Contract No. W-7405-ENG-36) Contact:
G. Gray, (505) 667-5452

Measurements of dynamic stress-strain and fracture behavior of materials used for nuclear weapons. Development of plastic constitutive relations.

Keywords: Dynamic, Strength, Fracture, Microstructure

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

374. **TARGET FABRICATION**
$1,500,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LANL (Contact No. W-7405-ENG-36) Contact:
L. Foreman, (505) 667-1846
LLNL Contact: W. Hatcher, (510) 422-1100
General Atomics Contact: Ken Schultz,
(619) 455-4304

ICF/AGEX targets are fabricated using PVD, CVD, precision micromachining, and polymer chemistry techniques. After the parts are fabricated, the components are assembled using a variety of techniques. These targets are used to provide laser materials interactions data for the inertial confinement fusion community.

Keywords: Inertial Fusion, Target Fabrication

375. **FILAMENT WINDER**
$100,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LANL (Contract No. W-7405-ENG-36) Contact:
B. Benicewicz, (505) 665-0101

The Entec filament winder in MST-7 Plastics is a 4-axis computer-programmed machine with a winding envelope extending up to 4 feet in diameter and 10 feet in length. It is being utilized to wind circumferential or helical cylinders, cones, spheres, and closed-end vessels from a variety of fibers including glass, kevlar, carbon, tungsten, and aluminum oxide. The applications cover a host of programs from within the Laboratory as well as from outside agencies.

Keywords: Filament Winding, Composites

376. **HIGH ENERGY DENSITY WELDING IN HAZARDOUS ENVIRONMENTS**
$800,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LANL (Contract No. W-7405-ENG-36) Contact:
G. Lewis, (505) 667-9663

High power Nd/YAG lasers combined with fiber optic beam delivery systems have been evaluated for welding applications in hazardous environments. Applications include the manufacture of nuclear weapons components and nuclear power reactor repair. High quality structural welds have been achieved without exposing the operators or the welding power supplies to the hazardous environment.

Keywords: Laser Welding, Fiber Optic Beam Delivery, Hazardous Environments, Nuclear Applications

377. **URANIUM SCRAP CONVERSION AND RECOVERY**
$1,500,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LANL (Contract No. W-7405-ENG-36) Contact:
Dan Knobeloch, (505) 667-4417

Maintain and develop technologies for conversion and recovery of uranium scrap. Maintain and upgrade facilities for processing enriched uranium and managing uranium inventories.

Keywords: Uranium, Uranium Scrap, Enriched Uranium, Recovery, Processing, Inventories

LABORATORY DIRECTED RESEARCH AND DEVELOPMENT

378. **ELECTRONICALLY CORRELATED MATERIALS AT AMBIENT AND EXTREME CONDITIONS**
$328,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36) Contact:
J. D. Thompson, (505) 667-6416

This coordinated program was aimed specifically at an in-depth description of the many-body ground state in correlated electron systems. This research examined heavy-electron compounds under extreme conditions of pressure, temperature, and magnetic field, thereby allowing unique insights into the correlated ground states.

Keywords: Heavy Electron Systems, Materials Under Extreme Conditions

379. **ORGANOMETALLIC CHEMICAL VAPOR DEPOSITION**
$248,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36) Contact:
D. C. Smith, (505) 667-2424

Most conventional metal halide based chemical vapor deposition processes take place at temperatures in excess of 800°C and produce corrosive gases (e.g., HCl, HF). Organometallic complexes as CVD precursors are a simple and powerful method for producing coatings at low temperatures, eliminating deleterious byproducts, and removing the halide from the process completely. In this effort, new routes to metal and metal carbide thin films from volatile organometallic precursors have been developed. Potential applications for these new low-temperature materials include: weapons diagnostics, oxidation protection coatings for polymers, barrier materials for use in nuclear fuels and high-temperature (>2000°C) environments, and coatings for solid propellants.

Keywords: Metal Thin Films, Metal Carbide Thin Films, Chemical Vapor Deposition

380. **POLYMER SORBENTS FOR HAZARDOUS METAL UPTAKE**
$164,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36) Contact:
B. Jorgensen, (505) 667-3619

Polymer sorbents with immobilized metal complexing agents are being developed for treatment of radioactive and mixed waste. The polymers are applicable to treatment of process streams, waste streams and environmental remediation. The polymers will remove hazardous metals and radionuclides from aqueous solutions. Two types of systems are being investigated. One of these is a water soluble polymer-supported extraction system for use in ultrafiltration technology and the other utilizes chelating resins. In each case, selective ligands are covalently bound to polymers and the polymers tested for metal ion uptake. Los Alamos is involved in the design, synthesis, and evaluation of actinide selective ligands in collaboration with several universities. Ligands developed in this program and other promising ligands are used in the polymer sorbents. The polymers are being tested on simulated waste mixtures and we hope to be able to test them on actual DOE radioactive waste.

Keywords: Metal Complexes, Radioactive Waste, Mixed Waste, Polymer Sorbents

381. **MICROSCOPIC MATERIALS MODELING: TEXTURES AND DYNAMICS**
$109,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36) Contact:
A. Bishop, (505) 667-6491

We applied analytical techniques developed in nonlinear science and simulation techniques using massively parallel computation to study textures and their dynamical consequences in areas of condensed matter and materials science. Specifically we have (1) implemented a Langevin MD code on the CM-2 that allows for study of large 2D Josephson junction arrays and 2D magnets; (2) simulated spiral surface growth in the presence of Frank-Read dislocation sources; (3) developed a nonlinear-nonlocal elasticity formalism for 2D martensitic materials; (4) discovered a new "glassy" relaxation response for large arrays of Josephson junctions in the presence of thermal noise and structural disorder; (5) used collective coordinate and MC-MD techniques to analyze the classical anisotropic Heisenberg model and relate dynamics of vortices to recent experiments.

Keywords: Textures, Condensed Matter, Materials Science, CM-2, Frank-Read Dislocations, Josephson Junctions, Heisenberg Model

382. **SURFACE MODIFICATION OF MATERIALS**
$315,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36) Contact:
M. Nastasi, (505) 667-7007

A combination of surface processing techniques, including reactive and non-reactive physical vapor deposition (PVD), ion implantation alloying, ion beam and excimer laser mixing, have been used to synthesize intermetallic, ceramic, and composite coatings with amorphous and/or ultrafine-microstructures. The influence of synthesis variables on microstructural evolution and phase formation was evaluated using X-ray diffraction and transmission electron microscopy. Composition analysis was carried out using ion backscattering. The surface mechanical properties of these materials were evaluated for hardness and modulus using nanoindentation techniques and, in some instance, the friction and wear performance was also evaluated using a pin-on-disk tribometer.

Keywords: Physical Vapor Deposition, Ion Implantation, Ion Beam/Laser Mixing, Intermetallic Coatings, Ceramic Coatings, Composites

383. **INTEGRATION OF FUNDAMENTAL KNOWLEDGE IN PLASTICITY AND TEXTURES TO PROVIDE TECHNICAL TOOLS FOR MICROSCOPIC APPLICATIONS**
$290,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36) Contact:
U. F. Kocks, (505) 667-9323

The individual components of understanding that have been developed in basic research on mechanical properties are being integrated into a complete, coherent description of material behavior in plasticity. This involves the kinetics of flow and strain hardening, as well as texture development and the influence of textures on plastic anisotropy. Methods are established for determining the parameters required for applications of the model. User-friendly computer codes are maintained for the analysis of experimental textures, as well as for the prediction of current anisotropies on the basis of measured textures, and for the future development of texture and anisotropy during deformation through simulation of polycrystal plasticity. One aim is to foster development of a universal materials response package for incorporation into large engineering design codes for structures as well as processing. Conversely, these codes are used to derive properties of heterogeneous materials.

Keywords: Texture, Plastic Anisotropy, Plastic Deformation, Polycrystal Plasticity, Modeling

384. **HIGH RESOLUTION ELECTRON MICROSCOPY OF MATERIALS**
$350,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36) Contact:
T. E. Mitchell, (505) 667-0938

The high resolution electron microscopy (HREM) facility is based on a Philips CM30T microscope operating at 300 kV. Its point-to-point resolution of 1.9A makes it possible to obtain structure images of most materials at the atomic level. Image processing and enhancement procedures are being used to optimize the images obtained. Multi-slice image simulations on proposed structures are used to compare with experimental images and obtain information on atomic positions around defects such as dislocation and interfaces. HREM is being used on a wide range of materials applications. These include interfaces in semiconductor multilayers, grain boundaries in high temperature superconductors, twin boundaries in molybdenum disilicide, interfaces between silicon carbide and silicon nitride, and dislocations in refractory oxides.

Keywords: High Resolution Electron Microscopy, Materials at the Atomic Level, Molybdenum Disilicide, Silicon Carbide/Silicon Nitride Interfaces, Refractory Oxides

385. **NANO-FABRICATION**
$255,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36) Contact:
Robert Day, (505) 667-2957

This project combines theory and experiment to investigate the limits of nano-fabrication technology. We are primarily using molecular dynamics (MD) to simulate the actions and interaction of materials at the nanometer size. MD is used to study the stability of nanofeatures and to simulate nanomachining.

Keywords: Nano-fabrication, Molecular Dynamics, Nanomachining

386. **THIN FILM MICRO-ELECTROCHEMICAL SENSOR DEVELOPMENT**
$210,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36) Contact:
F. H. Garzon, (505) 667-6643

The objective of this project is the development of solid state microelectrochemical sensors that are applicable to the monitoring of hazardous gases such as: chlorine containing solvent vapors, sulfur dioxide, and halogen gases.

Keywords: Chemical Sensors, Chlorinated Hydrocarbons, Sulfur Oxides, Halogen Gases

387. **LIQUID CRYSTAL THERMOSETS**
$200,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36) Contact:
B. C. Benicewicz, (505) 665-0101

Designing composite materials at the nano-scale or molecular level is predicted to lead to mechanical properties several orders of magnitude greater than current materials. In the area of organic polymer composites, it has been shown that increases in properties are possible, but the usefulness of such materials is limited because of phase separation of the immiscible liquid crystal reinforcement and isotropic matrix components. This effort is a study of a new concept to make stable molecular composites using high performance liquid crystal polymers and newly developed liquid crystal thermoset matrices.

Keywords: Liquid Crystal Polymers

388. **NEUTRON AND RESONANT X-RAY SCATTERING BY MATERIALS**
$350,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36) Contact:
A. C. Lawson, (505) 667-8844

The techniques of pulsed neutron scattering and resonant X-ray diffraction are used to study materials such as actinides, f-electron ferromagnets and structural materials.

Keywords: Neutron Scattering, X-ray Scattering, Actinides, Ferromagnets

389. **STRUCTURAL AND ELECTRONIC COMPETITIONS IN LOW-DIMENSIONAL MATERIALS**
$360,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36) Contact:
B. I. Swanson, (505) 667-5814

This represents a combined theoretical and experimental study of the structural and electronic properties of low-dimensional electronic materials as they are tuned to the phase boundary region between different broken symmetry states (charge-density-and spin-density-wave, CDW and SDW). Within the CDW/SDW phase boundary region, competitions arise between the ground and local states (doping, photoinduced) that give rise to large changes in the transport (electrical) and optical properties. Work to date has focused on (1) developing new approaches to chemically tuning these materials through the phase boundary region, (2) studies (theory and experiment) of weak CDW and SDW materials, and (3) studies of mixed-halide materials, where the properties of the dominant species can be used to control the structure and electronics of the doped species. Key findings to date include (1) a new approach to tuning these materials through a structural "template" effect, (2) many-body modeling of species near the phase boundary region that shows evidence for CDW/SDW transitions and complex new structures, and (3) observation of the quenching of the Peierls distortion and the CDW in MX' segments of chains doped into a host MS lattice.

Keywords: Me Phase Boundary Tuning, Low-Dimensional Electronic Materials

390. **FUNDAMENTAL ASPECTS OF PHOTOELECTRON SPECTROSCOPY IN HIGHLY CORRELATED ELECTRONIC SYSTEMS**
$300,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36) Contact:
A. K. Arko, (505) 665-0758

Materials displaying strong electron-electron correlations continue to occupy condensed matter physicists, particularly in view of high T_c materials, where these correlations may be all important. Several variations of the Hubbard model are proposed as possible representations of this electronic structure. Photoelectron spectroscopy plays a major role in this research since it is one of the few experimental tools via which it is possible to observe the electronic structure directly without resorting to interpretation. We have performed numerous photoelectron spectroscopy tests on a large number of Ce- and Yb-based heavy fermions and compared the results to predictions of the model. Our single crystal data continue to indicate that the features usually identified as arising from the magnetic, or Kondo interaction, are much more logically described to first order as simple core levels.

Keywords: Photoemission Spectroscopy, Electronic Correlations

391. **DEVELOPMENT OF HIGH STRENGTH HIGH CONDUCTIVITY MATERIALS FOR HIGH MAGNETIC FIELD DEVICES**
$100,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36) Contact:
F. M. Mueller, (505) 667-9244

The project will cover the fabrication analysis and design of high strength high conductivity materials for pulsed magnet applications of relevance to NHMFL. New methods of fabrication will be considered based on the use of rapid solidification and cryogenic forming. An analysis of the materials will be conducted based on measurement of mechanical properties, characterization of the structure by SEM and TEM methods and measurement of the ratio of the electrical conductivity at 293K and 77K as a function of the material's thermal-mechanical history. Attempts will be made to link the results of the study directly to the needs of NHMFL in terms of both magnetic coil design and optimization of relevant fabrication methods.

Keywords: Conductive Materials, Magnetic Coil Designs

392. **LOW TEMPERATURE STM FOR STRUCTURAL AND SPECTROSCOPIC STUDIES OF HIGH TEMPERATURE SUPERCONDUCTORS AND OTHER ELECTRONIC MATERIALS**
$50,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36) Contact:
M. Hawley, (505) 665-3600

The STM is a powerful probe of the local density of states in the study of electronic materials. The extension of this capability to low temperatures creates an opportunity to apply this technique to such studies as phase transitions in low dimensional electronic materials and in superconductors, i.e., I-V gap measurements and vortex lattices. To this end, this program includes the design and construction of a variable low temperature STM for the study of these materials. Where possible, we will explore the utility of this technique in the study of changes in morphology of structural materials with lower temperature applications and to the fabrication of nanoscale features.

Keywords: Scanning Tunneling Microscope, Electronic Materials, Low Temperature Scanning

393. **MATERIALS WITH FINE MICROSTRUCTURES**
$365,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36) Contact:
R. B. Schwarz, (505) 667-8454

The refinement of the microstructure of multiphase alloys can lead to significant enhancements in the mechanical properties of engineered materials. One synthesis route for such materials is the consolidation of powders with fine microstructures. This program addresses both the problem of synthesizing powders with fine microstructures and the problem of consolidating these powders while preserving their fine microstructure.

Keywords: Multiphase Alloys, Microstructure, Powder Consolidation

394. **ION BEAM MATERIALS RESEARCH**
$330,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36) Contact:
C. J. Maggiore, (505) 667-6133

The synthesis of any new material cannot proceed efficiently without the quantitative characterization of the composition and structure of the material actually fabricated. The use of MeV ions is a well understood means of quantitative analysis and is routinely available at the IBML (Ion Beam Materials Laboratory). However, the continued development of new materials with better defined structure and composition on a finer scale has placed more stringent requirements on existing analytical methods. The objective of this program is to extend the analytical range and applicability of the IBML to the classes of new synthetic materials of current technological interest. Samples will be prepared by a variety of collaborators that are suitable for studying the fundamental limitations of multiple straggling on depth resolution using ion beams, improving sensitivity limits for light elements in complex samples using prompt and delayed nuclear reaction analysis, and bulk detection of hydrogen.

Keywords: Ion Beam Characterization

395. **TEXTURE STUDIES OF HIGHLY DEFORMED COMPOSITE MATERIALS**
$192,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36) Contact:
A. C. Larson, (505) 667-2942

Recently scientists have become interested in creating composite materials, such as high Tc-superconductors encased in silver wire and then deformed to prepare a tape, aluminum with SiC whiskers embedded in the aluminum matrix and copper metal containing tungsten wires. These composite materials are an effort to prepare materials displaying an optimal combination of the properties of the component materials. It is important to recognize that, in the deformation of two-phase systems, two processes become of importance: (a) the development of accommodation strain or arrays of geometrically necessary dislocations around the particles of the more rigid phase and (b) a change in the patterns of the flow in each phase due to the presence of the other phase. The occurrence of these processes is dependent on the relative fractions of the phases. We propose to study the relationships among the phases present in a composite by examination of the texture or orientation distribution of the crystallites in each phase.

Keywords: Silicon Carbide Whisker Reinforced Aluminum, Tungsten Wire Reinforced Copper, Two Phase Deformation

396. **PRESSURE DEPENDENCY OF THE STRUCTURE OF HIGH EXPLOSIVES: NITROMETHANE**
$192,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36) Contact:
R. B. VonDreele, (505) 667-3630

This program examines the structural changes as a function of pressure for nitromethane and correlates them with the pressure dependence of solid state ionization processes proposed as an explosion front propagation mechanism.

Keywords: Nitromethane, Pressure Dependencies, Explosive Front Propagation Mechanisms

397. **NEUTRON REFLECTION STUDIES OF THIN FILM AND MULTILAYER STRUCTURES**
$300,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36) Contact:
M. R. Fitzsimmons, (505) 665-4045

The purpose of this research program is to understand magnetism in thin film and multilayer structures using polarized neutron reflection (PNR). In order to obtain meaningful measurements of the magnetic structures and properties of surfaces and interfaces, the capability to manufacture thin films and multilayers, while PNR measurements are made, is essential. Such a capability-a first for a neutron source-will be developed. Topics to be explored by this research program are: two-dimensional magnetism, the kinetics of diffusion within multilayers, diffusion-induced changes of the magnetic properties of multilayers, the correlation between the magnetic properties of surfaces and interfaces with their roughness, and the design of improved super-mirrors for neutron applications.

Keywords: Magnetic Properties of Thin Films, Polarized Neutron Diffusion in Multilayers

398. **NEUTRON REFLECTIVITY STUDIES OF IN SITU CORROSION OF METAL SURFACES**
$145,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36) Contact:
G. S. Smith, (505) 665-2842

Corrosion of metallic surfaces have been studied for many years by several techniques. These studies have looked at the problem of corrosion both as a problem to be eradicated and as a useful end to the electroplating process. Never before has anyone been able to look at the microscopic details of composition as well as surface roughness at the metal-electrolyte interface. This program uses neutron reflectometry to study these features.

Keywords: Corrosion, Neutron Reflectometry

399. **THE DYNAMICS OF AMORPHOUS MATERIALS**
$330,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36) Contact:
R. A. Robinson, (505) 667-3626

This research program studies the vibrational and magnetic dynamics of amorphous materials, using inelastic neutron scattering. While atomic and magnetic fluctuations are well understood as collective excitations (e.g., phonons, magnons) in single crystals, much less is understood in amorphous materials. The materials to be studied include silica, porous silica aerogels, a metallic glass and metglas.

