DOE/ER-0625

ENERGY MATERIALS COORDINATING COMMITTEE (EMaCC)

Fiscal Year 1993

July 1994

Annual Technical Report

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

DOE/ER-0625

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U.S. Department of Energy
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Washington, D.C. 20585

TABLE OF CONTENTS

TABLE OF CONTENTS (Continued)

TABLE OF CONTENTS (Continued)

TABLE OF CONTENTS (Continued)

INTRODUCTION

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

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

Electrochemical Technologies - Richard Kelly, ER-132, (301) 903-6051
Metals and Intermetallics - Matthew McMonigle, EE-231, (202) 586-2082
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 four 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 1993 and describes the materials research programs of various offices and divisions within the Department.

The Chairman of EMaCC for FY 1993 was Alan Dragoo. The compilation of this report was performed by Cynthia Carter, EMaCC Executive Secretary for FY 1994, with the assistance of FM Technologies, Inc.

Brian G. Volintine
Office of Industrial Technologies
Chairman of EMaCC, FY 1994

MEMBERSHIP LIST
DEPARTMENT OF ENERGY
ENERGY MATERIALS COORDINATING COMMITTEE

Organization	Representative	Phone No.
ENERGY EFFICIENCY AND RENEWABLE ENERGY		
Building Technologies		
Building Systems and Materials	Peter Scofield, EE-421	202/586-9193
Industrial Technologies		
Industrial Energy Efficiency	Scott Richlen, EE-221	202/586-2078
Waste Materials Management	Donald Walter, EE-222	202/586-6750
Improved Energy Productivity	Matthew McMonigle, EE-231	202/586-2082
Advanced Industrial Materials	Charles Sorrell, EE-232	202/586-1514
Transportation Technologies		
Advanced Transportation Materials	Sidney Diamond, EE-34	202/586-0832
Utility Technologies		
Wind/Hydro/Ocean Technologies	William Richards, EE-121	202/586-5410
Geothermal Technology	Raymond LaSala, EE-122	202/586-4198
Photovoltaic Technology	Morton B. Prince, EE-131	202/586-1725
Advanced Utility Concepts	James Daley, EE-142	202/586-1165

MEMBERSHIP LIST (Continued)

Organization	Representative	Phone No.
ENERGY RESEARCH		
Basic Energy Sciences		
Materials Sciences	Iran L. Thomas, ER-13	301/903-3426
Metallurgy and Ceramics	Robert J. Gottschall, ER-131	301/903-3428
Solid State Physics and Materials Chemistry	W. Oosterhuis, 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
Program Analysis	Timothy Fitzsimmons, ER-32	301/903-9830
Health and Environmental Research		
Physical and Technology Research	Gerald Goldstein, ER-74	301/903-5348
Fusion Energy		
Fusion Technologies	F. W. (Bill) Wiffen, ER-533	301/903-4963
NUCLEAR ENERGY		
Civilian Reactor Development		
Advanced Reactor Programs	Andrew Van Echo, NE-45	301/903-3930
Space and Defense Power Systems		
Defense Energy Projects	C. Chester Bigelow, NE-52	301/903-4299
Special Applications	William Barnett, NE-53	301/903-3097

MEMBERSHIP LIST (Continued)

Organization	Representative	Phone No.
NUCLEAR ENERGY (continued)		
Naval Reactors	Robert H. Steele, NE-60	703/603-5565
Nuclear Safety Self-Assessment		
Nuclear Quality Assurance	John Dowicki, NE-84	301/903-7729
DEFENSE PROGRAMS		
Research and Advanced Technology		
Research and Technology Development	Gregory J. D'Alessio, DP-242	301/903-6688
Inertial Confinement Fusion	Carl B. Hilland, DP-28	301/903-3687
ENVIRONMENTAL RESTORATION AND WASTE MANAGEMENT		
Waste Operations		
Waste Management Projects	Mark Frei, EM-34	301/903-7201
Technology Development		
Transportation Management	Michael Conroy, EM-561	301/903-7967
Research and Development	Stanley M. Wolf, EM-54	301/903-7962

MEMBERSHIP LIST (Continued)

Organization	Representative	Phone No.
FOSSIL ENERGY		
Management, Fundamental Research, and Cooperative Development		
Technical Coordination	James P. Carr, FE-14	301/903-6519
CIVILIAN RADIOACTIVE WASTE MANAGEMENT		
Analysis and Verification	Alan Berusch, RW-22	202/586-9362

ORGANIZATION OF THE REPORT

The program descriptions consist of a funding summary for each Assistant Secretary office and the Office of Energy Research, and detailed project summaries with project goals and accomplishments.

The FY 1993 budget summary table for DOE Materials Activities in each of the programs is presented on pages 7 through 10.

FY 1993 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 1993
Office of Building Technologies	$ 750,000
Office of Building Energy Research	750,000
Buildings Systems and Materials Division	750,000
Office of Industrial Technologies	$23,956,000
Office of Waste Reduction Technologies	14,504,000
Industrial Energy Efficiency Division	10,974,000
Waste Material Management Division	3,530,000
Office of Industrial Processes	9,452,000
Office of Transportation Technologies	$32,000,000
Office of Transportation Materials	16,984,000
Office of Propulsion Systems	14,596,000
Advanced Propulsion Division	10,933,000
Electric Hybrid Propulsion Division	3,663,000
Office of Alternative Fuels	420,000

FY 1993 BUDGET SUMMARY TABLE FOR DOE MATERIALS ACTIVITIES

	FY 1993
Office of Utility Technologies	$ 37,650,000
Office of Solar Energy Conversion	19,400,000
Photovoltaic Energy Technology Division	19,400,000
Office of Renewable Energy Conversion	687,000
Geothermal Division	687,000
Office of Energy Management	17,563,000
Advanced Utility Concepts Division	17,563,000
Office of Energy Research	$324,512,190
Office of Basic Energy Sciences	285,128,044
Division of Materials Sciences	267,140,000
Division of Chemical Sciences	5,320,000
Division of Engineering and Geosciences	7,228,044
Engineering Sciences Research	5,278,392
Geosciences Research	1,949,642
Division of Advanced Energy Projects	5,440,000
Office of Fusion Energy	13,980,000
Small Business Innovation Research Program	25,404,146

FY 1993 BUDGET SUMMARY TABLE FOR DOE MATERIALS ACTIVITIES (Continued)

	FY 1993
Office of Environmental Management	$ 22,557,000
Office of Waste Management	8,890,000
Office of Technology Development	13,667,000
Office of Nuclear Energy	$123,047,000
Office of Uranium Programs	14,770,000
Office of Civilian Reactor Development	31,347,000
Actinide Recycle Programs	31,347,000
High Temperature Gas-Cooled Reactors	5,947,000
Liquid Metal Reactors	25,400,000
Office of Space and Defense Power Systems	24,930,000
Radioisotope Power Systems Division	2,630,000
Space Reactor Power Systems Division	22,300,000
Office of Naval Reactors	52,000,000
Office of Civilian Radioactive Waste Management	$ 1,700,000

FY 1993 BUDGET SUMMARY TABLE FOR DOE MATERIALS ACTIVITIES (Continued)

	FY 1993
Office of Defense Programs	$122,589,000
The Weapons Research Development and Test Program	122,589,000
Sandia National Laboratory	65,443,000
Lawrence Livermore National Laboratory	30,119,000
Los Alamos National Laboratory	27,027,000
Office of Fossil Energy	$ 6,739,000
Office of Advanced Research	6,739,000
TOTAL	**$695,500,190**

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 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 1993
1. Office of Building Technologies	$ 750,000
a. Office of Building Energy Research	750,000
(1) Buildings Systems and Materials Division	750,000
2. Office of Industrial Technologies	$23,956,000
a. Office of Waste Reduction Technologies	14,504,000
(1) Industrial Energy Efficiency Division	10,974,000
(2) Waste Material Management Division	3,530,000
b. Office of Industrial Processes	9,452,000
3. Office of Transportation Technologies	$32,000,000
a. Office of Transportation Materials	16,984,000
b. Office of Propulsion Systems	14,596,000
(1) Advanced Propulsion Division	10,933,000
(2) Electric Hybrid Propulsion Division	3,663,000
c. Office of Alternative Fuels	420,000

4. Office of Utility Technologies	$37,650,000
a. Office of Solar Energy Conversion	19,400,000
(1) Photovoltaic Energy Technology Division	19,400,000
b. Office of Renewable Energy Conversion	687,000
(1) Geothermal Division	687,000
c. Office of Energy Management	17,563,000
(1) Advanced Utility Concepts Division	17,563,000

OFFICE OF BUILDING TECHNOLOGIES

	FY 1993
Office of Building Technologies - Grand Total	$750,000
Office of Building Energy Research	$750,000
Building Systems and Materials Division	$750,000
Materials Properties, Behavior, Characterization or Testing	$750,000
Development of Non-CFC Foam Insulations	150,000
Evacuated Powder Panel Insulation	300,000
Gas-Filled Reflective Insulation Panel	150,000
High-R Test Procedure Development	150,000

OFFICE OF BUILDING TECHNOLOGIES

Office of Building Energy Research

The Office of Building Energy Research works to increase the energy efficiency of the buildings sector through performance of R&D on building systems and building equipment. In addition, it conducts research to support the establishment of appliance standards and labeling and building energy performance standards. Specific objectives include providing the technology to:

- reduce energy consumption in existing buildings and in new buildings;
- increase the energy efficiency of oil and gas combustion heating systems and of oil- and gas-fired heat pump systems; and
- improve the energy efficiency of advanced electric heat pump and refrigeration systems, and of light systems.

Building Systems and Materials Division

The goal of this Division 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 Peter Scofield, (202) 586-9193.

Materials Properties, Behavior, Characterization or Testing

1. Development of Non-CFC Foam Insulations

FY 1993
$150,000

DOE Contact: Peter Scofield, (202) 586-9193
ORNL Contact: Tom Kollie, (615) 574-7463

This is the initial 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 with five different blends of HCFC-123 and 141b will be manufactured by industry and sent to ORNL for testing and evaluation both in the laboratory and in outdoor test facilities. Tests will be conducted to determine mechanical and thermal properties and aging characteristics.

Keywords: CFC, Foam Insulation, Insulation Sheathing, Roofs

2. Evacuated Powder Panel Insulation

FY 1993
$300,000

DOE Contact: Peter Scofield, (202) 586-9193
ORNL Contact: Tom Kollie, (615) 574-7463

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-30 per inch panel. Improved powders and longer life encasing films are being developed.

Keywords: Insulation, Vacuum, Heat Transfer

3. Gas-Filled Reflective Insulation Panel

FY 1993
$150,000

DOE Contact: Peter Scofield, (202) 586-9193
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. High-R Test Procedure Development

FY 1993
$150,000

DOE Contact: Peter Scofield, (202) 586-9193
ORNL Contact: Tom Kollie, (615) 574-7463

This project is a joint project with the Appliance Research Consortium 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 and the modelling of the test specimen within the test configuration.

Keywords: Thermal Resistance, Test Procedures

OFFICE OF INDUSTRIAL TECHNOLOGIES

	FY 1993
Office of Industrial Technologies - Grand Total	$23,956,000
Office of Waste Reduction Technologies	$14,504,000
Industrial Energy Efficiency Division	$10,974,000
Materials Properties, Behavior, Characterization or Testing	$ 2,674,000
Advanced Heat Exchanger Material Technology Development	927,000
Assessment of Strength Limiting Flaws in Ceramic Heat Exchanger Components	17,000
Ceramic Fiber Residue Measurement	25,000
CFCC Supporting Technologies	1,705,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 4,119,000
CFCC Program - Industry Tasks	$ 4,119,000
Device or Component Fabrication, Behavior or Testing	$ 4,181,000
Ceramic Composite Heat Exchanger for the Chemical Industry	222,000
HiPHES System Design Study for Energy Production from Hazardous Wastes	406,000
HiPHES System Design Study for an Advanced Reformer	253,000
Ceramic Components for Stationary Gas Turbines in Cogeneration Service	2,500,000
Long-Term Testing of Ceramic Components for Stationary Gas Turbines	800,000

OFFICE OF INDUSTRIAL TECHNOLOGIES

	FY 1993
Office of Waste Reduction Technologies (continued)	
Waste Material Management Division	$ 3,530,000
Waste Utilization and Conversion	$ 2,700,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 2,700,000
Wood Wastes to Adhesives	700,000
Waste Rubber-Polymer Composite	1,100,000
Electrochemical Removal of Zinc from Steel Scrap	0
Silicon Oxide Recovery-Conversion	500,000
Bioconversion of High-Starch Food Wastes into High-Value Products	400,000
Solar Materials Research	$ 830,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 830,000
Solar Materials Processing	594,000
Photocatalysts Based on Titanium Dioxide	236,000
Office of Industrial Processes	$ 9,452,000
Advanced Industrial Materials Program	$ 9,452,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 4,344,000
Combustion Chemical Vapor Deposition of Coatings	50,000
Synthesis and Design of Intermetallic Materials	690,000
Polymers with Improved Surface Properties	280,000
Development of Weldable, Corrosion Resistant Iron-Aluminide Alloys	214,000
Composites Through Reactive Metal Infiltration	350,000
Magnetic Field Processing of Inorganic Polymers	250,000