Keywords: Vibration Dynamics, Magnetic Dynamics, Silica, Silica Aerogels, Metallic Glasses

400. **ADVANCED MATERIAL SCIENCE ALGORITHMS FOR SUPERCOMPUTER ARCHITECTURES**
$75,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36) Contact:
J. E. Gubernatis, (505) 667-6727

This project is concerned with exploiting the potential new computer architectures offer to improving the understanding and modeling of material properties and behavior through computer simulation. The focus is on developing the simulation ability to study flux line dynamics, noise, melting, and pinning in London and Ginzburg-Landau phenomenological models of thin films on high temperature superconducting materials. The emphasis of the program is also on parallizing the world-line quantum Monte Carlo method and developing procedures to extract dynamical information from imaginary-time quantum Monte Carlo data.

Keywords: High Temperature Superconducting Materials, London Phenomenological Models, Ginzburg-Landau Phenomenological Models

401. **METAL VAPOR SYNTHESIS IN ORGANOMETALLIC CHEMISTRY**
$235,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36) Contact:
J. G. Watkin, (505) 667-4546

This program will employ the rare synthetic technique of metal vapor synthesis (MVS) to prepare a series of organometallic complexes of middle- and late-transition metals and lanthanides. Applications include catalytic processes and/or organic synthesis. The technique of metal vapor synthesis has been employed to prepare many examples of low-valent early transition metal complexes which have been shown to exhibit high reactivity, but the technique has rarely been applied to the later transition metals such as Rh, Ir, Pd, Pt and the lanthanides.

Keywords: Metal Vapor Synthesis, Lanthanides

402. **SEPARATION CHEMISTRY OF TOXIC METALS**
$250,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36) Contact:
P. H. Smith, (505) 667-1604

The goal of this research is to develop a new class of chelators for toxic metals which have the capacity to bind two species and where the binding of one substrate affects the binding of the second. In the process we hope to gain a fundamental understanding of the key parameters which govern toxic metal ion selective binding as it relates to separations chemistry. We will synthesize and evaluate a class of chelators which add a new dimension to coordination chemistry, namely cooperative/antagonistic binding. The chemistry involves the development and synthesis of ditopical receptors which contain two binding sites in close proximity to each other. In systems with cation and anion sites, the simultaneous binding of both a cation and an anion can enhance the overall binding constants relative to either one binding alone.

Keywords: Cooperative/Antagonistic Binding Sites, Chelates, Ditopical Receptors

403. **POLYMERS FOR INTEGRATED OPTICAL INTERCONNECTS**
$266,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36) Contact:
B. Laurich, (505) 665-0333

The recent discovery of electroluminescent polymers opens up, for the first time, the possibility of using optical interconnects for conventional silicon integrated circuits. If this capability can be realized, it will have a tremendous impact on the architecture and performance of the complex computing and communications systems.

Keywords: Electroluminescent Polymers, Integrated Optical Interconnects

404. **HIGH TEMPERATURE MATERIALS SYNTHESIS WITHOUT HEAT: OXIDE LAYER GROWTH ON ELECTRONIC MATERIALS USING HIGH KINETIC ENERGY ATOMIC SPECIES**
$164,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36) Contact:
M. A. Hoffbauer, (505) 667-4878

This research program examines high temperature materials synthesis using high kinetic energy atomic species instead of heat. Emphasis is being placed on the direct growth of oxide and nitride insulating layers on compound semiconducting electronic materials such as GaAs where we have already shown the unprecedented formation of oxide layers that are thick, uniform, and of extremely high quality. Research into this novel material synthesis process with the aim of producing and demonstrating device-quality oxide layers is being emphasized. Application of this materials synthesis technology to space-based manufacturing technology is also being pursued.

Keywords: Ceramic Oxides, Ceramic Nitrides, Insulating Layers, KE Atomic Heating

405. **DYNAMIC DEFORMATION OF ADVANCED MATERIALS**
$855,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36) Contact:
G. T. Gray, (505) 667-5452

Composites, metal or ceramic matrix, and advanced materials, such as intermetallics, are receiving increasing attention due to their higher specific strengths, stiffness, and high temperature properties. Advanced composites also allow other physical properties besides mechanical properties to be custom tailored to specific applications.

Increased utilization of these material classes under dynamic loading conditions requires an understanding of the relationship between high-rate/shock-wave response as a function of microstructure if predictive material behavior capabilities are to be attained. This program is a multidisciplinary effort to investigate the influence of microstructure, anisotropy, orientation, and structural ordering on the high-strain-rate and shock-wave deformation behavior of advanced composites and intermetallics. The long-term objective is to provide high quality experimental measurements on advanced materials to facilitate the development of predictive computational models.

Keywords: High-Strain Rate Deformation, Shock-Wave Deformation, Composites, Intermetallics

406. **STRAIN MEASUREMENTS IN INDIVIDUAL PHASES OF MULTI-PHASE MATERIALS**
$130,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36) Contact:
J. A. Goldstone, (505) 667-3629

Employment of metal matrix and ceramic composites in high-technology aerospace applications or as lighter (more economic) material in the auto industry requires the development of analytical methods capable of predicting the durability, debonding, and damage tolerance during the mechanical and thermal loads expected during service. Neutron diffraction has been used to measure residual stress in composites, steels, and compacted powders. We wish to extend our capability by acquiring a stress rig with a furnace to make in situ measurements of material response. This will permit measurements on technologically important materials under conditions close to service. Preliminary studies will address an Al/TiC composite (under consideration for automotive use) and $MoSi_2$.

Keywords: Neutron Diffraction, Aluminum/Titanium Carbide Composites, Molybdenum Disilicide Composites

407. **ARTIFICIALLY STRUCTURED NONLINEAR OPTIC AND ELECTRO-OPTIC MATERIALS**
$465,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36) Contact:
B. I. Swanson, (505) 667-5814

New artificially structured materials that are optimized for nonlinear optic (NLO) and electro-optic applications will be synthesized, characterized, and modeled. Materials based on two new synthetic strategies will be pursued. Chromophores with optical absorptions tuned to the red and near-IR portion of the spectrum will be directly attached to optical surfaces through the use of covalent bonding of self-assembled (CBSA) mono- and multilayers. The second strategy is based on the construction of single hetero-junctions or multiple hetero-junctions in superlattice materials where charge separation across the junctions results in optimal NLO and electro-optic properties. The overall goal is to further develop these two synthetic approaches through a combined synthesis, characterization, and theory effort where materials modeling, benchmarked by observed physical properties, is used to guide rational synthesis of advanced materials.

Keywords: Nonlinear Optic Materials, Electro-Optic Materials, Superlattice Materials

408. **STRUCTURAL PHASE TRANSITIONS IN NON-STOICHIOMETRIC OXIDES**
$275,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36) Contact:
A. Migliori, (505) 667-2515

Structural phase transitions (SPT) have profound effects on mechanical, magnetic, and electronic properties. In Stoichiometric compounds, SPTs are well understood and produce the magnetism in ferrites and the ferroelectricity in piezoelectric oxides that make these materials so important. However, for non-stoichiometric compounds, the situation is very far from clear, and the puzzles are not merely academic. For example, the high T_c perovskite $La_{2-x}Sr_xCuO_4$ undergoes a second-order SPT from a tetragonal to an orthorhombic structure upon cooling through $T_s(x)$. As T_s is approached from either direction, one shear modulus collapses, making the material mechanically partially unstable, a non-trivial consequence for applications. The surprise is that this collapse begins 100K above T_s, not at 2K predicted by the best theoretical approach. Resonant Ultrasound Spectroscopic (RUS) studies of this and other SPTs reveal additional and subtle problems with current theory, not observed with any other experimental problem. Lack of just this sort of observation has stymied the theory of SPTs in heavily doped crystals because a simple observation of modulus collapse cannot distinguish between several competing possibilities. An understanding of the effects of doping on material properties near SPTs is of extreme fundamental interest and is crucial for a very broad spectrum of applications; recent observations by us suggest that only LANL's unique RUS capability can provide the necessary clues.

Keywords: Resonant Ultrasound Spectroscopy, Structural Phase Transitions

409. **STRONGLY CORRELATED ELECTRONIC MATERIALS**
$495,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36) Contact:
K. S. Bedell, (505) 665-0478

New, novel materials have a number of extraordinary and often unexpected properties and, it is likely, they will play a major role in the high-technology electronic materials of the future. To better design materials for specific applications it is necessary to understand the microscopic origins of their novel physical characteristics. To relate the microscopic models of these strongly correlated systems to specific materials properties requires the extension of and the development of new many-body techniques. This program provides the basic science component for a number of new initiatives that include the Presidential initiative in materials science, the Advanced Computing Laboratory (ACL), the use of novel electronic materials for device applications, the National High Magnetic Field Laboratory (NHMFL), the UC Los Alamos INCOR program in high temperature superconductivity (HTS), and the Program in Correlated Electron Theory.

Keywords: High-Temperature Electronic Materials, Electronic Correlations

410. **PLASMA IMMERSION ION IMPLANTATION FOR SEMICONDUCTOR FILM GROWTH**
$261,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36) Contact:
M. Tuszewski, (505) 667-3566

An interdisciplinary team of plasma and semiconductor physicists will develop a novel plasma implanter for thin film growth on semiconductors with unprecedented control. The scientific objectives of this project are: (1) construction of a compact, inexpensive, and high-throughput implanter based on an inductive plasma source and on e plasma immersion ion implantation (PIII) technique; (2) extension of the PIII technique to higher frequencies, lower voltages, and higher dose rates; (3) characterization, optimization, and control of the plasma species concentrations and impurities; (4) generation of semiconductor dielectrics and alloys for new electronics device technologies.

Keywords: Plasma Ion Implantation, Semiconducting Materials

411. **ANALYSIS OF STRUCTURE AND ORIENTATION OF ADSORBED POLYMER IN SOLUTION SUBJECT TO DYNAMIC SHEAR STRESS**
$172,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36) Contact:
S. Baker, (505) 667-6069

Polymer based separation techniques rely on the ability of a binding portion of the polymer to interact with a specific molecule in a solution flowing past the polymer. The location of the binding site within or out of the entangled polymer chains is thus crucial to the effectiveness of these methods. For this reason, the details of flow induced deformation of the polymer chains is important in such applications as exclusion chromatography, waste water treatment, ultrafiltration, enhanced oil recovery and microbial adhesion. Few techniques exist to examine the structure and orientation of polymeric materials, and even fewer to examine systems in a dynamic fluid flow. The goal of this program is to understand the molecular structure and orientation of adsorbed polymers with and without active binding ligands as a function of solvent shear rate, solvent ower, polymer molecular weight, surface polymer coverage, and heterogeneity of the surface polymer chains by neutron reflectometry in a newly Designed shear cell. Geometrical effects on binding of molecules in the flow will also be studied subject to the same parameters.

Keywords: Polymer Molecules, Neutron Reflectometry, Flow Induced Deformation

412. **DEVELOPMENT OF PAIR DISTRIBUTION FUNCTION ANALYSIS OF MESOSTRUCTURAL DETAILS IN SINGLE CRYSTAL PEROVSKITES AND NANOCRYSTALLINE MATERIALS**
$170,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36) Contact:
G. H. Kwei, (505) 667-8840

It has become increasingly evident that structural coherence in the CuO_2 planes of high-Tc superconducting (HTSC) materials over some intermediate length scale (in the nanometer range) is important to superconductivity. Significant progress has been made in understanding these structural instabilities using pair distribution function analysis of powder diffraction data. However, PDF diffraction data on single crystals is required, both because of the greater amount of information in the latter and because of the much greater sample quality that is available in single crystals. The goal of this program is to develop analysis techniques for obtaining PDF's from single crystal diffraction data and to use these techniques to study structural instabilities and structural coherence in HTSC and other interesting materials. PDF techniques are also planned for studying mesostructural features in nanocrystalline materials.

Keywords: Powder Diffraction Analysis, High Temperature Superconductors, Mesostructural Nanocrystals

413. **NEUTRON SCATTERING AS A PROBE OF THE STRUCTURE OF LIQUID CRYSTAL POLYMER-REINFORCED COMPOSITE MATERIALS**
$180,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36) Contact:
R. P. Hjelm, (505) 665-2372

The goal of this program is to obtain nanoscale and molecular level information on the mechanism of reinforcement 9n crystal polymer-reinforced composites, and to realize the production of molecularly-reinforced LCP composites. Small-angle neutron scattering methods are proposed to study the structures on length scales ranging from 10-1000 Å. The goal of the small-angle scattering measurements is to understand the morphology of separation of the reinforcing and matrix phases as a function of composition, mixing, temperature and other process conditions. This information will be correlated with mechanical properties to achieve a better understanding of the molecular mechanism of reinforcement.

Keywords: Small-Angle Neutron Scattering, Polymer Composites

414. **STRAIN MEASUREMENTS IN INDIVIDUAL PHASES OF MULTI-PHASED MATERIALS DURING THERMO-MECHANICAL LOADING: LANSCE NEUTRON SCATTERING EXPERIMENT SUPPORT**
$318,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36) Contact:
J. A. Goldstone, (505) 667-3629

Employment of metal matrix and ceramic composites in high-technology aerospace applications or as lighter (more economic) material, in the auto industry requires the development of analytical methods capable of predicting the durability, debonding, and damage tolerance during the mechanical and thermal loads expected during service. Neutron diffraction has been used to measure residual stress in composites, steels and compacted powders. We wish to extend our capability by acquiring a stress rig with a furnace to make in situ measurements of material response. This will permit measurements on technologically important materials under conditions close to service. Preliminary studies will address an Al/TiC composite (under consideration for automotive use) and $MoSi_2$.

Keywords: Neutron Diffraction, Metal Matrix Composites, Ceramic Matrix Composites

415. **A NEW APPROACH TO TEXTURE MEASUREMENTS: ODF DETERMINATION BY RIETVELD REFINEMENT**
$73,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36) Contact:
R. B. VonDreele, (505) 667-3630

This program centers on the development of the experimental procedures and the mathematical treatment needed to produce an orientation distribution function (ODF) directly from full diffraction patterns from a sample in a limited number of orientations.

Keywords: Texture Measurement, Orientation Distribution Function, Diffraction Patterns

416. **APPLICATIONS OF FULLERENES IN NUCLEAR TECHNOLOGY**
$360,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36) Contact:
D. K. Veirs, (505) 667-9291

The major focus of our research efforts is in the use of fullerene-based materials in the solution to problems in the nuclear research and industry. Fullerene encapsulation of nuclear waste is of interest in the storage of high-level nuclear waste. Fullerene-encapsulated uranium or plutonium may be very stable with respect to the environment and may provide a safe and efficient way of disposing of nuclear waste. The metal-in-fullerene aspect or metal-doped fullerene compounds in conjunction with the high thermal stability and low density of fullerene suggests the fabrication of efficient, high-yield targets for the production of radioactive beams. It is likely that a target composed fullerene, upon proton-induced fission or spallation of the uranium, will allow the efficient release of the fission or spallation products for the purpose of producing radioactive nuclear beams. We propose to explore the production of actinide fullerides and to develop the relevant technology to generate and separate them for these purposes.

Keywords: Fullerenes, Encapsulation, Nuclear Waste, Uranium, Plutonium

417. **CERAMIC OXIDE FOAMS FOR SEPARATION**
$400,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36) Contact:
P. C. Apen, (505) 665-7513

Ceramic oxide foams and novel foam structures are playing an important role in environmental R&D, specifically in the areas of chemical separations and filtration for removal of heavy metals and particulates from contaminated waste streams and effluent. This program focusses on the investigation of virgin oxide and surface-modified oxide foams in environmental remediation applications. Processes for the preparation and modification of porous ceramic structures will be developed and the products characterized for functionality in the separation of heavy metal and toxic particulates from waste streams.

Keywords: Silica Foams, Silica Sol-Gels, Heavy Metal Ligands, Metal Ion Chelating Agents

418. **MATERIALS MODELING PROJECT**
$125,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36) Contact:
R. LeSar, (505) 665-0420

This program involves the modeling of laser-assisted deposition processes with an emphasis on laser/solid interactions, plasma chemistry and dynamics, nucleation and growth, and the theoretical design of novel materials. The modeling will also involve analytical studies of strain-induced diffusion along specific interfaces and Monte Carlo studies of diffusion in polycrystalline materials. The goal of the program is to link this work with a micromechanical fracture model.

Keywords: Laser-Assisted Deposition Processes, Micromechanical Fracture Models, Plasma Chemistry

419. **SYNTHESIS AND OPTICAL CHARACTERIZATION OF NOVEL FULLERENE-BASED COMPOSITES**
$50,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36) Contact:
J. M. Robinson, (505) 665-4834

This program takes an interdisciplinary approach to develop and study a novel family of fullerene-based organic and inorganic composites for applications as photodiodes and photovoltaic devices. The emphasis of the program is on "proof of principle" for the synthesis of new composite materials which will guide further synthetic refinements. A novel "host-guest" chemistry will result in two new classes of materials. The first class utilizes sol-gel chemistry to incorporate fullerenes into optically transparent hosts that are processable into thick glass monoliths or thin film waveguides. The principal role of the host is to protect the fullerene guests from environmental degradation, and to provide a low loss transparent medium for light transmission. The second class of materials is based on fullerene/conjugated polymer composites.

Keywords: Fullerene Composites, Photodiodes, Photovoltaic Devices, Sol-Gels

TECHNOLOGY TRANSFER INITIATIVE

420. **A PILOT PROGRAM: CHEMICAL VAPOR DEPOSITION OF DIAMOND IN A FLUIDIZED-BED FOR CUTTING TOOL AND TRIBOLOGICAL APPLICATIONS**
$250,000
DOE Contact: W. P. Chernock (202) 586-7590
LANL (Contract No. W-7405-ENG-36) Contact:
David Carroll, (505) 667-2145

A program to develop and commercialize a process to generate high-quality diamond coatings for machine tools.

Keywords: Diamond Coatings, Chemical Vapor Deposition, Cutting Tools, Tribology

421. **ADVANCED BERYLLIUM PROCESSING**
$632,000
DOE Contact: W. P. Chernock (202) 586-7590
LANL (Contract No. W-7405-ENG-36) Contact:
Loren Jacobson, (505) 667-5151

A program to produce beryllium powders and rolled beryllium sheet using improved manufacturing techniques that minimize worker exposure and reduce the environmental consequences of beryllium processing.

Keywords: Beryllium Processing, Beryllium Alloy Processing, Centrifugal Atomization

422. **AUTOMATED PULSED LASER DEPOSITION SYSTEM**
$130,000
DOE Contact: W. P. Chernock (202) 586-7590
LANL (Contract No. W-7405-ENG-36) Contact:
Ross Muenchausen, (505) 665-4949

A program to design an automated pulsed laser deposition system to deposit high-temperature superconducting thin films.

Keywords: Pulsed-Laser-Deposition, High-Temperature Superconducting Films

423. **PLASMA SOURCE ION IMPLANTATION FOR THE AUTOMOTIVE INDUSTRY**
$1,326,000
DOE Contact: W. P. Chernock (202) 586-7590
LANL (Contract No. W-7405-ENG-36) Contact:
Donald Rej (505) 665-1883

A program to develop a production-scale plasma-source ion implantation system for improving the surface properties of auto parts.

Keywords: Plasmas, Ion Implantation, Tool Hardening

424. **PROCESSING MODELING AND CONTROL FOR U.S. STEEL INDUSTRY**
$1,195,000
DOE Contact: W. P. Chernock (202) 586-7590
LANL (Contract No. W-7405-ENG-36) Contact:
Brian Lally, (505) 667-9954

A program to develop new process models and control systems for the U.S. Steel Industry.