OFFICE OF INDUSTRIAL TECHNOLOGIES

	FY 1993
Office of Industrial Processes (continued)	
Advanced Industrial Materials Program (continued)	
Materials Preparation, Synthesis, Deposition, Growth or Forming (continued)	
Development of Improved Aerogel Superinsulation	300,000
Microwave-Driven Spray Drying and Filament Processing	350,000
Conducting Polymers: Synthesis and Industrial Applications	325,000
Microwave Assisted Chemical Vapor Infiltration	235,000
High Deposition Rate Chemical Vapor Deposition	350,000
Development of Chemical Vapor Composite Materials	950,000
Materials Properties, Behavior, Characterization, or Testing	$ 200,000
Three Dimensional X-ray Tomography of Composites	150,000
Computer Simulation Models of Thermal-Expansion-Anisotropic Induced Microcracking and Fracture Resistance Curves	50,000
Materials Structure and Composition	$ 3,474,000
The Development of Advanced Ceramic Membrane Technology	137,000
Ductility of Intermetallic Compounds Exposed to Aqueous Solutions	50,000
High-Temperature Precipitate-Strengthened Iron-Aluminide Alloys	155,000
Metallic and Intermetallic Bonded Ceramic Composites	500,000
Advanced NiAl and TiAl Intermetallic Alloys	237,000
Superior Metallic Alloys Through Rapid Solidification Processing by Design	250,000
Polymerization and Processing of Organic Polymers in a Magnetic Field	140,000
Microwave Joining of SiC	115,000
Microwave Processing of Materials	500,000
Chemical Vapor Infiltration of Ceramic Composites	290,000
Biomimetic Thin Film Synthesis	400,000
Recoverable Thermosets	200,000
Chemical Recycling of Plastics	500,000

OFFICE OF INDUSTRIAL TECHNOLOGIES

	FY 1993
Office of Industrial Processes (continued)	
Advanced Industrial Materials Program (continued)	
Device or Component Fabrication, Behavior or Testing	$ 1,434,000
Advanced Engineering Coatings Development	166,000
Assessment of Selective Dehydrogenation Catalysts	50,000
Ni_3Al Technology Transfer: Castability and Weldability of Ni_3Al	268,000
Advanced Microwave Processing Concepts	500,000
Chemically Specific Coatings	450,000

OFFICE OF INDUSTRIAL TECHNOLOGIES

The Office of Industrial Technologies conducts research and development to conserve energy in industry. The goal of these activities is to save energy, achieve higher efficiency, provide for fuel flexibility, and increase productivity in industrial unit operations and processes. To accomplish these objectives, the Office has adopted the basic strategy of identifying, in cooperation with private industry, the technological needs of energy conservation in the industrial sector; identifying what private industry is currently doing or will not do alone; selecting the highest priority targets not being pursued by the private sector; and negotiating cost-shared contracts with private industry or contracts with national laboratories or universities to carry out the necessary research.

Office of Waste Reduction Technologies

The mission of the Office of Waste Reduction is to develop and maintain a balanced program of research and development on generic technologies which contribute to enhanced industrial energy use efficiency and which have wide application throughout industry and agriculture. The program includes activities in waste heat recovery, improved thermal energy management, combustion systems, waste products utilization including municipal solid wastes, and waste stream detoxification.

Industrial Energy Efficiency Division

Materials Properties, Behavior, Characterization or Testing

5. Advanced Heat Exchanger Material Technology Development — FY 1993 $927,000

DOE Contact: G. Varga, (202) 586-0082
ORNL Contact: M. Karnitz, (615) 574-5150

This project conducts research to develop improved ceramic materials and fabrication processes and to expand the materials database for advanced heat exchangers. Currently the project is studying the effects of corrosive waste stream constituents on candidate ceramic and ceramic composite materials through coupon tests and exposure to high pressure exhaust gas environments and developing advanced wet forming techniques for monolithic ceramic components.

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

6. Assessment of Strength Limiting Flaws in Ceramic Heat Exchanger Components

FY 1993
$17,000

DOE Contact: G. Varga, (202) 586-0082
Babcock & Wilcox Contact: J. Bower, (804) 522-5742

This project studies the flaw populations and the effect of operating environments on flaw populations of ceramic heat exchanger components. Currently the project is correlating acoustic response to flaw growth. The goal of the project is to develop lifetime prediction correlations for ceramic components. Research is conducted cooperatively with the Idaho National Engineering Laboratory.

Keywords: Structural Ceramics, Structure, NDE, Industrial Waste Heat Recovery

7. Ceramic Fiber Residue Measurement

FY 1993
$25,000

DOE Contact: S. Richlen, (202) 586-2078
ORNL Contact: M. Karnitz, (615) 574-5150

This project determines whether whisker-like particles can be generated during the handling, processing, or machining of continuous ceramic fiber ceramic matrix composites. A test protocol has been written and is under review.

Keywords: Ceramic Composites, Whiskers

8. CFCC Supporting Technologies

FY 1993
$1,705,000

DOE Contact: S. Richlen, (202) 586-2078
ORNL Contact: M. Karnitz, (615) 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, and life prediction.

Keywords: Ceramic Composites, Fiber Architecture

Materials Preparation, Synthesis, Deposition, Growth or Forming

9. CFCC Program - Industry Tasks — FY 1993 $4,119,000

DOE Contact: S. Richlen, (202) 586-2078

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, which establishes performance requirements of applications and assesses feasibility of potential processing systems, is underway.

Keywords: Ceramic Composites, Continuous Fiber

Device or Component Fabrication, Behavior or Testing

10. Ceramic Composite Heat Exchanger for the Chemical Industry — FY 1993 $222,000

DOE Contact: G. Varga, (202) 586-0082
Babcock & Wilcox Contact: D. Hindman, (804) 522-5825

The third phase of this project has been initiated to design and build a prototype module heat exchanger using ceramic composite tubes to determine their performance under industrial conditions. Currently, ceramic composite tubes are being proof-tested in a high-temperature furnace to determine their viability for actual use.

Keywords: Ceramic Composites, Structure

11. HiPHES System Design Study for Energy Production from Hazardous Wastes — FY 1993 $406,000

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 for recovery of energy from hazardous wastes. A preliminary design of an advanced heat exchange process based on the use of ceramic composites has been developed. Research on critical material and design needs continues.

Keywords: Ceramic Composites, Heat Exchangers

12. HiPHES System Design Study for an Advanced Reformer FY 1993
$253,000

DOE Contact: G. Varga, (202) 586-0082
Stone & Webster Engineering Corp. Contact: J. Williams, (617) 589-7147

This project is in the second phase of a three-phase effort to develop high pressure heat exchange systems for an advanced convective reformer. A preliminary design of an advanced heat exchange process based on the use of ceramics has been developed. Research on critical material and design needs continues.

Keywords: Composites, Heat Exchangers

13. Ceramic Components for Stationary Gas Turbines in Cogeneration Service
FY 1993
$2,500,000

DOE Contact: W. Parks, (202) 586-2093
Solar Contact: M. van Roode, (619) 544-5549

This project will design and test three major ceramic components in 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

14. Long-Term Testing of Ceramic Components for Stationary Gas Turbines FY 1993
$800,000

DOE Contact: W. Parks, (202) 586-2093
ORNL Contact: M. Ferber, (615) 576-0818

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

Waste Material Management Division

Waste Utilization and Conversion

Industrial waste solid, liquid, and gaseous materials are waste because they have insufficient economic potential, thus they are landfilled or discharged to the environment. Economically useful wastes are termed by-products and constitute the objective of the Waste

Utilization and Conversion program. Materials research can provide technologies to upgrade wastes or create new commodity materials so that wastes can have economic, i.e., added, value to become by-product materials of value to industry or commerce. The DOE contact is Bruce Cranford, (202) 586-9496.

Materials Preparation, Synthesis, Deposition, Growth or Forming

15. Wood Wastes to Adhesives — FY 1993 $700,000

DOE Contact: Charles Russomanno, (202) 586-7543
NREL Contact: Helena Chum, (303) 231-7249

Wood wastes are pyrolyzed via a vortex reactor yielding pyrolysis oils. Oils are separated to give a phenols-neutrals fraction which is used to replace phenol in various phenolic resin applications. Because petroleum-based phenol is replaced by wood-based phenol, and because the overall process is cheaper, substantial energy savings of over 200 trillion BTU/year are projected for 2010.

Keywords: Wood, Wastes, Adhesives, Pyrolysis

16. Waste Rubber-Polymer Composite — FY 1993 $1,100,000

DOE Contact: Stuart Natof, (202) 586-2370
Air Products & Chemicals, Inc., Contact: Dr. Bernard Bauman, (215) 481-2449

A new process is being developed to activate the surface of finely ground waste tire rubber using chlorine. The surface-treated ground waste tire rubber can be used by molders to make new composites with cost savings and/or improved properties. This use of waste tires can result in a net savings of 80,000 BTUs per pound of tire rubber, as a result of displacing relatively energy intensive virgin materials.

Keywords: Tires, Composites, Surface Activation

17. Electrochemical Removal of Zinc from Steel Scrap — FY 1993 $0

DOE Contact: Bill Obenchain, (202) 586-3090
Argonne National Laboratory Contact: Fred Dudek, (708) 972-7797

A new process is being developed to economically remove the zinc from galvanized steel scrap, resulting in clean, specification grade, scrap steel and recyclable zinc. The process works on loose shredded scrap or baled scrap. Hot sodium hydroxide with anodic stripping and simultaneous electrowinning is employed. A pilot plant was built in FY92 for operation in FY93 and FY94.

Keywords: Dezincing, Steel, Galvanized, Zinc, Scrap Metal, Metals Recycling

18. Silicon Oxide Recovery-Conversion — FY 1993 $500,000

DOE Contact: Bruce Cranford, (202) 586-9496
Dow Corning Contact: James May, (517) 496-6047

A new process is being developed to economically capture waste SiO emitted from conventional silicon production furnaces and return the SiO to the furnace to increase the conversion of SiO_2 to Si metal. The CO emitted is also utilized for methanol production to improve the energy efficiency of the process. The process has been demonstrated at the pilot scale.

Keywords: Silicon Oxide, Waste Recovery, Waste Conversion

19. Bioconversion of High-Starch Food Wastes into High-Value Products — FY 1993 $400,000

DOE Contact: Merrill Smith, (202) 586-3646
Argonne National Laboratory Contact: Jim Frank, (708) 972-3268

ANL has been developing processes and products for the conversion of starchy waste to lactic acid and its derivative products. The primary focus of the program has been to develop rationale and integrated processes and products that can potentially result in energy savings by utilization of waste carbohydrates. Various uses for lactic acid have been investigated. The possibilities include biodegradable polymers, "green" solvents and propylene glycol (as an antifreeze).

Keywords: Biodegradable, Starch, Lactic Acid, Lactide Plastic, Fertilizer, Mulch, Irrigation, Propylene Glycol

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

20. Solar Materials Processing — FY 1993 $594,000

DOE Contact: Frank Wilkins, (202) 586-1684
NREL Contact: Allan Lewandowski, (303) 231-1972

The objective of this project 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, production of ceramic powders, solar assisted chemical vapor deposition of a variety of films on various substrates, rapid thermal heat treating and other surface modification techniques. Two Cooperative Research and Development Agreements (CRADAs) have been initiated to promote transfer of this technology to industry. One is for the metallization of berylia ceramics used in electronic packing and the other is for the production of small diameter, sinterable silicon carbide powders. Both of these CRADAs have demonstrated significant technical success and are currently being pursued beyond technical feasibility stages.

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

21. Photocatalysts Based on Titanium Dioxide — FY 1993 $236,000

DOE Contact: Frank Wilkins, (202) 586-1684
NREL Contact: Daniel M. Blake, (303) 231-1202

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. 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. Potential catalysts are prepared by NREL, subcontractors, or obtained from commercial sources.