Keywords: Steel, Electric-Arc-Furnace, Scrap Steels

OFFICE OF FOSSIL ENERGY

	FY 1995
Office of Fossil Energy - Grand Total	$7,668,000
Office of Advanced Research	$7,668,000
Fossil Energy AR&TD Materials Program	$7,668,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$3,293,000
Coating Process Development for Cr-Nb Alloys	90,000
Procurement of Advanced Austenitic and Aluminide Alloys	50,000
Development of Iron Aluminides	170,000
Ultrahigh Temperature Intermetallic Alloys	200,000
Microalloyed Iron Aluminides	78,000
Low-Aluminum Content Iron-Aluminum Alloys	75,000
Mo-Si Alloy Development	10,000
Technology Transfer - Iron Aluminides	60,000
Commercial-Scale Melting and Processing of Low-Aluminum Content Alloys	50,000
Development of a Modified 310 Stainless Steel	120,000
Technology Transfer - Advanced Austenitics	80,000
Influence of Processing on Microstructure and Properties of Aluminides	175,000
Investigation of Electrospark Deposited Coatings for Protection of Materials in Sulfidizing Atmospheres	75,000
Technology Transfer - Electrospark-Deposited Coatings for Protection of Materials in Sulfidizing Atmospheres	80,000
Engineering-Scale Development of the Vapor-Liquid-Solid (VLS) Process for the Production of Silicon Carbide Fibrils	PYF*
Ceramic Composite Processing Equipment	30,000
Fabrication of Fiber-Reinforced Composites by Chemical Vapor Infiltration and Deposition	150,000
Compliant Oxide Coating Development	75,000
Development of Oxidation/Corrosion-Resistant Composite Materials and Interfaces	127,000
Optimization of the Chemical Vapor Infiltration Technique for Ceramic Composites	85,000
Transport Properties of Ceramic Composites	148,000
Modeling of Fibrous Preforms for CVD Infiltration	50,000
Corrosion Protection of SiC-Based Ceramics with CVD Mullite Coatings	50,000
Feasibility of Synthesizing Oxide Films on Ceramic and Metal Substrates	100,000
Screening Analysis of Ceramic Hot-Gas Filter Materials	PYF
Environmental Effects on Ceramics	100,000
Ceramic Coating Evaluation	100,000
Metal Dusting Study	25,000
Low-Temperature Fabrication of Transparent Silicon Nitride	100,000
Microwave-Assisted Chemical Vapor Infiltration	25,000
Development of Microwave-Heated Diesel Particulate Filters	75,000

*PYF denotes that funding for this activity, active in FY 1995, was provided from prior year funds.

OFFICE OF FOSSIL ENERGY (Continued)

	FY 1995
Office of Advanced Research (continued)	
Fossil Energy AR&TD Materials Program (continued)	
Materials Preparation, Synthesis, Deposition, Growth or Forming (continued)	
Carbon Fiber Composite Molecular Sieves	275,000
Carbon Materials Equipment	15,000
Activation of Carbon Fiber Composite Molecular Sieves	75,000
Characterization of Coal and Coal Extracts	20,000
Production of Aluminum Reduction Electrodes from Solvent-Extracted Coal-Derived Carbon Feedstocks	PYF*
Exploration of Coal-Based Pitch Precursors for Ultra-High Thermal Conductivity Graphite Fibers	PYF*
Development of Carbon-Carbon Composites from Solvent-Extracted Pitch	PYF*
Conversion of Pitches and Cokes from Solvent-Extracted Materials	PYF*
Carbon Fiber Composite Molecular Sieves	155,000
Development of Precursors for Production of Graphites and Carbon Products	PYF*
Production of Yarn From VLS Whiskers	100,000
Radio-Wave Nano-Phase Silicon Nitride and Silicon Carbide Processes	100,000
Materials Properties, Behavior, Characterization or Testing	$2,117,000
Investigation of the Weldability of Polycrystalline Iron Aluminides	75,000
Aqueous Corrosion of Iron Aluminides	29,000
Evaluation of the Intrinsic and Extrinsic Fracture Behavior of Iron Aluminides	68,000
Investigation of Iron Aluminide Weld Overlays	56,000
Fireside Corrosion Tests of Candidate Advanced Austenitic Alloys, Coatings, and Claddings	80,000
Joining Techniques for Advanced Austenitic Alloys	50,000
Fatigue and Fracture Behavior of Cr-Nb Alloys	20,000
Corrosion and Mechanical Properties of Alloys in FBC and Mixed-Gas Environments	310,000
Mechanically Reliable Coatings and Scales for High-Temperature Corrosion Resistance	50,000
Environmental Effects on Iron Aluminides	145,000
Investigation of Moisture-Induced Embrittlement of Iron Aluminides	73,000
Corrosion Protection of Ultrahigh Temperature Intermetallic Alloys	146,000
Oxide Dispersion Strengthened (ODS) Iron Aluminide Equipment	35,000
Oxide Dispersion Strengthened (ODS) Iron Aluminides	222,000
Materials Support for HITAF	PYF*
Characterization of Low-Expansion Ceramic Materials and Development of Sol Gel-derived Coatings as Interfaces for SiC Composites	23,000

*PYF denotes that funding for this activity, active in FY 1995, was provided from prior year funds.

OFFICE OF FOSSIL ENERGY (Continued)

	FY 1995
Office of Advanced Research (continued)	
Fossil Energy AR&TD Materials Program (continued)	
Materials Properties, Behavior, Characterization or Testing (continued)	
Joining of Ceramics	50,000
Support Services for Ceramic Fiber-Ceramic Matrix Composites	25,000
Development of Nondestructive Evaluation Methods and Effects of Flaws on the Fracture Behavior of Structural Ceramics	310,000
Fracture Behavior of Advanced Ceramic Hot-Gas Filters	125,000
Ceramic Catalyst Materials	225,000
Device or Component Fabrication, Behavior or Testing	$1,819,000
Materials and Components in Fossil Energy Applications Newsletter	60,000
Ceramic Fiber Filter Technology	50,000
Fabrication of Full-Scale Fiber-Reinforced Hot-Gas Filters by Chemical Vapor Deposition	PYF*
Development of Ceramic Membranes for Gas Separation	400,000
Corrosion Protection of Ceramic Heat Exchanger Tubes	125,000
Investigation of the Mechanical Properties and Performance of Ceramic Composite Components	150,000
Stability of Solid Oxide Fuel Cell Materials	250,000
Mixed Oxygen Ion/Electron-Conducting Ceramics for Oxygen Separation and Fuel Cells	225,000
Proton-Conducting Cerate Ceramics	225,000
ODS Fe_3Al Tubes for High-Temperature Heat Exchangers	53,000
Porous Iron Aluminide Alloys	23,000
Iron Aluminide Filters	50,000
Evaluation of Ceramic Heat Exchanger Tubes and Joints	158,000
Thermal and Mechanical Analysis of a Ceramic Tubesheet	40,000
Ceramic Tubesheet Design Analysis	10,000
Instrumentation and Facilities	$ 439,000
Management of the Fossil Energy AR&TD Materials Program	400,000
General Technology Transfer Activities	35,000
Gordon Research Conference Support	4,000

*PYF denotes that funding for this activity, active in FY 1995, was provided from prior year funds.

OFFICE OF FOSSIL ENERGY

The Office of Fossil Energy responsibilities include management of the Department's fossil fuels (coal, oil and natural gas) research and development program. This research is generally directed by the Office of Coal Technology (OCT), the Office of Gas and Petroleum Technology, and the Office of Advanced Research and Special Technologies in support of the National Energy Strategy Goals for Increasing Energy Efficiency, Securing Future Energy Supplies, Respecting the Environment, and Fortifying our Foundations. Three specific fossil energy goals are currently being pursued:

- The first is to secure liquids supply and substitution. This goal targets the enhanced production of domestic petroleum and natural gas, the development of advanced, cost-competitive alternative fuels technology, and the development of coal-based, end-use technology to substitute for oil in applications traditionally fueled by liquid and gaseous fuel forms.

- The second is to develop power generation options with environmentally superior, high-efficiency technologies for the utility, industrial, and commercial sectors. This goal targets the development of super-clean, high-efficiency power generation technologies.

- The third is to pursue a global technology strategy to support the increased competitiveness of the U.S. in fossil fuel technologies, to maintain world leadership in our fossil fuel technology base, and provide expanded markets for U.S. fuels and technology. This crosscutting goal is supported by the activities in the above two technology goals.

OFFICE OF ADVANCED RESEARCH

FOSSIL ENERGY AR&TD MATERIALS PROGRAM

Fossil Energy (FE) materials-related research is conducted under an Advanced Research and Technology Development (AR&TD) Materials subactivity and is an integral part of the R&D conducted by the Office of Advanced Research and Special Technologies. The AR&TD Materials program includes cross-cutting research to obtain a fundamental understanding of materials and how they perform in fossil-based process environments and the development of new classes of generic materials that will allow the development of new fossil energy systems or major improvements in existing systems. The present program is focused on ceramics (composite structural ceramics, catalyst supports, solid state electrolytes, membranes, and ceramic filters), new alloys (aluminides, advanced austenitic steels, and coatings and claddings), corrosion research, and technology development and transfer.

The AR&TD research is carried through development and technology transfer to industry. Special emphasis is being given to technology transfer to ensure that the materials will be available for subsequent fossil commercial applications. This also enhances U.S. technological competitiveness not only in the fossil area but in the materials industry in general and other technology application areas as well. The research is conducted in industry, universities, not-for-profit agencies, and national laboratories. This widespread participation also helps maintain the U.S. materials technology capabilities.

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

425. **COATING PROCESS DEVELOPMENT FOR Cr-Nb ALLOYS**
$90,000
DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole, (423) 574-4824
Ohio State University Contact: R. A. Rapp, (614) 292-6178

Cr-Nb alloys are being developed for high temperature service, but require protection from high temperature environments, such as oxidation. Previously developed $MoSi_2$-base coatings have shown some promise for protecting Nb, and the principles learned may have applicability for protective coatings of Cr-Nb. The purpose of this work is to examine the protection of Cr-Nb alloys with either silicides or aluminides.

Keywords: Alloys, Aluminizing, Chromizing, Corrosion, Coatings

426. **PROCUREMENT OF ADVANCED AUSTENITIC AND ALUMINIDE ALLOYS**
$50,000
DOE Contacts: J. P. Carr, (301) 903-6519 and
E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole,
(423) 574-4824

This task provides funds for the procurement of alloys necessary for alloy development and testing activities of the AR&TD Materials Program.

Keywords: Alloys, Aluminides, Austenitic

427. **DEVELOPMENT OF IRON ALUMINIDES**
$170,000
DOE Contacts: J. P. Carr, (301) 903-6519 and
E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact:
C. G. McKamey, (423) 574-6917

The objective of this task is to develop low-cost and low-density intermetallic alloys based on Fe_3Al with an optimum combination of strength, ductility, weldability, and corrosion resistance for use as components in advanced fossil energy conversion systems. Emphasis is on the development of iron aluminides for heat recovery applications in coal gasification systems.

Keywords: Alloys, Aluminides, Intermetallic Compounds

428. **ULTRAHIGH TEMPERATURE INTERMETALLIC ALLOYS**
$200,000
DOE Contacts: J. P. Carr, (301) 903-6519 and
E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: C. T. Liu,
(423) 574-4459

The objective of this task is to develop high-strength, corrosion-resistant intermetallic alloys for use as hot components in advanced fossil energy conversion and power generation systems. The successful development of these alloys is expected to improve the thermal efficiency of fossil energy conversion systems through increased operating temperatures and to increase the service life of hot components exposed to corrosive environments at elevated temperatures (1000 °C). The work is focused on *in situ* composite alloys based on the $Cr-Cr_2Nb$ system.

Keywords: Alloys, Chromium-Niobium, Corrosion, Intermetallic Compounds

429. **MICROALLOYED IRON ALUMINIDES**
$78,000
DOE Contacts: J. P. Carr, (301) 903-6519 and
E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact:
C. G. McKamey, (423) 574-6917

The objective of this task is to use microalloying techniques to further develop the Fe_3Al-based alloys. Emphasis is on producing a low-cost, low-density, precipitation-strengthened Fe_3Al-based intermetallic alloy with improved high-temperature creep resistance while maintaining an optimum combination of room-temperature and high-temperature (600-700 °C) tensile properties, weldability, and corrosion resistance for use as structural components of advanced fossil energy conversion systems.

Keywords: Alloys, Aluminides, Microalloy

430. **LOW-ALUMINUM CONTENT IRON-ALUMINUM ALLOYS**
$75,000
DOE Contacts: J. P. Carr, (301) 903-6519 and
E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: V. K. Sikka,
(423) 574-5112

The objective of this task is to develop a conventionally fabricable low-cost and lower density iron-aluminum-based alloy with a good combination of strength, ductility, weldability, and corrosion resistance for use as components in advanced fossil energy systems. Initial emphasis is on the development of iron-aluminum alloys for heat-recovery applications in coal gasification systems.

Keywords: Alloys, Iron-Aluminum

431. **Mo-Si ALLOY DEVELOPMENT**
$10,000
DOE Contacts: J. P. Carr, (301) 903-6519 and
E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: C. T. Liu,
(423) 574-4559

The objective of this task is to develop new-generation corrosion-resistant Mo-Si alloys for use as hot components in advanced fossil energy conversion and power generation systems. The successful development of Mo-Si alloys is expected to improve the thermal efficiency and performance of fossil energy systems through increased operating temperature and to increase the service life of hot components exposed to corrosive environments at high temperatures (to 1600 °C). The initial effort is devoted to Mo_5Si_3-base alloys containing boron additions.

Keywords: Alloys, Molybdenum, Silicon

432. **TECHNOLOGY TRANSFER - IRON ALUMINIDES**
$60,000
DOE Contacts: J. P. Carr, (301) 903-6519 and
E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: V. K. Sikka,
(423) 574-5112

A Cooperative Research and Development Agreement (CRADA) has been established with ABB Combustion Engineering for the development of corrosion-resistant surface protection for fossil power systems.

Keywords: Alloys, Iron-Aluminum, Corrosion, Technology Transfer

433. **COMMERCIAL-SCALE MELTING AND PROCESSING OF LOW-ALUMINUM CONTENT ALLOYS**
$50,000
DOE Contacts: J. P. Carr, (301) 903-6519 and
E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: V. K. Sikka,
(423) 574-5112

The purpose of this activity is the preparation and evaluation of castings of FAPY alloy. The castings will be prepared in several types of molds including: (1) graphite, (2) sand, and (3) investment. Castings will be prepared primarily from the air-induction-melted material. Selected graphite and investment castings will also be prepared from the vacuum- induction-melted material. The graphite and sand castings will be prepared at ORNL and will also be procured from the commercial foundries. The castings will be evaluated for porosity, grain structure, mechanical properties, and weldability. The mechanical property evaluation will consist of Charpy, tensile, and creep testing.

Keywords: Alloys, Iron-Aluminum, Melting, Casting

434. **DEVELOPMENT OF A MODIFIED 310 STAINLESS STEEL**
$120,000
DOE Contacts: J. P. Carr, (301) 903-6519 and
E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact:
R. W. Swindeman, (423) 574-5108

The purpose of this task is to evaluate structural alloys for improved performance of high-temperature components in advanced combined-cycle and coal-combustion systems.

Keywords: Materials, Mechanical Properties, Austenitics, Hot-Gas

435. **TECHNOLOGY TRANSFER - ADVANCED AUSTENITICS**
$80,000
DOE Contacts: J. P. Carr, (301) 903-6519 and
E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact:
R. W. Swindeman, (423) 574-5108

A Cooperative Research and Development Agreement (CRADA) has been established with ABB Combustion Engineering for the development of advanced austenitic alloys for fossil power systems.

Keywords: Alloys, Austenitics, Technology Transfer

436. **INFLUENCE OF PROCESSING ON MICROSTRUCTURE AND PROPERTIES OF ALUMINIDES**
$175,000
DOE Contacts: J. P. Carr, (301) 903-6519 and
E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole,
(423) 574-4824
Idaho National Engineering Laboratory Contact:
R. N. Wright, (208) 526-6127

The purpose of this project is to determine the influence of processing on the properties of alloys based on Fe_3Al. Thermomechanical processing is pursued to improve their room-temperature ductility. The response of the microstructure to annealing will be characterized in terms of the establishment of equilibrium phases and degrees of long-range order. The mechanical properties are determined at room and elevated temperatures and related to the microstructure.

Keywords: Aluminides, Processing, Microstructure

437. **INVESTIGATION OF ELECTROSPARK DEPOSITED COATINGS FOR PROTECTION OF MATERIALS IN SULFIDIZING ATMOSPHERES**
$75,000
DOE Contacts: J. P. Carr, (301) 903-6519 and
E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole,
(423) 574-4824
Pacific Northwest National Laboratory Contact:
R. N. Johnson, (509) 375-6906

The purpose of this task is to examine the use of the electrospark deposition coating process for the application of corrosion-, erosion-, and wear-resistant coatings to candidate heat exchanger (including superheater and reheater) alloys. Materials to be deposited may include MCrAl, MCrAlY, highly wear-resistant carbides, and other hardsurfacing materials.

Keywords: Coatings, Materials, Deposition

438. **TECHNOLOGY TRANSFER - ELECTROSPARK DEPOSITED COATINGS FOR PROTECTION OF MATERIALS IN SULFIDIZING ATMOSPHERES**
$80,000
DOE Contacts: J. P. Carr, (301) 903-6519 and
E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole,
(423) 574-4824
Pacific Northwest National Laboratory Contact:
R. N. Johnson, (509) 375-6906

The purpose of this task is to transfer to industry the electrospark deposition coating process technology for the application of corrosion-, erosion-, and wear-resistant coatings to candidate heat exchanger [including superheater and reheater] alloys.

Keywords: Coatings, Materials, Deposition

439. **ENGINEERING-SCALE DEVELOPMENT OF THE VAPOR-LIQUID-SOLID (VLS) PROCESS FOR THE PRODUCTION OF SILICON CARBIDE FIBRILS**
$0 (PYF)*
DOE Contacts: J. P. Carr, (301) 903-6519 and
E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole,
(423) 574-4824
The Carborundum Company Contact: S. K. Lau,
(716) 278-2004

The purpose of this work is to transfer to industry a specific technology developed by the DOE AR&TD Materials Program for the production of silicon carbide fibrils for the reinforcement of ceramic matrices. The Vapor-Liquid-Solid (VLS) process was developed at Los Alamos National Laboratory for the growth of silicon carbide fibrils of up to 75 mm in length which can be reduced in length by subsequent processing. The purpose of the work is to develop the VLS process into an engineering-scale process that will enable the U.S. industrial sector to commercialize the process for the production of fibrils for the reinforcement of structural ceramic components.

Keywords: Whiskers, Fibers, Ceramic

440. **CERAMIC COMPOSITE PROCESSING EQUIPMENT**
$30,000
DOE Contacts: J. P. Carr, (301) 903-6519 and
E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: D. P. Stinton,
(423) 574-4556

This task provides funds for the procurement of major equipment items necessary for AR&TD Materials Program activities.

Keywords: Equipment

*PYF denotes that funding for this activity, active in FY 1995, was provided from prior year funds.

441. FABRICATION OF FIBER-REINFORCED COMPOSITES BY CHEMICAL VAPOR INFILTRATION AND DEPOSITION
$150,000
DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: D. P. Stinton, (423) 574-4556

The purpose of this task is to develop a process for the fabrication of fiber-reinforced ceramic composites having high fracture toughness and high strength. This process utilizes a steep temperature gradient and a pressure gradient to infiltrate low-density fibrous structures with gases, which deposit solid phases to form the matrix of the composite. Further development of this process is needed to fabricate larger components of more complex geometry, and to optimize infiltration for shortest processing time, greatest density and maximum strength.

Keywords: Composites, Fiber-Reinforced, Ceramics

442. COMPLIANT OXIDE COATING DEVELOPMENT
$75,000
DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: D. P. Stinton, (423) 574-4556

Monolithic SiC heat exchangers and fiber-reinforced SiC-matrix composite heat exchangers and filters are susceptible to corrosion by alkali metals at elevated temperatures. Protective coatings are currently being developed to isolate the SiC materials from the corrodents. Unfortunately, these coatings typically crack and spall when applied to SiC substrates. The purpose of this task is to determine the feasibility of using a compliant material between the protective coating and the substrate. The low-modulus compliant layer could absorb stresses and eliminate cracking and spalling of the protective coatings.

Keywords: Ceramics, Oxides, Coatings

443. DEVELOPMENT OF OXIDATION/CORROSION-RESISTANT COMPOSITE MATERIALS AND INTERFACES
$127,000
DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: D. P. Stinton, (423) 574-4556

Fiber-reinforced SiC-matrix composites have been observed to fail in fossil energy applications for two reasons. First, the mechanical properties of composites deteriorate under stressed oxidation because oxidants such as steam penetrate cracks formed in the SiC matrix and react with the carbon or boron nitride interface. The mechanical properties of composites may degrade because of corrosion due to sodium species typically present in fossil systems. Therefore, the purposes of this task are to first, develop fiber-matrix interfaces that are resistant to oxidation and yet optimize the mechanical behavior of composites, and second, to develop protective overcoats or oxide matrices that are resistant to oxidation and corrosion.

Keywords: Composites, Ceramics, Fiber-Reinforced, Interfaces

444. OPTIMIZATION OF THE CHEMICAL VAPOR INFILTRATION TECHNIQUE FOR CERAMIC COMPOSITES
$85,000
DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole, (423) 574-4824
University of Tennessee Contact: Peter Liaw, (423) 974-6356

This project is focused on an optimization of the forced chemical vapor infiltration technique for fabrication of ceramic matrix composites (CMCs) using process models. In particular, a process model developed at the Georgia Tech Research Institute shall be thoroughly investigated. Experimental verification of the process model shall be conducted in light of microstructural characterization using both destructive and nondestructive evaluation techniques. An optimized process for manufacturing CMCs shall be demonstrated. Moreover, mechanistic understanding regarding the effects of processing parameters on microstructural features, and fatigue and fracture behavior of CMCs shall be provided.

Keywords: Composites, Fiber-Reinforced, Ceramics

445. TRANSPORT PROPERTIES OF CERAMIC COMPOSITES
$148,000
DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole, (423) 574-4824
Georgia Institute of Technology Contact: T. L. Starr, (404) 853-0579

The purpose of this research effort is to conduct a theoretical and experimental program to identify new compositions and processing methods to improve the physical and mechanical properties of selected fiber-reinforced ceramics. The ceramic matrix material is amorphous fused silica or modified silica glass, and the focus is the development of fiber-reinforced silica. Parameters studied include: (1) differences in elastic modulus between matrix and fiber, (2) differences in thermal expansion, (3) nature of interfacial bond, (4) densification of matrix, (5) nature of fiber fracture/pull-out, (6) fiber diameter and fiber length-to-diameter ratio, (7) fiber loading, and (8) fiber dispersion and orientation. A model will be developed based on the information generated in the experimental phase of the program.

Keywords: Ceramics, Composites, Fiber-Reinforced

446. **MODELING OF FIBROUS PREFORMS FOR CVD INFILTRATION**
$50,000
DOE Contacts: J. P. Carr, (301) 903-6519 and
E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole, (423) 574-4824
Georgia Institute of Technology Contact: T. L. Starr, (404) 853-0579

The purpose of this project is to conduct a theoretical and experimental program to develop an analytical model for the fabrication and infiltration of fibrous preforms. The analytical model will: (1) predict preform structure (density, porosity, fiber orientation, etc.) based on fabrication technique and fundamental fiber parameters (diameter, aspect ratio, etc.), and (2) predict permeation and heat conduction through the preform structure and, thus, predict the CVD infiltration performance.

Keywords: Ceramics, Composites, Modeling

447. **CORROSION PROTECTION OF SiC-BASED CERAMICS WITH CVD MULLITE COATINGS**
$50,000
DOE Contacts: J. P. Carr, (301) 903-6519 and
E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole, (423) 574-4824
Boston University Contact: Vinod Sarin, (617) 353-6451

This project involves the growth of dense mullite coatings on SiC-based substrates by chemical vapor deposition. SiC and SiC-based composites have been identified as the leading candidate materials for stringent elevated temperature applications. At moderate temperatures and pressures, the formation of a thin self-healing layer of SiO_2 is effective in preventing catastrophic oxidation by minimizing the diffusion of O_2 to the substrate. The presence of impurities can increase the rate of passive oxidation by modifying the transport rate of oxygen through the protective scale, can cause active oxidation via formation of SiO which accelerates the degradation process, or can produce compositions such as Na_2SO_3 which chemically attack the ceramic via rapid corrosion. There is therefore a critical need to develop adherent oxidation/corrosion-resistant, and thermal-shock-resistant coatings that can withstand such harsh environments. Mullite has been identified as an excellent candidate material due to its desirable properties of toughness, corrosion resistance, and a good coefficient of thermal expansion match with SiC.

Keywords: Ceramics, Coatings

448. **FEASIBILITY OF SYNTHESIZING OXIDE FILMS ON CERAMIC AND METAL SUBSTRATES**
$100,000
DOE Contacts: J. P. Carr, (301) 903-6519 and
E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole, (423) 574-4824
Lawrence Berkeley Laboratory Contact: Ian Brown, (510) 486-4174

The objective of this project is the study of the feasibility of synthesizing metal oxide ceramic films on ceramic and metal substrates. This feasibility will be demonstrated by use of plasma-based deposition and ion mixing techniques. The films shall be characterized for properties such as composition, structure, hardness, high temperature oxidation resistance, adhesion to the substrate, and stability to high temperature cycling. The value of intermediate transition or buffer layers, composed of materials with suitably matched thermal expansion characteristics and atomically graded interfaces, as a technique for improving the high temperature survivability of the films, shall be explored. Samples shall be formed on substrates of various shapes and sizes, including perhaps on the inside and outside of pipes, as well as on small flat coupons. The issue of deposition onto and atomic mixing into substrates which are insulating shall be addressed experimentally. The work is divided into two parts: (1) Al_2O_3 films on alumina-forming alloy substrates, and (2) oxides on SiC.

Keywords: Ceramics, Films, Oxides

449. **SCREENING ANALYSIS OF CERAMIC HOT-GAS FILTER MATERIALS**
$0 (PYF)*
DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole, (423) 574-4824
Pennsylvania State University Contact: R. E. Tressler, (814) 865-7961

This project will include a screening analysis of candidate ceramic hot-gas filter materials. A flow-through screening test will be developed to test ceramic hot-gas filter elements in simulated coal combustion environments.

Keywords: Ceramics, Corrosion, Coatings

450. **ENVIRONMENTAL EFFECTS ON CERAMICS**
$100,000
DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contacts: P. F. Tortorelli, (423) 574-5119

The purpose of this work is to support the development of advanced ceramics and ceramic composites for applications in fossil environments by examining critical issues related to high-temperature corrosion resistance. More specifically, the overall objective of this task is to examine the chemical compatibility and reliability of potentially corrosion-resistant ceramics being developed as protective overcoats and/or structural materials as parts of other work elements funded by the AR&TD Program.

Keywords: Coatings, Corrosion

451. **CERAMIC COATING EVALUATION**
$100,000
DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contacts: P. F. Tortorelli, (423) 574-5119

The purpose of this work is to generate the information needed for the development of improved (slow growing, adherent, sound) protective oxide coatings and scales. The specific objectives are to (1) systematically investigate the relationships among substrate composition and surface oxide structure, adherence, soundness, and micromechanical properties, (2) use such information to predict scale and coating failures, and (3) identify and evaluate compositions and synthesis routes for producing materials with damage-tolerant scales and coatings.

Keywords: Coatings, Corrosion

452. **METAL DUSTING STUDY**
$25,000
DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contacts: P. F. Tortorelli, (423) 574-5119

The objective of this task is to establish the potential risk of operating problems due to carbon deposition and metal dusting in advanced coal gasification processes and to identify methods for avoiding carbon deposition. The work involves a literature search, compilation of a bibliography of relevant articles, and a summary of the current state of knowledge.

Keywords: Coatings, Corrosion

453. **LOW-TEMPERATURE FABRICATION OF TRANSPARENT SILICON NITRIDE**
$100,000
DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole, (423) 574-4824
National Institute of Standards and Technology Contact: S. G. Malghan, (301) 975-6101

The objective of this research is the production of dense, hard, transparent ceramics from nanosize particles without the use of sintering aids. The work will concentrate on the fabrication of samples of transparent silicon nitride using the cryogenic compaction technique. TEM, SEM, X-ray diffraction, and laser light scattering will be used to characterize the microstructure. Hardness at various temperatures will be measured to assess the creep resistance of the material. Fracture toughness and bending strength will also be measured.

Keywords: Ceramics, Mechanical Properties

*PYF denotes that funding for this activity, active in FY 1995, was provided from prior year funds.

454. MICROWAVE-ASSISTED CHEMICAL VAPOR INFILTRATION
$25,000
DOE Contacts: J. P. Carr, (301) 903-6519 and
E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: M. A. Janney,
(423) 574-4281

The purpose of this research effort is to explore the feasibility of using microwave heating to enhance the *chemical vapor infiltration* (CVI) process developed under the Fossil Energy Materials Program (FEMP) sponsorship. The goal is to achieve faster deposition rates, greater control over deposition conditions and resulting microstructures, and perhaps lower temperature infiltration.

Keywords: Ceramics, Microwave Processing

455. DEVELOPMENT OF MICROWAVE-HEATED DIESEL PARTICULATE FILTERS
$75,000
DOE Contacts: J. P. Carr, (301) 903-6519 and
E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: M. A. Janney,
(423) 574-4281

The purpose of this research, which derives from our work on ceramic filters for coal systems, is to help develop microwave-heated diesel engine particulate filter/burner devices. The goal is to develop materials that will perform both as filter and heater in such a device. A Cooperative Research and Development Agreement (CRADA) between Lockheed Martin Energy Systems and the Cummins Engine Company is in place that supports this work, CRADA No. ORNL93-0172. We propose to develop a ceramic composite structure of SiC-coated ceramic fiber that can be used as a diesel engine particulate filter. For commercial usage a particulate filter must: (1) filter carbon particles from high temperature diesel exhaust gas at an acceptable (low) backpressure; (2) survive thousands of thermal transients caused by regeneration (cleaning) of the filter by oxidizing the collected carbon; (3) be durable and reliable over the life of the filter, which is in excess of 300,000 miles (10,000 hours of operation); and (4) provide a low overall operating cost which is competitive with other filtering techniques.

Keywords: Ceramics, Microwave Processing

456. CARBON FIBER COMPOSITE MOLECULAR SIEVES
$275,000
DOE Contacts: J. P. Carr, (301) 903-6519 and
E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact:
T. D. Burchell, (423) 576-8595

Hydrogen recovery technologies are required to allow the upgrading of heavy hydrocarbons to transport fuels, thus reducing the amount of carbon rejected during the conversion of fossil resources into hydrocarbon products. The purpose of this work is to develop carbon molecular sieves (CMS) starting with porous carbon fiber composites (CFC) manufactured from petroleum pitch derived carbon fibers. The carbon fiber composite molecular sieves (CFCMS) will be utilized in pressure swing adsorption units for the efficient recovery of hydrogen from synthesis gas, refinery purge gases, and for other gas separation operations associated with hydrogen recovery.

Keywords: Carbon Fibers, Sieves, Composites

457. CARBON MATERIALS EQUIPMENT
$15,000
DOE Contacts: J. P. Carr, (301) 903-6519 and
E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact:
T. D. Burchell, (423) 576-8595

This task provides funds for the procurement of major equipment items necessary for AR&TD Materials Program activities.

Keywords: Equipment

458. ACTIVATION OF CARBON FIBER COMPOSITE MOLECULAR SIEVES
$75,000
DOE Contacts: J. P. Carr, (301) 903-6519 and
E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole,
(423) 574-4824
University of Kentucky Contact: Frank Derbyshire,
(606) 257-0305

A novel monolithic adsorbent carbon, manufactured from carbon fibers, has been invented jointly by researchers at Oak Ridge National Laboratory (ORNL) and the University of Kentucky Center for Applied Energy Research. The novel material, referred to as a carbon-fiber composite molecular sieve (CFCMS) is fabricated at ORNL in the Carbon Materials Technology Group. The purpose of this activity is to activate samples of the CFCMS and to perform subsequent analyses of the surface area, pore width distributions, and micropore volume. Activities are directed toward an understanding of the relationships between the activation process and the micro- or mesopore structure that develops.

Keywords: Carbon Fibers, Sieves, Composites

459. **CHARACTERIZATION OF COAL AND COAL EXTRACTS**
$20,000
DOE Contacts: J. P. Carr, (301) 903-6519 and
E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole,
(423) 574-4824
University of Tennessee Contact: E. L. Fuller,
(423) 974-6356

The objective of this work is to characterize coal and coal extracts and to assist Oak Ridge National Laboratory in the research activities connected with the Cooperative Research Partnership on Carbon Products and the Non Fuel Uses of Coal. Work involves the characterization of coal and coal extracts obtained form West Virginia University. Activation and reactivity studies of carbon materials, including carbon fiber composite molecular sieves, shall be performed. Analysis of the pore structures of activated carbons, including carbon fiber composite molecular sieves, shall be performed.

Keywords: Carbon Fibers, Sieves, Composites

460. **PRODUCTION OF ALUMINUM REDUCTION ELECTRODES FROM SOLVENT-EXTRACTED COAL-DERIVED CARBON FEEDSTOCKS**
$0 (PYF)*
DOE Contacts: J. P. Carr, (301) 903-6519 and
E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole,
(423) 574-4824
Alcoa Aluminum Company Contact: Dave Belitskus,
(412) 337-4812

This research is directed toward the objective of producing aluminum reduction electrodes from solvent-extracted coal-derived carbon feedstocks obtained from West Virginia University (WVU) and Koppers Industries, Inc.

Keywords: Carbon, Feedstocks, Coal-Derived

461. **EXPLORATION OF COAL-BASED PITCH PRECURSORS FOR ULTRA-HIGH THERMAL CONDUCTIVITY GRAPHITE FIBERS**
$0 (PYF)*
DOE Contacts: J. P. Carr, (301) 903-6519 and
E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole,
(423) 574-4824
Amoco Performance Products, Inc. Contact:
G. V. Deshpande

The preparation of high-performance carbon (graphite) fibers requires a mesophase pitch precursor. Traditionally, in the USA, this has been derived from a petroleum precursor. Overseas suppliers have, however, developed high-performance fibers from coal derived precursors. Amoco Performance Products' goal is to explore coal-based pitch precursors' utility for use in ultra-high thermal conductivity graphite fibers.

Keywords: Carbon, Fibers, Graphite, Precursors

462. **DEVELOPMENT OF CARBON-CARBON COMPOSITES FROM SOLVENT-EXTRACTED PITCH**
$0 (PYF)*
DOE Contacts: J. P. Carr, (301) 903-6519 and
E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole,
(423) 574-4824
Fiber Materials, Inc. Contact: Cliff Baker,
(207) 282-5911

The manufacture of carbon-carbon composites for use in the aerospace industry has been heavily reliant on petroleum and coal tar pitches as matrix precursors. It is of great importance to strategic materials production for the Department of Defense that a stable, long-lived source of pitch be developed. Consequently, Fiber Materials, Inc. will work with staff members at the Oak Ridge National Laboratory and at West Virginia University to develop carbon-carbon composite materials from pitches derived from coal via a solvent extraction process. The objectives of this project shall be twofold. First, FMI shall use solvent extracted pitch to develop carbon-carbon composites with similar or improved properties over those currently manufactured from Allied 15V coal tar or Ashland A-240 petroleum pitches. Second, FMI shall develop improved, lower-cost composites from improved solvent extracted pitches supplied by WVU.

Keywords: Carbon, Composites, Pitch

*PYF denotes that funding for this activity, active in FY 1995, was provided from prior year funds.

463. **CONVERSION OF PITCHES AND COKES FROM SOLVENT-EXTRACTED MATERIALS**
$0 (PYF)*
DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole, (423) 574-4824
Koppers Industries, Inc. Contact: R. McHenry, (412) 826-3989

The closure of by-product coke ovens has caused the domestic production of coal tar pitch to decline at 3 percent to 4 percent per annum during the mid-1990s. This reduction has directly affected Koppers' capability to produce required quantities of quality binder and impregnating pitches used in the aluminum and commercial carbon and graphite industries. Moreover, the other major constituent of carbon anodes and graphites is a coke, usually produced from petroleum pitch precursors, 50 percent of which are imported. The objectives of this research are to develop dependable domestic coal-based raw materials for the production of: binder pitches for aluminum cell anodes and commercial carbon and graphite products; impregnating pitches for commercial carbon and graphite products and specialty materials; oils for wood treatment and carbon black production; chemicals for phthalic anhydride and other products; and metallurgical and foundry grade cokes.

Keywords: Coke, Pitch, Conversion

464. **CARBON FIBER COMPOSITE MOLECULAR SIEVES**
$155,000
DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: T. D. Burchell, (423) 576-8595

Hydrogen and Methane gas recovery technologies are required to: (1) allow the upgrading of heavy hydrocarbons to transport fuels, thus reducing the amount of carbon rejected during crude oil refining and (2) to improve the yield and process economics of natural gas wells. The purpose of this work is to develop carbon fiber composite molecular sieves (CFCMS) from porous carbon fiber composites manufactured from solvent extracted coal tar pitch derived carbon fibers. The work will be performed in collaboration with other members of the Cooperative Research Partnership on Carbon Products and the Non Fuel Uses of Coal.

Keywords: Consortium, Carbon Products

465. **DEVELOPMENT OF PRECURSORS FOR PRODUCTION OF GRAPHITES AND CARBON PRODUCTS**
$0 (PYF)*
DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole, (423) 574-4824
UCAR Carbon Company Contact: Irv Lewis, (216) 676-2203

The manufacture of graphite utilizes cokes and pitches derived from petroleum refining by-products and by-product coke ovens. These include isotropic and anisotropic cokes, binder, and impregnant pitches. Assuring feedstock quality is of great importance to the graphite industry. Therefore, a stable long-lived source of feedstock pitch (and hence coke) would be of considerable benefit to the industry. Consequently, UCAR Carbon Company Inc. shall work with staff members at the Oak Ridge National Laboratory and at the West Virginia University to develop suitable precursor pitches, binders, impregnants, and cokes for the production of graphites and other carbon products.