Keywords: Photocatalyst, Titanium Dioxide, Oxidation

Office of Industrial Processes

Advanced Industrial Materials Program

The Advanced Industrial Materials program mission is to unite National Laboratory/ industry/university teams to bring materials from basic research, through applied research, development and engineering to industrial application to strengthen the competitive position of U.S. industry and save energy. The program works with materials suppliers, manufacturers and end users to identify opportunities for improving system efficiencies and product quality, and increasing service lives with the implementation of new materials. The Advanced Industrial Materials program has research efforts in four areas: Intermetallic and Metallic Alloys, Ceramics - Composites and Coatings, Ceramics - Microwave Processing, and Innovative Materials - Materials and Processing. The Program Manager is Charles A. Sorrell, (202) 586-1514.

Materials Preparation, Synthesis, Deposition, Growth or Forming

22. Combustion Chemical Vapor Deposition of Coatings — FY 1993 $50,000

DOE Contact: Charles A. Sorrell, (202) 586-1514
Georgia Institute of Technology Contact: W. B. Carter, (404) 894-6762

Chemical vapor deposition is a well known process for the production of high quality thin and thick coatings that are used in a variety of industrial applications. Conventional CVD processing is performed in a reactor (cold-wall or hot-wall) that is often a vacuum chamber. Combustion chemical vapor deposition (CCVD) is a CVD process that is performed in the open atmosphere without the use of a reaction chamber. The CCVD of ceramic oxide and some metal coatings involves the dissolution of reagents containing the metallic constituents of the coatings in a flammable, organic solvent. The resulting solution is burned in the open air, either in a diffusion flame or a premixed flame. Deposition will occur on the back sides (away from the flame) of substrates as well as on the front side of the substrate. The objective of this project is to develop dense, adherent yttria stabilized zirconia (YSZ) coatings using combustion chemical vapor deposition. Current efforts have resulted in the deposition of YSZ onto single crystal MgO and single crystal sapphire, and onto type 430 stainless steel, 2-ethylhexanoates of zirconium and yttrium dissolved in toluene.

Keywords: Combustion Chemical Vapor Deposition, Chemical Vapor Deposition, Coatings

23. Synthesis and Design of Intermetallic Materials FY 1993
$690,000

DOE Contact: Charles A. Sorrell, (202) 586-1514
Los Alamos National Laboratory Contacts: J. J. Petrovic, (505) 667-0125 and A. D. Rollett, (505) 667-6133

Los Alamos is developing advanced intermetallic materials for high temperature applications in oxidizing atmospheres (i.e. gas turbines, heat exchangers, and furnaces). These materials are typically composites based on molybdenum disilicide that have excellent intrinsic resistance to oxidation but require improvement in their fracture toughness at room temperature and their high temperature creep strength. Efforts are currently focused on obtaining a $MoSi_2$ with both improved fracture toughness at room temperature (with ZrO_2 additions), and improved creep resistance (with SiC additions). These efforts have resulted in advanced fabrication techniques, such as plasma arc spray that are currently being used to successfully produce in situ composites, and to generate prototypical shapes (i.e. tubes).

Keywords: Composites, Intermetallics, Toughening, Micro-Mechanical Modeling

24. Polymers with Improved Surface Properties FY 1993
$280,000

DOE Contact: Charles A. Sorrell, (202) 586-1514
ORNL Contact: E. H. Lee, (615) 574-5058

Ion beam treatments have been shown to significantly alter and improve several surface related properties of polymeric materials. The purpose of this project is to investigate the use of ion-beam treatments for improving various surface sensitive properties of polymers for technological, industrial, and military applications. Several basic and high performance engineering polymers such as polyethylene, polypropylene, polystryene, polycarbonate, poly-ether-ether-ketone and polyimide have been implanted with various ions such as He, B, N, C, Ar, Fe, Ag, and Ti. In most cases significant improvements in near-surface hardness up to several thousand percent were obtained. Additionally, the tribological properties of several polymers were also found to improve significantly after ion implantation.

Keywords: Polymers, Surface Modification, Ion Beam Processing

25. Development of Weldable, Corrosion Resistant Iron-Aluminide Alloys FY 1993
$214,000

DOE Contact: Charles A. Sorrell, (202) 586-1514
ORNL Contact: G. M. Goodwin, (615) 574-4809 and P. J. Maziasz, (615) 574-5082

Iron-aluminides show excellent corrosion/oxidation resistance to at least 1100°C. Alloying has shown to considerable 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 and properties related to structural applications of weldable, corrosion resistant FeAl alloys and to develop FeAl alloys for Weld-overlay coating applications on conventional structural steels and alloys. Efforts have included: (1) producing large and multiple layer overlay deposits; (2) characterizing and evaluating the microstructure, composition and mechanical integrity of the FeAl cladding deposits; and (3) exploring the production of FeAl weld consumables by commercially viable processes. Current results have shown that minor alloying element additions (and combinations) can improve the threshold stress for hot-cracking, which is comparable to that of 304 and 316 austenitic stainless steels.

Keywords: Iron Aluminides, Coatings, Claddings, Thermophysical Properties

26. Composites Through Reactive Metal Infiltration FY 1993
$350,000

DOE Contact: Charles A. Sorrell, (202) 586-1514
Sandia National Laboratories Contact: R. E. Loehman, (505) 844-2222

Reactive metal infiltration is a versatile new method for the synthesis and processing of a wide range of ceramic and metal-matrix composites. The technique involves infiltrating a ceramic preform with a molten metal that reacts with the ceramic to produce a fine scale composite of ceramic particles within a continuous metal matrix. One major advantage of this process is that the technique can be used to form parts to near-net-shape while controlling both composition and microstructure. Current efforts focus on determining the reaction mechanisms, kinetics, and the effects of different process variables on the final product.

Keywords: Metal Matrix Composites, Reactive Metal Infiltration, Ceramics

27. Magnetic Field Processing of Inorganic Polymers FY 1993
$250,000

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.

Keywords: Polymers, Magnetic Field Processing

28. Development of Improved Aerogel Superinsulation — FY 1993 $300,000

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 advanced material processing methods for producing nanostructured aerogel materials via sol-gel processing and supercritical drying for very high R-value insulation and a whole new class of composite materials. Current efforts have resulted in processing methods to incorporate nanostructured carbon into aerogels that absorb infrared radiation. In addition, photoluminescent and magnetic nanocomposites materials have been developed.