Keywords: Carbon Products, Precursors, Graphites

466. **PRODUCTION OF YARN FROM VLS WHISKERS**
$100,000
DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole, (423) 574-4824

In order to exploit the superior thermomechanical properties of fibrils produced by the Vapor-Liquid-Solid (VLS) Process, the feasibility of scaled-up production of the SiC fibril will be demonstrated in this activity. Through time-series study and computer simulation, the parameters affecting the growth process and properties of the fibrils will be examined.

Keywords: Whiskers, Fibers, Ceramic

*PYF denotes that funding for this activity, active in FY 1995, was provided from prior year funds.

467. **RADIO-WAVE NANO-PHASE SILICON CARBIDE AND SILICON NITRIDE PROCESSES**
$100,000
DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole, (423) 574-4824
Sandia National Laboratories Contact: R. J. Buss, (505) 844-3504

This program examines the use of radio-frequency plasma discharges as a synthetic route to nanometer-size silicon carbide and silicon nitride particles.

Keywords: Nanophase, Silicon Nitride, Silicon Carbide

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

468. **INVESTIGATION OF THE WELDABILITY OF POLYCRYSTALLINE IRON ALUMINIDES**
$75,000
DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole, (423) 574-4824
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

469. **AQUEOUS CORROSION OF IRON ALUMINIDES**
$29,000
DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole, (423) 574-4824
University of Tennessee Contact: R. A. Buchanan, (423) 974-4858

The objective of this project is to investigate (1) evaluation of the effects of surface conditions on the corrosion and embrittlement of Fe-Al alloys, and (2) corrosion fatigue properties of Fe-Al alloys.

Keywords: Alloys, Aluminides, Corrosion, Stress

470. **EVALUATION OF THE INTRINSIC AND EXTRINSIC FRACTURE BEHAVIOR OF IRON ALUMINIDES**
$68,000
DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole, (423) 574-4824
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

471. **INVESTIGATION OF IRON ALUMINIDE WELD OVERLAYS**
$56,000
DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole, (423) 574-4824
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

472. **FIRESIDE CORROSION TESTS OF CANDIDATE ADVANCED AUSTENITIC ALLOYS, COATINGS, AND CLADDINGS**
$80,000
DOE Contacts: J. P. Carr, (301) 903-6519 and
E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole,
(423) 574-4824
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

473. **JOINING TECHNIQUES FOR ADVANCED AUSTENITIC ALLOYS**
$50,000
DOE Contacts: J. P. Carr, (301) 903-6519 and
E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole,
(423) 574-4824
University of Tennessee Contact: C. D. Lundin,
(423) 974-5310

Weldability is an important consideration in the selection of a suitable alloy for the fabrication of boiler components such as superheaters and reheaters. It is often a challenge to select joining materials and establish procedures that will allow advanced materials to function at their full potential. The purpose of this research is to examine important aspects of newly developed austenitic tubing alloys intended for service in the temperature range 550 to 700°C.

Keywords: Alloys, Austenitics, Joining, Welding

474. **FATIGUE AND FRACTURE BEHAVIOR OF Cr-Nb ALLOYS**
$20,000
DOE Contacts: J. P. Carr, (301) 903-6519 and
E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole,
(423) 574-4824
University of Tennessee Contact: Peter Liaw,
(423) 974-6356

The objective of this research shall be to characterize the fatigue and fracture behavior of Cr_2Nb-based alloys and other intermetallic materials at ambient and elevated temperatures in controlled environments. These studies are expected to lead to mechanistic understanding of the fatigue and fracture behavior of these alloys. Fatigue tests shall be conducted for the purpose of evaluating crack initiation and fatigue life of Cr_2Nb-based alloys as well as other intermetallic alloys. The fatigue properties shall be evaluated as functions of test environment, cyclic frequency and test temperature. Additional tensile tests will be required to characterize the fracture behavior of these structural alloys. Mechanical tests shall be performed to determine the fatigue and fracture behavior of Cr_2Nb-based alloys. The microstructure of the alloys shall be characterized and correlated with the mechanical properties.
Keywords: Fracture, Fatigue, Alloys

475. **CORROSION AND MECHANICAL PROPERTIES OF ALLOYS IN FBC AND MIXED-GAS ENVIRONMENTS**
$310,000
DOE Contacts: J. P. Carr, (301) 903-6519 and
E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole,
(423) 574-4824
Argonne National Laboratory Contact: K. Natesan,
(708) 252-5103

The purposes of this task are to: (1) evaluate the corrosion mechanisms for chromia- and alumina-forming alloys in mixed-gas environments, (2) develop an understanding of the role of several microalloy constituents in the oxidation/sulfidation process, (3) evaluate transport kinetics in oxide scales as functions of temperature and time, (4) characterize surface scales that are resistant to sulfidation attack, and (5) evaluate the role of deposits in corrosion processes.

Keywords: Corrosion, Gasification, Creep Rupture, Fluidized-Bed Combustion

476. **MECHANICALLY RELIABLE COATINGS AND SCALES FOR HIGH-TEMPERATURE CORROSION RESISTANCE**
$50,000
DOE Contacts: J. P. Carr, (301) 903-6519 and
E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole, (423) 574-4824
Argonne National Laboratory Contact: K. Natesan, (708) 252-5103

This project involves the development of mechanically reliable coatings and scales for high-temperature corrosion resistance. ANL shall systematically generate the knowledge required to establish a scientific basis for design and synthesis of improved (slow growing, adherent, sound) protective oxide coatings and scales on high temperature materials, without compromising the requisite bulk material properties. In addition, ANL shall provide information on the performance of advanced candidate materials from the standpoint of corrosion resistance and residual mechanical properties, after exposure in simulated combustion environments typical of indirectly-fired gas turbines. The work shall emphasize corrosion evaluation of materials in air, salt, and coal/ash environments at temperatures between 1000° and 1400°C, and measurement of residual toughness properties of the materials after corrosion.

Keywords: Corrosion, Coatings, Scales

477. **ENVIRONMENTAL EFFECTS ON IRON ALUMINIDES**
$145,000
DOE Contacts: J. P. Carr, (301) 903-6519 and
E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: P. F. Tortorelli, (423) 574-5119

The purpose of this task is to evaluate the high-temperature corrosion behavior of iron-aluminum alloys as part of the effort to develop highly corrosion-resistant iron-aluminide alloys and coatings for fossil energy applications. A primary objective is to investigate the resistance of the alloys to mixed-oxidant (oxygen-sulfur-chlorine-carbon) environments that arise in the combustion or gasification of coal. This includes the determination of the influence of sulfur and other reactive gaseous species on corrosion kinetics and oxide micro-structures and the effects of alloying additions and oxide dispersoids on sulfidation and oxidation resistance.

Keywords: Corrosion, Aluminides, Mixed-Gas, Scales

478. **INVESTIGATION OF MOISTURE-INDUCED EMBRITTLEMENT OF IRON ALUMINIDES**
$73,000
DOE Contacts: J. P. Carr, (301) 903-6519 and
E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole, (423) 574-4824
Rensselaer Polytechnic Institute Contact: N. S. Stoloff, (518) 276-6371

The purpose of this work is to study hydrogen embrittlement of iron aluminide alloys. Moisture in air can significantly reduce the room-temperature tensile ductility of Fe_3Al-based alloys by combining with the aluminum in the alloys to form atomic hydrogen. The atomic hydrogen diffuses rapidly into the material causing embrittlement. Experiments are being conducted on selected Fe_3Al alloys that will lead to an understanding of the phenomenon. The work focuses on the effects of moisture on relevant mechanical properties such as fatigue and tensile strengths, and correlates important microstructural variables such as degree of order, grain size, and phases present with the alloy's susceptibility to embrittlement.

Keywords: Aluminides, Embrittlement, Moisture

479. **CORROSION PROTECTION OF ULTRAHIGH TEMPERATURE INTERMETALLIC ALLOYS**
$146,000
DOE Contacts: J. P. Carr, (301) 903-6519 and
E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: P. F. Tortorelli, (423) 574-5119

The objective of this task is to develop high-strength, corrosion-resistant intermetallic alloys for use as hot components in advanced fossil energy conversion and combustion systems. The successful development of these alloys is expected to improve the thermal efficiency of fossil energy conversion systems through increased operating temperatures and to increase the service life of hot components exposed to corrosive environments at elevated temperatures (1000°C). The initial effort will be devoted to in situ composite alloys based on the Cr-Cr_2Nb system.

Keywords: Corrosion, Chromium-Niobium, Mixed-Gas, Scales

480. **OXIDE DISPERSION STRENGTHENED (ODS) IRON ALUMINIDE EQUIPMENT**
$35,000
DOE Contacts: J. P. Carr, (301) 903-6519 and
E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: I. G. Wright,
(423) 574-4451

This task provides funds for the procurement of major equipment items necessary for AR&TD Materials Program activities.

Keywords: Equipment

481. **OXIDE DISPERSION STRENGTHENED (ODS) IRON ALUMINIDES**
$222,000
DOE Contacts: J. P. Carr, (301) 903-6519 and
E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: I. G. Wright,
(423) 574-4451

The purpose of this task is to develop fabrication procedures for making oxide dispersion-strengthened (ODS) iron-aluminum alloys based on Fe_3Al. The suitability of the procedures is measured in terms of the high-temperature oxidation and sulfidation resistance and creep strength of the ODS alloys compared with Fe_3Al alloys fabricated by conventional ingot and powder processes.

Keywords: Aluminides

482. **MATERIALS SUPPORT FOR HITAF**
$0 (PYF)*
DOE Contacts: J. P. Carr, (301) 903-6519 and
E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: K. Breder,
(423) 574-5089

This task involves the measurement of selected mechanical and physical properties of structural ceramics which are proposed for use in the construction of the High Temperature Advanced Furnace (HITAF) air heater design being developed under the Combustion 2000 program for PETC/DOE. The purpose of the research is to evaluate candidate structural ceramics for this application by studying the fast fracture and fatigue (both dynamic and interrupted static) properties at temperatures from 1100 to 1400°C in air, their corrosion behavior, property uniformity of components and long term degradation of ceramic properties due to exposure in prototype HITAF systems. This work is continuing with funding from the Combustion 2000 Program.

Keywords: Furnace, Materials, HITAF

483. **CHARACTERIZATION OF LOW-EXPANSION CERAMIC MATERIALS AND DEVELOPMENT OF SOL GEL-DERIVED COATINGS AS INTERFACES FOR SIC COMPOSITES**
$23,000
DOE Contacts: J. P. Carr, (301) 903-6519 and
E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole,
(423) 574-4824
University of Tennessee Contact: Peter Liaw,
(423) 974-6356

The purpose of this activity is the experimental study of low-expansion ceramic materials and the development of sol-gel derived coatings as interfaces for Nicalon®/SiC composites

Keywords: Composites, Ceramics

484. **JOINING OF CERAMICS**
$50,000
DOE Contacts: J. P. Carr, (301) 903-6519 and
E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole,
(423) 574-4824
Idaho National Engineering Laboratory Contact:
B. H. Rabin, (208) 526-0058

The purpose of this project is to explore and develop joining techniques for silicon carbide fiber-reinforced silicon carbide ceramics produced by chemical vapor infiltration and deposition (CVID). The research goals include identifying appropriate joining methods, establishing experimental procedures for fabricating joints, and characterizing the structure and properties of joined materials. An understanding of the factors that control joint performance is sought through studies of the relationships among processing variables, joint microstructures, and mechanical properties. Additional funds for this project are provided by the DOE Pittsburgh Energy Technology Center.

Keywords: Ceramics, Joining, Technology Transfer

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*PYF denotes that funding for this activity, active in FY 1995, was provided from prior year funds.

485. **SUPPORT SERVICES FOR CERAMIC FIBER-CERAMIC MATRIX COMPOSITES**
$25,000
DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole, (423) 574-4824
University of North Dakota Energy and Environmental Research Center Contact: J. P. Hurley, (701) 777-5159

This task will review and, if appropriate, propose modifications to plans, materials, and tests planned by researchers on the AR&TD Materials Program in work to test materials for coal-fueled energy systems. The changes shall be suggested in order to make the corrosion experiments more reflective of the actual conditions that will be encountered by the materials in the energy systems. UNDEERC shall accomplish this task by reviewing the major advanced energy system projects being funded by the DOE, and by working with the company's technical monitor and staff to prepare a summary of the expected corrosion problems. Both gasification and combustion systems will be included. Ceramic materials in two subsystems will be the focus of this work: (1) hot gas cleanup systems and (2) high-temperature heat exchangers. UNDEERC shall review and suggest improvements to materials testing procedures that are used to determine material behavior when used in hot-gas cleanup or heat exchanger applications. A limited amount of computer modeling and laboratory experimentation shall be a part of this effort.

Keywords: Composites, Ceramics, Fibers

486. **DEVELOPMENT OF NONDESTRUCTIVE EVALUATION METHODS AND EFFECTS OF FLAWS ON THE FRACTURE BEHAVIOR OF STRUCTURAL CERAMICS**
$310,000
DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole, (423) 574-4824
Argonne National Laboratory Contacts: W. A. Ellingson, (708) 252-5068 and J. P. Singh, (708) 252-5123

The purpose of this project is to study and develop acoustic and radiographic techniques and possible novel techniques such as nuclear magnetic resonance, to characterize structural ceramics with regard to presence of porosity, cracking, inclusions, amount of free silicon, and mechanical properties, and to establish the type and character of flaws that can be found by nondestructive evaluation (NDE) techniques. Both fired and unfired specimens are being studied to establish correlations between NDE results and failure of specimens.

Keywords: Nondestructive Evaluation, Ceramics, Flaws, Fracture

487. **FRACTURE BEHAVIOR OF ADVANCED CERAMIC HOT-GAS FILTERS**
$125,000
DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole, (423) 574-4824
Argonne National Laboratory Contacts: J. P. Singh, (708) 252-5123

The purpose of this project is to study the fracture behavior of ceramic hot-gas filters. ANL shall evaluate mechanical/physical properties and microstructure, identify critical flaws and failure modes, and correlate mechanical/physical properties with microstructure and critical flaws to provide much needed information for selection of materials and optimization of fabrication procedures for hot-gas ceramic filter modules. As part of the information base, requirements for strength and fracture toughness of the filter material shall be established from stress and fracture mechanics analyses of typical filters subjected to loadings expected during operation and pulse-cleaning cycles.

Keywords: Ceramics, Flaws, Fracture, Failure

488. **CERAMIC CATALYST MATERIALS**
$225,000
DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole, (423) 574-4824
Sandia National Laboratories Contact: A. G. Sault, (505) 844-8723

The purpose of this research is to investigate the role of ceramic material properties in the catalytic activity of a novel class of catalytic supports, known as hydrous titanium oxides (HTO). Catalysts prepared on these materials show particular promise as economically and environmentally attractive alternatives to present commercial catalysts for the direct liquefaction of coal. In these studies, improved understanding and control of the synthesis process is being pursued in order to tailor the composition, molecular structure, microporosity, and physical/mechanical properties of the HTO thin films. The effects of altered structure, composition, and other material properties of the thin film ceramic support material on catalytic activity are being assessed.

Keywords: Ceramics, Catalysts

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

489. ***MATERIALS AND COMPONENTS IN FOSSIL ENERGY APPLICATIONS* NEWSLETTER**
$60,000
DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: I. G. Wright, (423) 574-4451

The purpose of this task is to publish a periodic (bimonthly) DOE-EPRI newsletter to address current developments in materials and components in fossil energy applications. Equal funding is provided by EPRI.

Keywords: Materials, Components

490. **CERAMIC FIBER FILTER TECHNOLOGY**
$50,000
DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: M. A. Janney, (614) 424-4281

The purpose of this effort is to develop the fabrication technology necessary to make ceramic-fiber based filters for a variety of filtration applications of interest to the Fossil Energy community.

Keywords: Filters, Ceramics, Fibers

491. **FABRICATION OF FULL-SCALE FIBER-REINFORCED HOT-GAS FILTERS BY CHEMICAL VAPOR DEPOSITION**
$0 (PYF)*
DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole, (423) 574-4824
3M Company Contact: M. A. Leitheiser, (612) 733-9394

The purpose of this project is to scale-up the chemical vapor infiltration and deposition (CVID) process developed at Oak Ridge National Laboratory for fabricating ceramic fiber-ceramic matrix composites. The goal is to use the scaled-up CVID process to produce composite filters that have the requisite strength and toughness, but which also have sufficient porosity to be permeable to gas streams and the appropriate size and distribution of porosity to be an effective filter. A practical process for fabricating porous ceramic fiber-ceramic matrix candle filters (full-size) with increased surface area has been developed.

Keywords: Ceramics, Composites, Filters

492. **DEVELOPMENT OF CERAMIC MEMBRANES FOR GAS SEPARATION**
$400,000
DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole, (423) 574-4824
Oak Ridge K-25 Site Contact: D. E. Fain, (423) 574-9932

The purpose of this activity is to fabricate inorganic membranes for the separation of gases at high temperatures and/or in hostile environments, typically encountered in fossil energy conversion processes such as coal gasification. This work is performed in conjunction with a separate research activity that is concerned with the development and testing of the ceramic membranes.

Keywords: Ceramics, Membranes, Filters, Separation

493. **CORROSION PROTECTION OF CERAMIC HEAT EXCHANGER TUBES**
$125,000
DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole, (423) 574-4824
Pennsylvania State University Contact: R. E. Tressler, (814) 865-7961

This project addresses the development of ceramic heat exchanger materials with chromia surface treatments for corrosion resistance. High chromia-content refractories have been demonstrated to be resistant to corrosion by coal slags. This project will focus on improving the corrosion resistance of ceramics by incorporating chromia into the surface layers.

Keywords: Ceramics, Corrosion, Filters

*PYF denotes that funding for this activity, active in FY 1995, was provided from prior year funds.

494. **INVESTIGATION OF THE MECHANICAL PROPERTIES AND PERFORMANCE OF CERAMIC COMPOSITE COMPONENTS**
$150,000
DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole, (423) 574-4824
Virginia Polytechnic Institute Contact: K. L. Reifsnider, (703) 231-5259

The purpose of this project is to develop a test system and test methods to obtain information on the properties and performance of ceramic composite materials. The work involves a comprehensive mechanical characterization of composite engineering components such as tubes, plates, shells, and beams subjected to static and cyclic multiaxial loading at elevated temperatures for extended time periods.

Keywords: Ceramics, Composites, Mechanical Properties, Testing

495. **STABILITY OF SOLID OXIDE FUEL CELL (SOFC) MATERIALS**
$250,000
DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole, (423) 574-4824
Pacific Northwest Laboratory Contact: L. R. Pederson, (509) 375-2579

The purpose of this task is to evaluate the chemical and physical stability of fuel cell materials and interfaces under conditions relevant to an operating SOFC and to identify features in SOFC operation that would limit system performance.

Keywords: Fuel Cells, SOFC

496. **MIXED OXYGEN ION/ELECTRON-CONDUCTING CERAMICS FOR OXYGEN SEPARATION AND FUEL CELLS**
$225,000
DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole, (423) 574-4824
Pacific Northwest Laboratory Contact: L. R. Pederson, (509) 375-2579

The purpose of this task is to develop ceramic compositions and physical forms that will provide the highest possible oxygen separation efficiencies from air at the lowest cost.

Keywords: Fuel Cells, Electrochemical, Electrolytes

497. **PROTON-CONDUCTING CERATE CERAMICS**
$225,000
DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole, (423) 574-4824
Pacific Northwest Laboratory Contact: L. R. Pederson, (509) 375-2579

The purpose of this task is to develop cerate perovskites for use as hydrogen separation membranes, as hydrogen sensors, in membrane reactors, and in gas cleanup.

Keywords: Fuel Cells, Electrochemical, Electrolytes

498. **ODS Fe_3Al TUBES FOR HIGH-TEMPERATURE HEAT EXCHANGERS**
$53,000
DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole, (423) 574-4824
PM Hochtemperatur-Metall. GmbH Contact: Dieter Sporer, 011-43-5672-70-2923

The goal of the work is to produce tubes of Fe_3Al-0.5 wt. percent Y_2O_3 which have properties suitable for application as heat transfer surfaces in very high-temperature heat exchangers. The alloy is produced by a powder metallurgical (mechanical alloying) process, the main purpose of which is to obtain a uniform distribution of sub-micron Y_2O_3 particles in the Fe_3Al matrix. The required high-temperature creep strength is derived largely by developing very large, elongated grains which are effectively pinned by the oxide dispersion. Development of the necessary grain structure is dependent on the characteristics of the mechanically-alloyed powder, and on thermomechanical processing of the consolidated powder.

Keywords: Aluminide, Tubes, Heat Exchangers

499. **POROUS IRON ALUMINIDE ALLOYS**
$23,000
DOE Contacts: J. P. Carr, (301) 903-6519 and
E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole, (423) 574-4824
Oak Ridge K-25 Site Contact: D. E. Fain, (423) 574-9932

This project is directed to the development of porous iron aluminide structures for applications such as hot-gas filters

Keywords: Filters, Aluminides

500. **IRON ALUMINIDE FILTERS**
$50,000
DOE Contacts: J. P. Carr, (301) 903-6519 and
E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: P. F. Tortorelli, (423) 574-5119

The purpose of this project is to provide technical support to the Pall Corporation in its development of porous sintered iron-aluminide filters for hot-particle removal from product streams in coal gasification systems. The ORNL role is to provide specialized expertise in the areas of corrosion analysis, microstructural characterization, alloy selection, and processing based on extensive experience with iron aluminides and materials performance in fossil energy systems. ORNL's contribution via this project should aid the success and timely completion of Pall's development and demonstration efforts.

Keywords: Filters, Aluminides

501. **EVALUATION OF CERAMIC HEAT EXCHANGER TUBES AND JOINTS**
$158,000
DOE Contacts: J. P. Carr, (301) 903-6519 and
E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole, (423) 574-4824
Pennsylvania State University Contact: R. E. Tressler, (814) 865-7961

This project has two principal parts: (1) screening analysis of candidate ceramic hot-gas filter materials, and (2) development of ceramic heat exchanger materials with chromium surface treatments for corrosion resistance. A flow-through screening test will be developed to test ceramic hot-gas filter elements in simulated coal combustion environments. Corrosion-resistant heat exchanger tubes will be fabricated by incorporating chromium in the surface layers.

Keywords: Ceramics, Corrosion, Filters

502. **THERMAL AND MECHANICAL ANALYSIS OF A CERAMIC TUBESHEET**
$40,000
DOE Contacts: J. P. Carr, (301) 903-6519 and
E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole, (423) 574-4824
Mallett Technology Contact: R. H. Mallett, (919) 406-1500

A transport combustor is being commissioned at the Southern Services facility in Wilsonville, Alabama, to provide a gaseous product for the assessment of hot-gas filtering systems. These hot-gas filtration systems will include granular-bed and barrier filter concepts. Filters will be evaluated for carbonizer and gasifier gaseous products. In addition, a pressurized fluidized-bed combustor (PFBC) will be installed to burn the carbonizer product, and a hot gas filter will be installed in the PFBC gas stream. Compositions of the gas streams will range from oxidizing to reducing, and the partial pressures of oxygen and sulfur will vary substantially. Temperatures of the gas streams will range from 840 to 980°C (or higher). One of the barrier filters under consideration incorporates a ceramic tubesheet to support the candle filters. This system, to be designed and built by Industrial Filter & Pump Manufacturing Company (IF&PM) is unique and may offer distinct advantages over metal/ceramic systems that have been tested extensively in other EPRI/DOE projects. To gain an insight that could prove to be useful in the scaleup of a commercial-size, all-ceramic system, work will be undertaken to develop a design methodology applicable to the thermal-mechanical analysis of the all-ceramic system.

Keywords: Ceramics, Tubesheet

503. **CERAMIC TUBESHEET DESIGN ANALYSIS**
$10,000
DOE Contacts: J. P. Carr, (301) 903-6519 and
E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact:
R. W. Swindeman, (423) 574-5108

The purpose of this task is to perform thermal and mechanical analyses of critical regions in a ceramic tubesheet support for barrier filters in a hot gas cleanup vessel designed for use in gasifier, carbonizer, and pressurized fluidized bed combustion gas streams.

Keywords: Ceramics, Tubesheet

INSTRUMENTATION AND FACILITIES

504. **MANAGEMENT OF THE FOSSIL ENERGY AR&TD MATERIALS PROGRAM**
$400,000
DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole, (423) 574-4824

The overall objective of the Fossil Energy Advanced Research and Technology Development (AR&TD) Materials program is to conduct a fundamental, long-range research and development program that addresses, in a generic way, the materials needs of fossil energy systems and ensures the development of advanced materials and processing techniques. The purpose of this task is to manage the Fossil Energy AR&TD Materials program in accordance with procedures described in the Program Management Plan approved by DOE. This task is responsible for preparing the technical program implementation plan for DOE approval; submitting budget proposals for the program; recommending work to be accomplished by subcontractors, other national laboratories, and by Oak Ridge National Laboratory (ORNL); placing and managing subcontracts for fossil energy materials development at industrial research centers, universities, and other government laboratories; and for reporting the progress of the program.

Keywords: Management, Materials Program

505. **GENERAL TECHNOLOGY TRANSFER ACTIVITIES**
$35,000
DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole, (423) 574-4824

The task provides funds for the initiation of technology transfer activities to identify and develop relationships with industrial partners for the transfer of AR&TD Materials Program technologies to industry.

Keywords: Technology Transfer

506. **GORDON RESEARCH CONFERENCE SUPPORT**
$4,000
DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole, (423) 574-4824

The task provides funds to support the annual Gordon Research Conference.

Keywords: Technology Transfer

507. **Mo-Si ALLOY DEVELOPMENT**
$10,000
DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: C. T. Liu, (423) 574-4559

The objective of this task is to develop new-generation corrosion-resistant Mo-Si alloys for use as hot components in advanced fossil energy conversion and power generation systems. The successful development of Mo-Si alloys is expected to improve the thermal efficiency and performance of fossil energy systems through increased operating temperature and to increase the service life of hot components exposed to corrosive environments at high temperatures (to 1600°C). The initial effort is devoted to Mo_5Si_3-base alloys containing boron additions.

Keywords: Alloys, Molybdenum, Silicon

508. **TECHNOLOGY TRANSFER - IRON ALUMINIDES**
$60,000
DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: V. K. Sikka, (423) 574-5112

A Cooperative Research and Development Agreement (CRADA) has been established with ABB Combustion Engineering for the development of corrosion-resistant surface protection for fossil power systems.

Keywords: Alloys, Iron-Aluminum, Corrosion, Technology Transfer

509. **COMMERCIAL-SCALE MELTING AND PROCESSING OF LOW-ALUMINUM CONTENT ALLOYS**
$50,000
DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: V. K. Sikka, (423) 574-5112

The purpose of this activity is the preparation and evaluation of castings of FAPY alloy. The castings will be prepared in several types of molds including: (1) graphite, (2) sand, and (3) investment. Castings will be prepared primarily from the air-induction-melted material. Selected graphite and investment castings will also be prepared from the vacuum- induction-melted material. The graphite and sand castings will be prepared at ORNL and will also be procured from the commercial foundries. The castings will be evaluated for porosity, grain structure, mechanical properties, and weldability. The mechanical property evaluation will consist of Charpy, tensile, and creep testing.

Keywords: Alloys, Iron-Aluminum, Melting, Casting

510. **DEVELOPMENT OF A MODIFIED 310 STAINLESS STEEL**
$120,000
DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: R. W. Swindeman, (423) 574-5108

The purpose of this task is to evaluate structural alloys for improved performance of high-temperature components in advanced combined-cycle and coal-combustion systems.

Keywords: Materials, Mechanical Properties, Austenitics, Hot-Gas

511. **TECHNOLOGY TRANSFER - ADVANCED AUSTENITICS**
$80,000
DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: R. W. Swindeman, (423) 574-5108

A Cooperative Research and Development Agreement (CRADA) has been established with ABB Combustion Engineering for the development of advanced austenitic alloys for fossil power systems.

Keywords: Alloys, Austenitics, Technology Transfer

512. **INFLUENCE OF PROCESSING ON MICROSTRUCTURE AND PROPERTIES OF ALUMINIDES**
$175,000
DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole, (423) 574-4824
Idaho National Engineering Laboratory Contact: R. N. Wright, (208) 526-6127

The purpose of this project is to determine the influence of processing on the properties of alloys based on Fe_3Al. Thermomechanical processing is pursued to improve their room-temperature ductility. The response of the microstructure to annealing will be characterized in terms of the establishment of equilibrium phases and degrees of long-range order. The mechanical properties are determined at room and elevated temperatures and related to the microstructure.

Keywords: Aluminides, Processing, Microstructure

513. **INVESTIGATION OF ELECTROSPARK DEPOSITED COATINGS FOR PROTECTION OF MATERIALS IN SULFIDIZING ATMOSPHERES**
$75,000
DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole, (423) 574-4824
Pacific Northwest National Laboratory Contact: R. N. Johnson, (509) 375-6906

The purpose of this task is to examine the use of the electrospark deposition coating process for the application of corrosion-, erosion-, and wear-resistant coatings to candidate heat exchanger (including superheater and reheater) alloys. Materials to be deposited may include MCrAl, MCrAIY, highly wear-resistant carbides, and other hardsurfacing materials.

Keywords: Coatings, Materials, Deposition

514. TECHNOLOGY TRANSFER - ELECTROSPARK DEPOSITED COATINGS FOR PROTECTION OF MATERIALS IN SULFIDIZING ATMOSPHERES
$80,000
DOE Contacts: J. P. Carr, (301) 903-6519 and
E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole,
(423) 574-4824
Pacific Northwest National Laboratory Contact:
R. N. Johnson, (509) 375-6906

The purpose of this task is to transfer to industry the electrospark deposition coating process technology for the application of corrosion-, erosion-, and wear-resistant coatings to candidate heat exchanger [including superheater and reheater] alloys.

Keywords: Coatings, Materials, Deposition

515. ENGINEERING-SCALE DEVELOPMENT OF THE VAPOR-LIQUID-SOLID (VLS) PROCESS FOR THE PRODUCTION OF SILICON CARBIDE FIBRILS
$0 (PYF)*
DOE Contacts: J. P. Carr, (301) 903-6519 and
E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole,
(423) 574-4824
The Carborundum Company Contact: S. K. Lau,
(716) 278-2004

The purpose of this work is to transfer to industry a specific technology developed by the DOE AR&TD Materials Program for the production of silicon carbide fibrils for the reinforcement of ceramic matrices. The Vapor-Liquid-Solid (VLS) process was developed at Los Alamos National Laboratory for the growth of silicon carbide fibrils of up to 75 mm in length which can be reduced in length by subsequent processing. The purpose of the work is to develop the VLS process into an engineering-scale process that will enable the U.S. industrial sector to commercialize the process for the production of fibrils for the reinforcement of structural ceramic components.

Keywords: Whiskers, Fibers, Ceramic

*PYF denotes that funding for this activity, active in FY 1995, was provided from prior year funds.

516. CERAMIC COMPOSITE PROCESSING EQUIPMENT
$30,000
DOE Contacts: J. P. Carr, (301) 903-6519 and
E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: D. P. Stinton,
(423) 574-4556

This task provides funds for the procurement of major equipment items necessary for AR&TD Materials Program activities.

Keywords: Equipment

517. FABRICATION OF FIBER-REINFORCED COMPOSITES BY CHEMICAL VAPOR INFILTRATION AND DEPOSITION
$150,000
DOE Contacts: J. P. Carr, (301) 903-6519 and
E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: D. P. Stinton,
(423) 574-4556

The purpose of this task is to develop a process for the fabrication of fiber-reinforced ceramic composites having high fracture toughness and high strength. This process utilizes a steep temperature gradient and a pressure gradient to infiltrate low-density fibrous structures with gases, which deposit solid phases to form the matrix of the composite. Further development of this process is needed to fabricate larger components of more complex geometry, and to optimize infiltration for shortest processing time, greatest density and maximum strength.

Keywords: Composites, Fiber-Reinforced, Ceramics

518. COMPLIANT OXIDE COATING DEVELOPMENT
$75,000
DOE Contacts: J. P. Carr, (301) 903-6519 and
E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: D. P. Stinton,
(423) 574-4556

Monolithic SiC heat exchangers and fiber-reinforced SiC-matrix composite heat exchangers and filters are susceptible to corrosion by alkali metals at elevated temperatures. Protective coatings are currently being developed to isolate the SiC materials from the corrodents. Unfortunately, these coatings typically crack and spall when applied to SiC substrates. The purpose of this task is to determine the feasibility of using a compliant material between the protective coating and the substrate. The low-modulus compliant layer could absorb stresses and eliminate cracking and spalling of the protective coatings.

Keywords: Ceramics, Oxides, Coatings

519. **DEVELOPMENT OF OXIDATION/CORROSION-RESISTANT COMPOSITE MATERIALS AND INTERFACES**
$127,000
DOE Contacts: J. P. Carr, (301) 903-6519 and
E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: D. P. Stinton,
(423) 574-4556

Fiber-reinforced SiC-matrix composites have been observed to fail in fossil energy applications for two reasons. First, the mechanical properties of composites deteriorate under stressed oxidation because oxidants such as steam penetrate cracks formed in the SiC matrix and react with the carbon or boron nitride interface. The mechanical properties of composites may degrade because of corrosion due to sodium species typically present in fossil systems. Therefore, the purposes of this task are to first, develop fiber-matrix interfaces that are resistant to oxidation and yet optimize the mechanical behavior of composites, and second, to develop protective overcoats or oxide matrices that are resistant to oxidation and corrosion.

Keywords: Composites, Ceramics, Fiber-Reinforced, Interfaces

520. **OPTIMIZATION OF THE CHEMICAL VAPOR INFILTRATION TECHNIQUE FOR CERAMIC COMPOSITES**
$85,000
DOE Contacts: J. P. Carr, (301) 903-6519 and
E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole,
(423) 574-4824
University of Tennessee Contact: Peter Liaw,
(423) 974-6356

This project is focused on an optimization of the forced chemical vapor infiltration technique for fabrication of ceramic matrix composites (CMCs) using process models. In particular, a process model developed at the Georgia Tech Research Institute shall be thoroughly investigated. Experimental verification of the process model shall be conducted in light of microstructural characterization using both destructive and nondestructive evaluation techniques. An optimized process for manufacturing CMCs shall be demonstrated. Moreover, mechanistic understanding regarding the effects of processing parameters on microstructural features, and fatigue and fracture behavior of CMCs shall be provided.

Keywords: Composites, Fiber-Reinforced, Ceramics

521. **TRANSPORT PROPERTIES OF CERAMIC COMPOSITES**
$148,000
DOE Contacts: J. P. Carr, (301) 903-6519 and
E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole,
(423) 574-4824
Georgia Institute of Technology Contact: T. L. Starr,
(404) 853-0579

The purpose of this research effort is to conduct a theoretical and experimental program to identify new compositions and processing methods to improve the physical and mechanical properties of selected fiber-reinforced ceramics. The ceramic matrix material is amorphous fused silica or modified silica glass, and the focus is the development of fiber-reinforced silica. Parameters studied include: (1) differences in elastic modulus between matrix and fiber, (2) differences in thermal expansion, (3) nature of interfacial bond, (4) densification of matrix, (5) nature of fiber fracture/pull-out, (6) fiber diameter and fiber length-to-diameter ratio, (7) fiber loading, and (8) fiber dispersion and orientation. A model will be developed based on the information generated in the experimental phase of the program.

Keywords: Ceramics, Composites, Fiber-Reinforced

522. **MODELING OF FIBROUS PREFORMS FOR CVD INFILTRATION**
$50,000
DOE Contacts: J. P. Carr, (301) 903-6519 and
E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole,
(423) 574-4824
Georgia Institute of Technology Contact: T. L. Starr,
(404) 853-0579

The purpose of this project is to conduct a theoretical and experimental program to develop an analytical model for the fabrication and infiltration of fibrous preforms. The analytical model will: (1) predict preform structure (density, porosity, fiber orientation, etc.) based on fabrication technique and fundamental fiber parameters (diameter, aspect ratio, etc.), and (2) predict permeation and heat conduction through the preform structure and, thus, predict the CVD infiltration performance.

Keywords: Ceramics, Composites, Modeling

523. **CORROSION PROTECTION OF SiC-BASED CERAMICS WITH CVD MULLITE COATINGS**
$50,000
DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole, (423) 574-4824
Boston University Contact: Vinod Sarin, (617) 353-6451

This project involves the growth of dense mullite coatings on SiC-based substrates by chemical vapor deposition. SiC and SiC-based composites have been identified as the leading candidate materials for stringent elevated temperature applications. At moderate temperatures and pressures, the formation of a thin self-healing layer of SiO_2 is effective in preventing catastrophic oxidation by minimizing the diffusion of O_2 to the substrate. The presence of impurities can increase the rate of passive oxidation by modifying the transport rate of oxygen through the protective scale, can cause active oxidation via formation of SiO which accelerates the degradation process, or can produce compositions such as Na_2SO_3 which chemically attack the ceramic via rapid corrosion. There is therefore a critical need to develop adherent oxidation/corrosion-resistant, and thermal-shock-resistant coatings that can withstand such harsh environments. Mullite has been identified as an excellent candidate material due to its desirable properties of toughness, corrosion resistance, and a good coefficient of thermal expansion match with SiC.

Keywords: Ceramics, Coatings

524. **FEASIBILITY OF SYNTHESIZING OXIDE FILMS ON CERAMIC AND METAL SUBSTRATES**
$100,000
DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole, (423) 574-4824
Lawrence Berkeley Laboratory Contact: Ian Brown, (510) 486-4174

The objective of this project is the study of the feasibility of synthesizing metal oxide ceramic films on ceramic and metal substrates. This feasibility will be demonstrated by use of plasma-based deposition and ion mixing techniques. The films shall be characterized for properties such as composition, structure, hardness, high temperature oxidation resistance, adhesion to the substrate, and stability to high temperature cycling. The value of intermediate transition or buffer layers, composed of materials with suitably matched thermal expansion characteristics and atomically graded interfaces, as a technique for improving the high temperature survivability of the films, shall be explored. Samples shall be formed on substrates of various shapes and sizes, including perhaps on the inside and outside of pipes, as well as on small flat coupons. The issue of deposition onto and atomic mixing into substrates which are insulating shall be addressed experimentally. The work is divided into two parts: (1) Al_2O_3 films on alumina-forming alloy substrates, and (2) oxides on SiC.