Keywords: Thermal Insulation, Sol-Gel, Processing

29. Microwave-Driven Spray Drying and Filament Processing — FY 1993 $350,000

DOE Contact: Charles A. Sorrell, (202) 586-1514
Los Alamos National Laboratory Contact: F. D. Gac, (505) 667-5126

The purpose of this project is to develop a generic microwave process to heat ceramic oxide filaments by direct absorption of 2.45 GHz microwaves for drying, prefiring, and sintering to produce flexible, high-strength continuous ceramic fibers. Microwave processing is an alternative to conventional thermal processing of ceramic oxide filaments from green sol-gel filaments. During filament processing, microwave energy is volumetrically absorbed by the entire filament, resulting in rapid heating of individual filaments. The major advantages of rapid heating include faster processing, and greater energy efficiency. Current results indicated that microwave energy readily couples with oxide filaments for drying and burning out organic residues. Ceramic filaments can also be sintered with the proper control of heating rates. In addition, sintering temperatures can be obtained by using a coating with a high dielectric loss to preheat the filament to a lossy state for direct heating to higher temperatures.

Keywords: Microwave Processing, Spray Drying, Filaments

30. Conducting Polymers: Synthesis and Industrial Applications — FY 1993 $325,000

DOE Contact: Charles A. Sorrell, (202) 586-1514
Los Alamos National Laboratory Contact: S. Gottesfeld, (505) 667-0853

This project is pursuing new methods for the synthesis of electronically conducting polymers, and the development of new industrial applications for these materials, which will result in significant reductions in energy usage or industrial waste. Recent applications specifically addressed included: (1) supercapacitors based on conducting polymer active materials for power trains in electric vehicles; (2) improved industrial metallization methods that could replace current costly and environmentally damaging technologies; and (3) conducting polymer membranes for gas separation. Current efforts have focused on active materials for electrochemical capacitors, metallization processes based on conducting polymer precoats, and optimization of conducting polymer films for gas separations.

Keywords: Electrically Conducting Polymers, Metallization, Capacitors, Coatings and Films

31. Microwave Assisted Chemical Vapor Infiltration — FY 1993 $235,000

DOE Contact: Charles A. Sorrell, (202) 586-1514
Los Alamos National Laboratory: R. P. Currier, (505) 665-3601

The purpose of this investigation is to develop a chemical vapor infiltration process utilizing microwave heating to establish inverted thermal gradients in a fiber preform. Efforts resulted in steep thermal gradients in SiC (Nicalon) cloths. Initial demonstration of "inside out" deposition has been performed on SiC, Si-rich SiC, and Si_3N_4 on Nicalon cloth substrates. Future efforts will focus on the impact of interfacial coatings (pyrolytic carbon and BN) on microwave heating. If successful, microwave assisted infiltration has the potential to eliminate many limitations encountered with conventional approaches to composite fabrication by chemical vapor infiltration. This process could remove constraints on substrate geometry and produce partially uniform, high density composites with relatively short processing times.

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

32. High Deposition Rate Chemical Vapor Deposition FY 1993
$350,000

DOE Contact: Charles A. Sorrell, (202) 586-1514
Sandia National Laboratories 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 and the objective of this project is to develop a quantitative understanding of the chemical and physical mechanisms that result in high deposition rates and fully dense materials. Current efforts are focused on (1) deposition of silicon carbide from methyltrichorosilane, and (2) a flame-spray process for the formation of metal-ceramic and metal-polymer wear-resistant coatings. These models will provide insight into the mechanism of each process, facilitating and accelerating process optimization.

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

33. Development of Chemical Vapor Composite Materials FY 1993
$950,000

DOE Contact: Charles A. Sorrell, (202) 586-1514
Thermotrex Corporation Contact: P. Reagan, (617) 622-1347

The purpose of this project is to develop a reliable, flexible and economic process to fabricate strong, fracture tough ceramic composites to net shape without machining in a single step. Chemical vapor composite (CVC) process has the potential to produce low cost ceramic composites. The CVC process mixes particulates (powder and/or fibers) with vapor reactants that are co-deposited on a machined substrate. This process is a 100 times faster than chemical vapor infiltration (CVI), does not require a woven preform and can produce net-shaped composites on one side without machining. Current efforts have focused on developing a basic understanding of the mechanical properties and their relationship to the microstructure and deposition conditions.

Keywords: Chemical Vapor Deposition, Ceramics, Composites

Materials Properties, Behavior, Characterization, or Testing

34. Three Dimensional X-ray Tomography of Composites FY 1993
$150,000

DOE Contact: Charles A. Sorrell, (202) 586-1514
LLNL Contact: J. H. Kinney, (415) 243-6669

Densification mechanisms in chemical vapor infiltrated (CVI) ceramic matrix composites need to be better understood if porosity is to be controlled and minimized. X-ray tomographic microscopy (XTM) is a new technique for nondestructively imaging materials microstructures in three dimensions. The microporosity between individual filaments in the fiber bundles, the channel porosity between individual cloth layers, and the connectivity of the large through-ply holes that remain after processing can all be examined without destroying the sample. Current XTM research is focused on monitoring the CVI processing of silicon carbide matrix - Nicalon fiber composites. Direct visualization of the evolving microstructure during CVI can be compared to model calculations and the role that fiber architecture plays in densification and final state porosity.

Keywords: X-ray, Tomography, Composites

35. Computer Simulation Models of Thermal-Expansion-Anisotropic Induced Microcracking and Fracture Resistance Curves — FY 1993 $50,000

DOE Contact: Charles A. Sorrell, (202) 586-1514
National Institute of Standards and Technology Contacts: Edwin R. Fuller, Jr., (301) 975-5795 and Tee-Jer Chuang, (301) 975-5773

Ceramic materials can have significant positive impact on innumerable energy-related applications at elevated temperature. Brittleness, however, is a major concern in designing with these materials. A general stratagem has been to improve the fracture toughness by developing ceramic microstructures, including ceramic composite systems. This project will focus on the development of micro-mechanic computer simulations which could elucidate important microstructural and stochastic aspects of the strength and fracture toughness of advanced ceramic materials. Current efforts have resulted in two algebraically formulated microstructural, micro-mechanic fracture models, and several simulations based on an initial computer code.

Keywords: Anisotropic Microcracking, Fracture Resistance, Computer Modeling

Materials Structure and Composition

36. The Development of Advanced Ceramic Membrane Technology — FY 1993 $137,000

DOE Contact: Charles A. Sorrell, (202) 586-1514
ORNL Contact: Peter Angelini, (615) 574-4565
General Magnaplate Corporation Contact: Michael L. Pearce, (908) 862-6200

The objective of this project is to develop high performance engineering coatings of modest cost with good potential for on-site application. The technical approach is to examine the feasibility of using a light weight, portable flame spray system to deposit coatings comprised of high modulus disperse phases in lower modulus metal and thermoplastic matrices and characterize the products. Current results show that nylon, polyetheretherketone (PEEK) and nickel aluminide matrices offer the greatest promise for providing excellent wear resistance and bond strength (especially with tungsten carbide and silicon nitride dispersions). In addition, with the possible exception of PEEK, all show great promise for on-site application via a one-step, low cost, environmentally benign process.