Keywords: Ceramics, Films, Oxides

525. **SCREENING ANALYSIS OF CERAMIC HOT-GAS FILTER MATERIALS**
$0 (PYF)*
DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole, (423) 574-4824
Pennsylvania State University Contact: R. E. Tressler, (814) 865-7961

This project will include a screening analysis of candidate ceramic hot-gas filter materials. A flow-through screening test will be developed to test ceramic hot-gas filter elements in simulated coal combustion environments.

Keywords: Ceramics, Corrosion, Coatings

526. **ENVIRONMENTAL EFFECTS ON CERAMICS**
$100,000
DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contacts: P. F. Tortorelli, (423) 574-5119

The purpose of this work is to support the development of advanced ceramics and ceramic composites for applications in fossil environments by examining critical issues related to high-temperature corrosion resistance. More specifically, the overall objective of this task is to examine the chemical compatibility and reliability of potentially corrosion-resistant ceramics being developed as protective overcoats and/or structural materials as parts of other work elements funded by the AR&TD Program.

Keywords: Coatings, Corrosion

*PYF denotes that funding for this activity, active in FY 1995, was provided from prior year funds.

527. **CERAMIC COATING EVALUATION**
$100,000
DOE Contacts: J. P. Carr, (301) 903-6519 and
E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contacts:
P. F. Tortorelli, (423) 574-5119

The purpose of this work is to generate the information needed for the development of improved (slow growing, adherent, sound) protective oxide coatings and scales. The specific objectives are to systematically investigate the relationships among substrate composition and surface oxide structure, adherence, soundness, and micromechanical properties, (2) use such information to predict scale and coating failures, and (3) identify and evaluate compositions and synthesis routes for producing materials with damage-tolerant scales and coatings.

Keywords: Coatings, Corrosion

528. **METAL DUSTING STUDY**
$25,000
DOE Contacts: J. P. Carr, (301) 903-6519 and
E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contacts:
P. F. Tortorelli, (423) 574-5119

The objective of this task is to establish the potential risk of operating problems due to carbon deposition and metal dusting in advanced coal gasification processes and to identify methods for avoiding carbon deposition. The work involves a literature search, compilation of a bibliography of relevant articles, and a summary of the current state of knowledge.

Keywords: Coatings, Corrosion

529. **LOW-TEMPERATURE FABRICATION OF TRANSPARENT SILICON NITRIDE**
$100,000
DOE Contacts: J. P. Carr, (301) 903-6519 and
E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole, (423) 574-4824
National Institute of Standards and Technology Contact: S. G. Malghan, (301) 975-6101

The objective of this research is the production of dense, hard, transparent ceramics from nanosize particles without the use of sintering aids. The work will concentrate on the fabrication of samples of transparent silicon nitride using the cryogenic compaction technique. TEM, SEM, X-ray diffraction, and laser light scattering will be used to characterize the microstructure. Hardness at various temperatures will be measured to assess the creep resistance of the material. Fracture toughness and bending strength will also be measured.

Keywords: Ceramics, Mechanical Properties

530. **MICROWAVE-ASSISTED CHEMICAL VAPOR INFILTRATION**
$25,000
DOE Contacts: J. P. Carr, (301) 903-6519 and
E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact:
M. A. Janney, (423) 574-4281

The purpose of this research effort is to explore the feasibility of using microwave heating to enhance the chemical vapor infiltration (CVI) process developed under the Fossil Energy Materials Program (FEMP) sponsorship. The goal is to achieve faster deposition rates, greater control over deposition conditions and resulting microstructures, and perhaps lower temperature infiltration.

Keywords: Ceramics, Microwave Processing

531. **DEVELOPMENT OF MICROWAVE-HEATED DIESEL PARTICULATE FILTERS**
$75,000
DOE Contacts: J. P. Carr, (301) 903-6519 and
E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact:
M. A. Janney, (423) 574-4281

The purpose of this research, which derives from our work on ceramic filters for coal systems, is to help develop microwave-eated diesel engine particulate filter/burner devices. The goal is to develop materials that will perform both as filter and heater in such a device. A Cooperative Research and Development Agreement (CRADA) between Lockheed Martin Energy Systems and the Cummins Engine Company is in place that supports this work, CRADA No. ORNL93-0172. We propose to develop a ceramic composite structure of SiC-coated ceramic fiber that can be used as a diesel engine particulate filter. For commercial usage a particulate filter must: (1) filter carbon particles from high temperature diesel exhaust gas at an acceptable (low) backpressure; (2) survive thousands of thermal transients caused by regeneration (cleaning) of the filter by oxidizing the collected carbon; (3) be durable and reliable over the life of the filter, which is in excess of 300,000 miles (10,000 hours of operation); and (4) provide a low overall operating cost which is competitive with other filtering techniques.

Keywords: Ceramics, Microwave Processing

532. **CARBON FIBER COMPOSITE MOLECULAR SIEVES**
$275,000
DOE Contacts: J. P. Carr, (301) 903-6519 and
E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact:
T. D. Burchell, (423) 576-8595

Hydrogen recovery technologies are required to allow the upgrading of heavy hydrocarbons to transport fuels, thus reducing the amount of carbon rejected during the conversion of fossil resources into hydrocarbon products. The purpose of this work is to develop carbon molecular sieves (CMS) starting with porous carbon fiber composites (CFC) manufactured from petroleum pitch derived carbon fibers. The carbon fiber composite molecular sieves (CFCMS) will be utilized in pressure swing adsorption units for the efficient recovery of hydrogen from synthesis gas, refinery purge gases, and for other gas separation operations associated with hydrogen recovery.

Keywords: Carbon Fibers, Sieves, Composites

533. **CARBON MATERIALS EQUIPMENT**
$15,000
DOE Contacts: J. P. Carr, (301) 903-6519 and
E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact:
T. D. Burchell, (423) 576-8595

This task provides funds for the procurement of major equipment items necessary for AR&TD Materials Program activities.

Keywords: Equipment

534. **ACTIVATION OF CARBON FIBER COMPOSITE MOLECULAR SIEVES**
$75,000
DOE Contacts: J. P. Carr, (301) 903-6519 and
E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole,
(423) 574-4824
University of Kentucky Contact: Frank Derbyshire,
(606) 257-0305

A novel monolithic adsorbent carbon, manufactured from carbon fibers, has been invented jointly by researchers at Oak Ridge National Laboratory (ORNL) and the University of Kentucky Center for Applied Energy Research. The novel material, referred to as a carbon-fiber composite molecular sieve (CFCMS) is fabricated at ORNL in the Carbon Materials Technology Group. The purpose of this activity is to activate samples of the CFCMS and to perform subsequent analyses of the surface area, pore width distributions, and micropore volume. Activities are directed toward an understanding of the relationships between the activation process and the micro- or mesopore structure that develops.

Keywords: Carbon Fibers, Sieves, Composites

535. **CHARACTERIZATION OF COAL AND COAL EXTRACTS**
$20,000
DOE Contacts: J. P. Carr, (301) 903-6519 and
E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole,
(423) 574-4824
University of Tennessee Contact: E. L. Fuller,
(423) 974-6356

The objective of this work is to characterize coal and coal extracts and to assist Oak Ridge National Laboratory in the research activities connected with the Cooperative Research Partnership on Carbon Products and the Non Fuel Uses of Coal. Work involves the characterization of coal and coal extracts obtained form West Virginia University. Activation and reactivity studies of carbon materials, including carbon fiber composite molecular sieves, shall be performed. Analysis of the pore structures of activated carbons, including carbon fiber composite molecular sieves, shall be performed.

Keywords: Carbon Fibers, Sieves, Composites

536. **PRODUCTION OF ALUMINUM REDUCTION ELECTRODES FROM SOLVENT-EXTRACTED COAL-DERIVED CARBON FEEDSTOCKS**
$0 (PYF)*
DOE Contacts: J. P. Carr, (301) 903-6519 and
E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole,
(423) 574-4824
Alcoa Aluminum Company Contact: Dave Belitskus,
(412) 337-4812

This research is directed toward the objective of producing aluminum reduction electrodes from solvent-extracted coal-derived carbon feedstocks obtained from West Virginia University (WVU) and Koppers Industries, Inc.

Keywords: Carbon, Feedstocks, Coal-Derived

*PYF denotes that funding for this activity, active in FY 1995, was provided from prior year funds.

537. **EXPLORATION OF COAL-BASED PITCH PRECURSORS FOR ULTRA-HIGH THERMAL CONDUCTIVITY GRAPHITE FIBERS**
$0 (PYF)*
DOE Contacts: J. P. Carr, (301) 903-6519 and
E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole,
(423) 574-4824
Amoco Performance Products, Inc. Contact:
G. V. Deshpande

The preparation of high-performance carbon (graphite) fibers requires a mesophase pitch precursor. Traditionally, in the USA, this has been derived from a petroleum precursor. Overseas suppliers have, however, developed high-performance fibers from coal derived precursors. Amoco Performance Products' goal is to explore coal-based pitch precursors' utility for use in ultra-high thermal conductivity graphite fibers.

Keywords: Carbon, Fibers, Graphite, Precursors

538. **DEVELOPMENT OF CARBON-CARBON COMPOSITES FROM SOLVENT-EXTRACTED PITCH**
$0 (PYF)*
DOE Contacts: J. P. Carr, (301) 903-6519 and
E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole,
(423) 574-4824
Fiber Materials, Inc. Contact: Cliff Baker,
(207) 282-5911

The manufacture of carbon-carbon composites for use in the aerospace industry has been heavily reliant on petroleum and coal tar pitches as matrix precursors. It is of great importance to strategic materials production for the Department of Defense that a stable, long-lived source of pitch be developed. Consequently, Fiber Materials, Inc. will work with staff members at the Oak Ridge National Laboratory and at West Virginia University to develop carbon-carbon composite materials from pitches derived from coal via a solvent extraction process. The objectives of this project shall be twofold. First, FMI shall use solvent extracted pitch to develop carbon-carbon composites with similar or improved properties over those currently manufactured from Allied 15V coal tar or Ashland A-240 petroleum pitches. Second, FMI shall develop improved, lower-cost composites from improved solvent extracted pitches supplied by WVU.

Keywords: Carbon, Composites, Pitch

539. **CONVERSION OF PITCHES AND COKES FROM SOLVENT-EXTRACTED MATERIALS**
$0 (PYF)*
DOE Contacts: J. P. Carr, (301) 903-6519 and
E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole,
(423) 574-4824
Koppers Industries, Inc. Contact: R. McHenry,
(412) 826-3989

The closure of by-product coke ovens has caused the domestic production of coal tar pitch to decline at 3 percent to 4 percent per annum during the mid-1990s. This reduction has directly affected Koppers' capability to produce required quantities of quality binder and impregnating pitches used in the aluminum and commercial carbon and graphite industries. Moreover, the other major constituent of carbon anodes and graphites is a coke, usually produced from petroleum pitch precursors, 50 percent of which are imported. The objectives of this research are to develop dependable domestic coal-based raw materials for the production of: binder pitches for aluminum cell anodes and commercial carbon and graphite products; impregnating pitches for commercial carbon and graphite products and specialty materials; oils for wood treatment and carbon black production; chemicals for phthalic anhydride and other products; and metallurgical and foundry grade cokes.

Keywords: Coke, Pitch, Conversion

540. **CARBON FIBER COMPOSITE MOLECULAR SIEVES**
$155,000
DOE Contacts: J. P. Carr, (301) 903-6519 and
E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact:
T. D. Burchell, (423) 576-8595

Hydrogen and Methane gas recovery technologies are required to: (1) allow the upgrading of heavy hydrocarbons to transport fuels, thus reducing the amount of carbon rejected during crude oil refining and (2) to improve the yield and process economics of natural gas wells. The purpose of this work is to develop carbon fiber composite molecular sieves (CFCMS) from porous carbon fiber composites manufactured from solvent extracted coal tar pitch derived carbon fibers. The work will be performed in collaboration with other members of the Cooperative

*PYF denotes that funding for this activity, active in FY 1995, was provided from prior year funds.

Research Partnership on Carbon Products and the Non Fuel Uses of Coal.

Keywords: Consortium, Carbon Products

541. **DEVELOPMENT OF PRECURSORS FOR PRODUCTION OF GRAPHITES AND CARBON PRODUCTS**
$0 (PYF)*
DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole, (423) 574-4824
UCAR Carbon Company Contact: Irv Lewis, (216) 676-2203

The manufacture of graphite utilizes cokes and pitches derived from petroleum refining by-products and by-product coke ovens. These include isotropic and anisotropic cokes, binder, and impregnant pitches. Assuring feedstock quality is of great importance to the graphite industry. Therefore, a stable long-lived source of feedstock pitch (and hence coke) would be of considerable benefit to the industry. Consequently, UCAR Carbon Company Inc. shall work with staff members at the Oak Ridge National Laboratory and at the West Virginia University to develop suitable precursor pitches, binders, impregnants, and cokes for the production of graphites and other carbon products.

Keywords: Carbon Products, Precursors, Graphites

542. **PRODUCTION OF YARN FROM VLS WHISKERS**
$100,000
DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole, (423) 574-4824

In order to exploit the superior thermomechanical properties of fibrils produced by the Vapor-Liquid-Solid (VLS) Process, the feasibility of scaled-up production of the SiC fibril will be demonstrated in this activity. Through time-series study and computer simulation, the parameters affecting the growth process and properties of the fibrils will be examined.

Keywords: Whiskers, Fibers, Ceramic

*PYF denotes that funding for this activity, active in FY 1995, was provided from prior year funds.

543. **RADIO-WAVE NANO-PHASE SILICON CARBIDE AND SILICON NITRIDE PROCESSES**
$100,000
DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole, (423) 574-4824
Sandia National Laboratories Contact: R. J. Buss, (505) 844-3504

This program examines the use of radio-frequency plasma discharges as a synthetic route to nanometer-size silicon carbide and silicon nitride particles.

Keywords: Nanophase, Silicon Nitride, Silicon Carbide

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

544. **INVESTIGATION OF THE WELDABILITY OF POLYCRYSTALLINE IRON ALUMINIDES**
$75,000
DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole, (423) 574-4824
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

545. **AQUEOUS CORROSION OF IRON ALUMINIDES**
$29,000
DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole, (423) 574-4824
University of Tennessee Contact: R. A. Buchanan, (423) 974-4858

The objective of this project is to investigate (1) evaluation of the effects of surface conditions on the corrosion and embrittlement of Fe-Al alloys, and (2) corrosion fatigue properties of Fe-Al alloys.

Keywords: Alloys, Aluminides, Corrosion, Stress

546. **EVALUATION OF THE INTRINSIC AND EXTRINSIC FRACTURE BEHAVIOR OF IRON ALUMINIDES**
$68,000
DOE Contacts: J. P. Carr, (301) 903-6519 and
E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole,
(423) 574-4824
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

547. **INVESTIGATION OF IRON ALUMINIDE WELD OVERLAYS**
$56,000
DOE Contacts: J. P. Carr, (301) 903-6519 and
E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole,
(423) 574-4824
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

548. **FIRESIDE CORROSION TESTS OF CANDIDATE ADVANCED AUSTENITIC ALLOYS, COATINGS, AND CLADDINGS**
$80,000
DOE Contacts: J. P. Carr, (301) 903-6519 and
E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole,
(423) 574-4824
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

549. **JOINING TECHNIQUES FOR ADVANCED AUSTENITIC ALLOYS**
$50,000
DOE Contacts: J. P. Carr, (301) 903-6519 and
E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole,
(423) 574-4824
University of Tennessee Contact: C. D. Lundin,
(423) 974-5310

Weldability is an important consideration in the selection of a suitable alloy for the fabrication of boiler components such as superheaters and reheaters. It is often a challenge to select joining materials and establish procedures that will allow advanced materials to function at their full potential. The purpose of this research is to examine important aspects of newly developed austenitic tubing alloys intended for service in the temperature range 550 to 700°C.

Keywords: Alloys, Austenitics, Joining, Welding

550. **FATIGUE AND FRACTURE BEHAVIOR OF Cr-Nb ALLOYS**
$20,000
DOE Contacts: J. P. Carr, (301) 903-6519 and
E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole, (423) 574-4824
University of Tennessee Contact: Peter Liaw, (423) 974-6356

The objective of this research shall be to characterize the fatigue and fracture behavior of Cr_2Nb-based alloys and other intermetallic materials at ambient and elevated temperatures in controlled environments. These studies are expected to lead to mechanistic understanding of the fatigue and fracture behavior of these alloys. Fatigue tests shall be conducted for the purpose of evaluating crack initiation and fatigue life of Cr_2Nb-based alloys as well as other intermetallic alloys. The fatigue properties shall be evaluated as functions of test environment, cyclic frequency and test temperature. Additional tensile tests will be required to characterize the fracture behavior of these structural alloys. Mechanical tests shall be performed to determine the fatigue and fracture behavior of Cr_2Nb-based alloys. The microstructure of the alloys shall be characterized and correlated with the mechanical properties.

Keywords: Fracture, Fatigue, Alloys

551. **CORROSION AND MECHANICAL PROPERTIES OF ALLOYS IN FBC AND MIXED-GAS ENVIRONMENTS**
$310,000
DOE Contacts: J. P. Carr, (301) 903-6519 and
E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole, (423) 574-4824
Argonne National Laboratory Contact: K. Natesan, (708) 252-5103

The purposes of this task are to: (1) evaluate the corrosion mechanisms for chromia- and alumina-forming alloys in mixed-gas environments, (2) develop an understanding of the role of several microalloy constituents in the oxidation/sulfidation process, (3) evaluate transport kinetics in oxide scales as functions of temperature and time, (4) characterize surface scales that are resistant to sulfidation attack, and (5) evaluate the role of deposits in corrosion processes.

Keywords: Corrosion, Gasification, Creep Rupture, Fluidized-Bed Combustion

552. **MECHANICALLY RELIABLE COATINGS AND SCALES FOR HIGH-TEMPERATURE CORROSION RESISTANCE**
$50,000
DOE Contacts: J. P. Carr, (301) 903-6519 and
E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole, (423) 574-4824
Argonne National Laboratory Contact: K. Natesan, (708) 252-5103

This project involves the development of mechanically reliable coatings and scales for high-temperature corrosion resistance. ANL shall systematically generate the knowledge required to establish a scientific basis for design and synthesis of improved (slow growing, adherent, sound) protective oxide coatings and scales on high temperature materials, without compromising the requisite bulk material properties. In addition, ANL shall provide information on the performance of advanced candidate materials from the standpoint of corrosion resistance and residual mechanical properties, after exposure in simulated combustion environments typical of indirectly-fired gas turbines. The work shall emphasize corrosion evaluation of materials in air, salt, and coal/ash environments at temperatures between 1000° and 1400°C, and measurement of residual toughness properties of the materials after corrosion.

Keywords: Corrosion, Coatings, Scales

553. **ENVIRONMENTAL EFFECTS ON IRON ALUMINIDES**
$145,000
DOE Contacts: J. P. Carr, (301) 903-6519 and
E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact:
P. F. Tortorelli, (423) 574-5119

The purpose of this task is to evaluate the high-temperature corrosion behavior of iron-aluminum alloys as part of the effort to develop highly corrosion-resistant iron-aluminide alloys and coatings for fossil energy applications. A primary objective is to investigate the resistance of the alloys to mixed-oxidant (oxygen-sulfur-chlorine-carbon) environments that arise in the combustion or gasification of coal. This includes the determination of the influence of sulfur and other reactive gaseous species on corrosion kinetics and oxide microstructures and the effects of alloying additions and oxide dispersoids on sulfidation and oxidation resistance.

Keywords: Corrosion, Aluminides, Mixed-Gas, Scales

554. **INVESTIGATION OF MOISTURE-INDUCED EMBRITTLEMENT OF IRON ALUMINIDES**
$73,000
DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole, (423) 574-4824
Rensselaer Polytechnic Institute Contact: N. S. Stoloff, (518) 276-6371

The purpose of this work is to study hydrogen embrittlement of iron aluminide alloys. Moisture in air can significantly reduce the room-temperature tensile ductility of Fe_3Al-based alloys by combining with the aluminum in the alloys to form atomic hydrogen. The atomic hydrogen diffuses rapidly into the material causing embrittlement. Experiments are being conducted on selected Fe_3Al alloys that will lead to an understanding of the phenomenon. The work focuses on the effects of moisture on relevant mechanical properties such as fatigue and tensile strengths, and correlates important microstructural variables such as degree of order, grain size, and phases present with the alloy's susceptibility to embrittlement.

Keywords: Aluminides, Embrittlement, Moisture

555. **CORROSION PROTECTION OF ULTRAHIGH TEMPERATURE INTERMETALLIC ALLOYS**
$146,000
DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: P. F. Tortorelli, (423) 574-5119

The objective of this task is to develop high-strength, corrosion-resistant intermetallic alloys for use as hot components in advanced fossil energy conversion and combustion systems. The successful development of these alloys is expected to improve the thermal efficiency of fossil energy conversion systems through increased operating temperatures and to increase the service life of hot components exposed to corrosive environments at elevated temperatures (1000°C). The initial effort will be devoted to in situ composite alloys based on the $Cr\text{-}Cr_2Nb$ system.

Keywords: Corrosion, Chromium-Niobium, Mixed-Gas, Scales

556. **OXIDE DISPERSION STRENGTHENED (ODS) IRON ALUMINIDE EQUIPMENT**
$35,000
DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: I. G. Wright, (423) 574-4451

This task provides funds for the procurement of major equipment items necessary for AR&TD Materials Program activities.

Keywords: Equipment

557. **OXIDE DISPERSION STRENGTHENED (ODS) IRON ALUMINIDES**
$222,000
DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: I. G. Wright, (423) 574-4451

The purpose of this task is to develop fabrication procedures for making oxide dispersion-strengthened (ODS) iron-aluminum alloys based on Fe_3Al. The suitability of the procedures is measured in terms of the high-temperature oxidation and sulfidation resistance and creep strength of the ODS alloys compared with Fe_3Al alloys fabricated by conventional ingot and powder processes.

Keywords: Aluminides

558. **MATERIALS SUPPORT FOR HITAF**
$0 (PYF)*
DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: K. Breder, (423) 574-5089

This task involves the measurement of selected mechanical and physical properties of structural ceramics which are proposed for use in the construction of the High Temperature Advanced Furnace (HITAF) air heater design being developed under the Combustion 2000 program for PETC/DOE. The purpose of the research is to evaluate candidate structural ceramics for this application by studying the fast fracture and fatigue (both dynamic and interrupted static) properties at temperatures from 1100 to 1400°C in air, their corrosion behavior, property uniformity of components and long term degradation of ceramic properties due to exposure in prototype HITAF systems.

*PYF denotes that funding for this activity, active in FY 1995, was provided from prior year funds.

This work is continuing with funding from the Combustion 2000 Program.

Keywords: Furnace, Materials, HITAF

559. **CHARACTERIZATION OF LOW-EXPANSION CERAMIC MATERIALS AND DEVELOPMENT OF SOL GEL-DERIVED COATINGS AS INTERFACES FOR SIC COMPOSITES**
$23,000
DOE Contacts: J. P. Carr, (301) 903-6519 and
E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole,
(423) 574-4824
University of Tennessee Contact: Peter Liaw,
(423) 974-6356

The purpose of this activity is the experimental study of low-expansion ceramic materials and the development of sol-gel derived coatings as interfaces for Nicalon®/SiC composites

Keywords: Composites, Ceramics

560. **JOINING OF CERAMICS**
$50,000
DOE Contacts: J. P. Carr, (301) 903-6519 and
E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole,
(423) 574-4824
Idaho National Engineering Laboratory Contact:
B. H. Rabin, (208) 526-0058

The purpose of this project is to explore and develop joining techniques for silicon carbide fiber-reinforced silicon carbide ceramics produced by chemical vapor infiltration and deposition (CVID). The research goals include identifying appropriate joining methods, establishing experimental procedures for fabricating joints, and characterizing the structure and properties of joined materials. An understanding of the factors that control joint performance is sought through studies of the relationships among processing variables, joint microstructures, and mechanical properties. Additional funds for this project are provided by the DOE Pittsburgh Energy Technology Center.

Keywords: Ceramics, Joining, Technology Transfer

561. **SUPPORT SERVICES FOR CERAMIC FIBER-CERAMIC MATRIX COMPOSITES**
$25,000
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(423) 574-4824
University of North Dakota Energy and Environmental Research Center Contact: J. P. Hurley,
(701) 777-5159

This task will review and, if appropriate, propose modifications to plans, materials, and tests planned by researchers on the AR&TD Materials Program in work to test materials for coal-fueled energy systems. The changes shall be suggested in order to make the corrosion experiments more reflective of the actual conditions that will be encountered by the materials in the energy systems. UNDEERC shall accomplish this task by reviewing the major advanced energy system projects being funded by the DOE, and by working with the company's technical monitor and staff to prepare a summary of the expected corrosion problems. Both gasification and combustion systems will be included. Ceramic materials in two subsystems will be the focus of this work: (1) hot gas cleanup systems and (2) high-temperature heat exchangers. UNDEERC shall review and suggest improvements to materials testing procedures that are used to determine material behavior when used in hot-gas cleanup or heat exchanger applications. A limited amount of computer modeling and laboratory experimentation shall be a part of this effort.

Keywords: Composites, Ceramics, Fibers

562. **DEVELOPMENT OF NONDESTRUCTIVE EVALUATION METHODS AND EFFECTS OF FLAWS ON THE FRACTURE BEHAVIOR OF STRUCTURAL CERAMICS**
$310,000
DOE Contacts: J. P. Carr, (301) 903-6519 and
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Oak Ridge National Laboratory Contact: N. C. Cole,
(423) 574-4824
Argonne National Laboratory Contacts:
W. A. Ellingson, (708) 252-5068 and
J. P. Singh, (708) 252-5123

The purpose of this project is to study and develop acoustic and radiographic techniques and possible novel techniques such as nuclear magnetic resonance, to characterize structural ceramics with regard to presence of porosity, cracking, inclusions, amount of free silicon, and mechanical properties, and to establish the type and character of flaws that can be found by nondestructive evaluation (NDE) techniques. Both fired and unfired specimens are being studied to establish correlations between NDE results and failure of specimens.

Keywords: Nondestructive Evaluation, Ceramics, Flaws, Fracture

563. **FRACTURE BEHAVIOR OF ADVANCED CERAMIC HOT-GAS FILTERS**
$125,000
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Oak Ridge National Laboratory Contact: N. C. Cole,
(423) 574-4824
Argonne National Laboratory Contacts: J. P. Singh,
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The purpose of this project is to study the fracture behavior of ceramic hot-gas filters. ANL shall evaluate mechanical/physical properties and microstructure, identify critical flaws and failure modes, and correlate mechanical/physical properties with microstructure and critical flaws to provide much needed information for selection of materials and optimization of fabrication procedures for hot-gas ceramic filter modules. As part of the information base, requirements for strength and fracture toughness of the filter material shall be established from stress and fracture mechanics analyses of typical filters subjected to loadings expected during operation and pulse-cleaning cycles.

Keywords: Ceramics, Flaws, Fracture, Failure

564. **CERAMIC CATALYST MATERIALS**
$225,000
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Oak Ridge National Laboratory Contact: N. C. Cole,
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(505) 844-8723

The purpose of this research is to investigate the role of ceramic material properties in the catalytic activity of a novel class of catalytic supports, known as hydrous titanium oxides (HTO). Catalysts prepared on these materials show particular promise as economically and environmentally attractive alternatives to present commercial catalysts for the direct liquefaction of coal. In these studies, improved understanding and control of the synthesis process is being pursued in order to tailor the composition, molecular structure, microporosity, and physical/mechanical properties of the HTO thin films. The effects of altered structure, composition, and other material properties of the thin film ceramic support material on catalytic activity are being assessed.

Keywords: Ceramics, Catalysts

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

565. ***MATERIALS AND COMPONENTS IN FOSSIL ENERGY APPLICATIONS* NEWSLETTER**
$60,000
DOE Contacts: J. P. Carr, (301) 903-6519 and
E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: I. G. Wright,
(423) 574-4451

The purpose of this task is to publish a periodic (bimonthly) DOE-EPRI newsletter to address current developments in materials and components in fossil energy applications. Equal funding is provided by EPRI.

Keywords: Materials, Components

566. **CERAMIC FIBER FILTER TECHNOLOGY**
$50,000
DOE Contacts: J. P. Carr, (301) 903-6519 and
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Oak Ridge National Laboratory Contact: M. A. Janney,
(614) 424-4281

The purpose of this effort is to develop the fabrication technology necessary to make ceramic-fiber based filters for a variety of filtration applications of interest to the Fossil Energy community.

Keywords: Filters, Ceramics, Fibers

567. **FABRICATION OF FULL-SCALE FIBER-REINFORCED HOT-GAS FILTERS BY CHEMICAL VAPOR DEPOSITION**
$0 (PYF)*
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Oak Ridge National Laboratory Contact: N. C. Cole,
(423) 574-4824
3M Company Contact: M. A. Leitheiser,
(612) 733-9394

The purpose of this project is to scale-up the chemical vapor infiltration and deposition (CVID) process developed at Oak Ridge National Laboratory for fabricating ceramic

*PYF denotes that funding for this activity, active in FY 1995, was provided from prior year funds.

fiber-ceramic matrix composites. The goal is to use the scaled-up CVID process to produce composite filters that have the requisite strength and toughness, but which also have sufficient porosity to be permeable to gas streams and the appropriate size and distribution of porosity to be an effective filter. A practical process for fabricating porous ceramic fiber-ceramic matrix candle filters (full-size) with increased surface area has been developed.

Keywords: Ceramics, Composites, Filters

568. **DEVELOPMENT OF CERAMIC MEMBRANES FOR GAS SEPARATION**
$400,000
DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole, (423) 574-4824
Oak Ridge K-25 Site Contact: D. E. Fain, (423) 574-9932

The purpose of this activity is to fabricate inorganic membranes for the separation of gases at high temperatures and/or in hostile environments, typically encountered in fossil energy conversion processes such as coal gasification. This work is performed in conjunction with a separate research activity that is concerned with the development and testing of the ceramic membranes.

Keywords: Ceramics, Membranes, Filters, Separation

569. **CORROSION PROTECTION OF CERAMIC HEAT EXCHANGER TUBES**
$125,000
DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole, (423) 574-4824
Pennsylvania State University Contact: R. E. Tressler, (814) 865-7961

This project addresses the development of ceramic heat exchanger materials with chromia surface treatments for corrosion resistance. High chromia-content refractories have been demonstrated to be resistant to corrosion by coal slags. This project will focus on improving the corrosion resistance of ceramics by incorporating chromia into the surface layers.

Keywords: Ceramics, Corrosion, Filters

570. **INVESTIGATION OF THE MECHANICAL PROPERTIES AND PERFORMANCE OF CERAMIC COMPOSITE COMPONENTS**
$150,000
DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole, (423) 574-4824
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The purpose of this project is to develop a test system and test methods to obtain information on the properties and performance of ceramic composite materials. The work involves a comprehensive mechanical characterization of composite engineering components such as tubes, plates, shells, and beams subjected to static and cyclic multiaxial loading at elevated temperatures for extended time periods.

Keywords: Ceramics, Composites, Mechanical Properties, Testing

571. **STABILITY OF SOLID OXIDE FUEL CELL (SOFC) MATERIALS**
$250,000
DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole, (423) 574-4824
Pacific Northwest Laboratory Contact: L. R. Pederson, (509) 375-2579

The purpose of this task is to evaluate the chemical and physical stability of fuel cell materials and interfaces under conditions relevant to an operating SOFC and to identify features in SOFC operation that would limit system performance.

Keywords: Fuel Cells, SOFC

572. **MIXED OXYGEN ION/ELECTRON-CONDUCTING CERAMICS FOR OXYGEN SEPARATION AND FUEL CELLS**
$225,000
DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole, (423) 574-4824
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The purpose of this task is to develop ceramic compositions and physical forms that will provide the highest possible oxygen separation efficiencies from air at the lowest cost.

Keywords: Fuel Cells, Electrochemical, Electrolytes

573. **PROTON-CONDUCTING CERATE CERAMICS**
$225,000
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Oak Ridge National Laboratory Contact: N. C. Cole,
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The purpose of this task is to develop cerate perovskites for use as hydrogen separation membranes, as hydrogen sensors, in membrane reactors, and in gas cleanup.

Keywords: Fuel Cells, Electrochemical, Electrolytes

574. **ODS Fe_3Al TUBES FOR HIGH-TEMPERATURE HEAT EXCHANGERS**
$53,000
DOE Contacts: J. P. Carr, (301) 903-6519 and
E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole,
(423) 574-4824
PM Hochtemperatur-Metall. GmbH Contact:
Dieter Sporer, 011-43-5672-70-2923

The goal of the work is to produce tubes of Fe_3Al-0.5 wt. percent Y_2O_3 which have properties suitable for application as heat transfer surfaces in very high-temperature heat exchangers. The alloy is produced by a powder metallurgical (mechanical alloying) process, the main purpose of which is to obtain a uniform distribution of sub-micron Y_2O_3 particles in the Fe_3Al matrix. The required high-temperature creep strength is derived largely by developing very large, elongated grains which are effectively pinned by the oxide dispersion. Development of the necessary grain structure is dependent on the characteristics of the mechanically-alloyed powder, and on thermomechanical processing of the consolidated powder.

Keywords: Aluminide, Tubes, Heat Exchangers

575. **POROUS IRON ALUMINIDE ALLOYS**
$23,000
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Oak Ridge National Laboratory Contact: N. C. Cole,
(423) 574-4824
Oak Ridge K-25 Site Contact: D. E. Fain,
(423) 574-9932

This project is directed to the development of porous iron aluminide structures for applications such as hot-gas filters

Keywords: Filters, Aluminides

576. **IRON ALUMINIDE FILTERS**
$50,000
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Oak Ridge National Laboratory Contact:
P. F. Tortorelli, (423) 574-5119

The purpose of this project is to provide technical support to the Pall Corporation in its development of porous sintered iron-aluminide filters for hot-particle removal from product streams in coal gasification systems. The ORNL role is to provide specialized expertise in the areas of corrosion analysis, microstructural characterization, alloy selection, and processing based on extensive experience with iron aluminides and materials performance in fossil energy systems. ORNL's contribution via this project should aid the success and timely completion of Pall's development and demonstration efforts.

Keywords: Filters, Aluminides

577. **EVALUATION OF CERAMIC HEAT EXCHANGER TUBES AND JOINTS**
$158,000
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(423) 574-4824
Pennsylvania State University Contact: R. E. Tressler,
(814) 865-7961

This project has two principal parts: (1) screening analysis of candidate ceramic hot-gas filter materials, and

(2) development of ceramic heat exchanger materials with chromium surface treatments for corrosion resistance. A flow-through screening test will be developed to test ceramic hot-gas filter elements in simulated coal combustion environments. Corrosion-resistant heat exchanger tubes will be fabricated by incorporating chromium in the surface layers.

Keywords: Ceramics, Corrosion, Filters

578. **THERMAL AND MECHANICAL ANALYSIS OF A CERAMIC TUBESHEET**
$40,000
DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole, (423) 574-4824
Mallett Technology Contact: R. H. Mallett, (919) 406-1500

A transport combustor is being commissioned at the Southern Services facility in Wilsonville, Alabama, to provide a gaseous product for the assessment of hot-gas filtering systems. These hot-gas filtration systems will include granular-bed and barrier filter concepts. Filters will be evaluated for carbonizer and gasifier gaseous products. In addition, a pressurized fluidized-bed combustor (PFBC) will be installed to burn the carbonizer product, and a hot gas filter will be installed in the PFBC gas stream. Compositions of the gas streams will range from oxidizing to reducing, and the partial pressures of oxygen and sulfur will vary substantially. Temperatures of the gas streams will range from 840 to 980°C (or higher). One of the barrier filters under consideration incorporates a ceramic tubesheet to support the candle filters. This system, to be designed and built by Industrial Filter & Pump Manufacturing Company (IF&PM) is unique and may offer distinct advantages over metal/ceramic systems that have been tested extensively in other EPRI/DOE projects. To gain an insight that could prove to be useful in the scaleup of a commercial-size, all-ceramic system, work will be undertaken to develop a design methodology applicable to the thermal-mechanical analysis of the all-ceramic system.

Keywords: Ceramics, Tubesheet

579. **CERAMIC TUBESHEET DESIGN ANALYSIS**
$10,000
DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (423) 576-0735
Oak Ridge National Laboratory Contact: R. W. Swindeman, (423) 574-5108

The purpose of this task is to perform thermal and mechanical analyses of critical regions in a ceramic tubesheet support for barrier filters in a hot gas cleanup vessel designed for use in gasifier, carbonizer, and pressurized fluidized bed combustion gas streams.

Keywords: Ceramics, Tubesheet

INSTRUMENTATION AND FACILITIES

580. **MANAGEMENT OF THE FOSSIL ENERGY AR&TD MATERIALS PROGRAM**
$400,000
DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (423) 576-0735
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The overall objective of the Fossil Energy Advanced Research and Technology Development (AR&TD) Materials program is to conduct a fundamental, long-range research and development program that addresses, in a generic way, the materials needs of fossil energy systems and ensures the development of advanced materials and processing techniques. The purpose of this task is to manage the Fossil Energy AR&TD Materials program in accordance with procedures described in the Program Management Plan approved by DOE. This task is responsible for preparing the technical program implementation plan for DOE approval; submitting budget proposals for the program; recommending work to be accomplished by subcontractors, other national laboratories, and by Oak Ridge National Laboratory (ORNL); placing and managing subcontracts for fossil energy materials development at industrial research centers, universities, and other government laboratories; and for reporting the progress of the program.

Keywords: Management, Materials Program

581. **GENERAL TECHNOLOGY TRANSFER ACTIVITIES**
$35,000
DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (423) 576-0735
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The task provides funds for the initiation of technology transfer activities to identify and develop relationships with industrial partners for the transfer of AR&TD Materials Program technologies to industry.

Keywords: Technology Transfer

582. **GORDON RESEARCH CONFERENCE SUPPORT**
$4,000
DOE Contacts: J. P. Carr, (301) 903-6519 and
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The task provides funds to support the annual Gordon Research Conference.

Keywords: Technology Transfer

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