Keywords: Ceramics, Composites, Coatings

37. Ductility of Intermetallic Compounds Exposed to Aqueous Solutions — FY 1993 $50,000

DOE Contact: Charles A. Sorrell, (202) 586-1514
National Institute of Standards and Technology Contact: R. E. Ricker, (301) 975-6023

When elemental aluminum comes into contact with either vapor phase or liquid phase water, the aluminum ionizes rapidly by giving its electrons to the hydrogen ions in the water molecule and forming atomic hydrogen. As a result, intermetallic compounds that are susceptible to hydrogen embrittlement and contain aluminum should be embrittled by hydrogen when exposed to either liquid phase or vapor phase water. The objective of this project is to evaluate the role of environment in determining the ductility of intermetallic compounds at room temperature. Current efforts are focused on the influence of the ordered structure on the electrochemical conditions required to generate hydrogen at the surface.

Keywords: Hydrogen Embrittlement, Intermetallics, Electrochemistry

38. High-Temperature Precipitate-Strengthened Iron-Aluminide Alloys — FY 1993 $155,000

DOE Contact: Charles A. Sorrell, (202) 586-1514
ORNL Contact: P. J. Maziasz, (615) 574-5082

The objective of this project is to produce weldable B_2-phase iron aluminide alloys with the best combination of high-temperature strength and room-temperature ductility. FeAl and Fe_3Al alloy compositions have been found which have good weldability (hot-cracking resistance). Some of these alloys also have good creep rupture resistance at 600-650°C due to precipitate-strengthening effects, while other alloys have been found to have good room-temperature ductility after proper heat-treatment/processing. Current efforts focus on optimizing the combination of properties by manipulation of both alloy composition and heat-treatment/processing conditions. Physical property characterization includes the melting point, thermal expansion and thermal conductivity of Fe_3Al, FeAl, and Ni_3Al Alloys.

Keywords: Iron Aluminide, Nickel Aluminides, Physical Properties

39. Metallic and Intermetallic Bonded Ceramic Composites FY 1993
$500,000

DOE Contact: Charles A. Sorrell, (202) 586-1514
ORNL Contacts: T. N. Tiegs and K. B. Alexander, (615) 574-0631
University of California, Berkeley 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 program consists of two efforts, one on alumina-based composites, and the other on nonoxide-based (primarily WC, TiN, and TiC) composites. Several powder processing routes have been successfully used to fabricate composites with variations in reinforcement size and aspect ratio. Current results show a two-fold increase in the fracture toughness over that of an alumina monolithic. Fractographic evidence indicates that extended or interconnected particles are required to maximize the fracture toughness contribution from bridging or deforming particles.

Keywords: Ceramics, Composites, Aluminides

40. Advanced NiAl and TiAl Intermetallic Alloys FY 1993
$237,000

DOE Contact: Charles A. Sorrell, (202) 586-1514
ORNL Contact: C. T. Liu, (615) 574-4459

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. NiAl and TiAl are of industrial interest because of their low density, high melting-point, and good oxidation and corrosion resistance at elevated temperatures. However, brittle fracture and poor ductility limit their use as engineering materials. Current efforts are focused on (1) the development of TiAl alloys, and (2) mechanical properties tailoring of NiAl and TiAl with alloy additions. Initial results have shown that TiAl-based alloy ribbons prepared by rapid solidification possess tensile ductility as high as 8 percent at room temperature. Additionally, alloying NiAl with Mo will increase room-temperature ductility and Nb, Ta, V, and Zr will enhance tensile strength and creep resistance at elevated temperatures.

Keywords: Intermetallics, Ordered Alloys, Ductility

41. Superior Metallic Alloys Through Rapid Solidification Processing by Design

FY 1993
$250,000

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. The fine and stable microstructures are being realized from the RSP research, and application of the principles to metallic alloys of interest to industry is underway. 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

42. Polymerization and Processing of Organic Polymers in a Magnetic Field

FY 1993
$140,000

DOE Contact: Charles A. Sorrell, (202) 586-1514
Los Alamos National Laboratory Contacts: N.E. Elliott, (505) 667-1587, R. K. Jahn, (505) 665-1751 and R. Liepins, (505) 667-2656

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. Two approaches will be explored: (1) applying the "dynamic film casting" technique to the formation of composites, and (2) exploring the "gravity induced flow shear/magnetic field" technique to composite materials. These materials could provide significant benefits to vehicles, aircraft and seacraft.

Keywords: Polymers, Magnetic Processing, Mechanical Properties

43. Microwave Joining of SiC

FY 1993
$115,000

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 was successful and a feasibility demonstration for the reaction bonded silicon carbide and sintered silicon carbide tube assemblies was performed. Leak-tight behavior was demonstrated before and after cycling between ambient temperature and 1100°C. Current work is focused on joining larger and longer tubes with single and multimode cavities.

Keywords: Microwave Processing, Microwave Joining, SiC

44. Microwave Processing of Materials

FY 1993
$500,000

DOE Contact: Charles A. Sorrell, (202) 586-1514
ORNL Contact: M. A. Janney and H. D. Kimrey, (615) 576-5183
University of Utah Contact: Magdy Iskander, (801) 581-6944

The purpose of this project is to develop ceramics for energy conversion systems with improved strength, toughness, reliability, and uniformity of properties. Microwave processing will be used to engineer and control critical component microstructures. Currently work has focused on two efforts: (1) development of a process for microwave sintering zirconia-toughened alumina and (2) development of a "quasi-optical" computer model for describing processing in the multimode cavities.

Keywords: Microwave Processing, Sintering, Zirconia-Toughened Alumina, Modeling

45. Chemical Vapor Infiltration of Ceramic Composites

FY 1993
$290,000

DOE Contact: Charles A. Sorrell, (202) 586-1514
ORNL Contact: T. M. Besmann, (615) 574-6852
Georgia Institute of Technology Contact: Tom Starr, (404) 583-0579

The objective of this task is to develop continuous filament reinforced TiB_2 matrix composites for use as cathodes in the Hall-Heroult electrolytic reduction of aluminum. These cathodes will provide an increased electrical efficiency and cell design versatility in the production of aluminum. Continuous filament reinforced TiB_2 composites have been produced using a forced flow chemical vapor infiltration method. Current efforts have focused on (1) preparing specimens for test at the Alcoa Technical Center, and (2) modeling the chemical vapor infiltration process.

Keywords: Chemical Vapor Infiltration, Composites, TiB, SiC, Cathodes, Modeling

46. Biomimetic Thin Film Synthesis — FY 1993 $400,000

DOE Contact: Charles A. Sorrell, (202) 586-1514
Pacific Northwest Laboratory Contact: B. J. Tarasevich, (509) 375-2078

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. Initial efforts have concentrated on the synthesis of chemically-resistant ceramic coatings for polymeric components used in fuel delivery systems of automobiles and iron oxide films for use as magnetic storage devices. The high particle density obtained in the biomimetic films, combined with the potential for crystallite orientation, holds promise for improved storage densities over current magnetic iron oxide tapes.

Keywords: Biomimetic, Organic Interfaces, Ceramic Coatings

47. Recoverable Thermosets — FY 1993 $200,000

DOE Contact: Charles A. Sorrell, (202) 586-1514
Polytechnic University Contact: G. Tesoro, (718) 643-5244

The objective of this project is to demonstrate the feasibility of thermoset recovery for a class of low cost, high volume resins (UPE). Current efforts are primarily focused on the optimization of neutral hydrolysis, hydrolysis, recovery and characterization of chemical compounds obtained and potential industrial applications of recovered products. Results show that neutral hydrolysis is a feasible approach to recover Phthalic acid. The use of recovered oligomer as a component of acid-curing epoxy resin systems has been identified as a potential application for the recovered products.

Keywords: Thermoset Resins, Plastics Recycle

48. Chemical Recycling of Plastics FY 1993
$500,000

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. Requirements for feed sorting and product purification are minimized by controlling reaction conditions so that target products can be collected with high yield. Control is achieved by taking advantage of differences in reaction rates, catalysis, and coreactants. Target waste streams are post-consumer wastes that can range from commodity plastics to high-value engineering blends. The most promising applications are recovering caprolactam from waste nylon 6 carpet, recovering diamines from the isocyanates and high-value oxygenates from the polyols in waste polyurethane, and recovering dimethlyterephthalate from wastes containing polyethyleneterephthalate.

Keywords: Plastics Recycling, Pyrolysis, Waste Streams

Device or Component Fabrication, Behavior or Testing

49. Advanced Engineering Coatings Development FY 1993
$166,000

DOE Contact: Charles A. Sorrell, (202) 586-1514
ORNL Contact: Peter Angelini, (615) 574-4565
K-25 Contact: Douglas Fain, (615) 574-9932
University of Wisconsin Contact: Marc A. Anderson, (608) 262-2674

The purpose of this work is to develop and evaluate a variety of ceramic membranes composed of nanoparticulate oxides. The application of these microporous ceramic materials include gas and liquid separations, photocatalysis, coatings, ceramic membrane reactors, and energy storage devices. Current efforts have resulted in the successful use of photocatalytic membrane materials in an actual field test at the Savannah River Site in Aiken, South Carolina. Porous TiO_2 semiconducting ceramics were used to completely mineralize trichloroethylene.

Keywords: Membranes, Separations, Sol-Gel, Photocatalysis

50. Assessment of Selective Dehydrogenation Catalysts FY 1993
$50,000

DOE Contact: Charles A. Sorrell, (202) 586-1514
Sandia National Laboratories Contact: Allen G. Sault, (505) 844-8723

The objective of this project is to design, synthesize and evaluate selective dehydrogenation catalysts specifically tailored for membrane reactor applications. Preliminary assessment of hydrous titanium oxide (HTO) ion-exchange materials as supports for iron-based ethylbenzene (EB) dehydrogenation catalysts has been performed. The results of this preliminary study indicate that HTO supported EB dehydrogenation catalysts can be made superior to current catalyst technology in the field. Besides providing superior performance as bulk catalysts materials, these catalysts also present significant advantages for membrane reactors with the ability to cast HTO supports in the form of thin films on a variety of substrates. The ability to achieve superior performance with HTO supported catalysts, coupled with the thin film capabilities inherent in HTO materials, offers great potential in catalytic membrane reactor systems.

Keywords: Dehydrogenation Catalysts, Membrane Reactors, Membranes

51. Ni_3Al Technology Transfer: Castability and Weldability of Ni_3Al FY 1993
$268,000

DOE Contact: Charles A. Sorrell, (202) 586-1514
ORNL Contacts: M. L. Santella, (615) 574-4805 and V. K. Sikka, (615) 574-5112

The Ni_3Al and Ni_3Al-based intermetallic alloys are of great interest for many high-temperature industrial applications because of the advantages they offer which include; (1) high-temperature oxidation resistance, (2) carburization resistance, and (3) high-temperature strength. The objective of this project is to facilitate the transfer of intermetallic alloy technology to industry by resolving technical issues (i.e. castability, weldability, hot workability, and fracture toughness) constraining the industrial application of alloy systems. Near-term applications have been identified and include heat-treating trays for carburizing furnaces, rollers for heat-treating steel plates, beams for walking-beam furnaces, hot-forming dies, and turbochargers for diesel engine applications. Current research has focused on weld repair of commercially cast components.

Keywords: Nickel Aluminides, Processing, Mechanical Properties

52. Advanced Microwave Processing Concepts FY 1993
$500,000

DOE Contact: Charles A. Sorrell, (202) 586-1514
ORNL Contact: R. J. Lauf, (615) 574-5176

The purpose of this project is to explore new techniques and uses for microwave processing, including polymer-matrix composites, and develop variable-frequency microwave sources. A variable-frequency microwave furnace has been built to conduct microwave processing studies over a wide frequency range. This design uses a high-power traveling wave tube and will permit (1) more efficient use of microwave energy in processing of materials, and (2) more effective microwave field uniformity. Initial polymer curing studies focused on the curing of neat resin samples. Samples cured at a fixed frequency of 6 GHz, using a 50 W power for 30 min, were completely charred. It appeared that thermal runaway was initiated at a local hot spot and then propagated to cover most of the specimen. In contrast, a sample cured for 30 min at 50 W while sweeping the frequency from 4.5 to 7.5 GHz, 5000 times per second, was uniformly cured and showed no evidence of overheating.

Keywords: Microwave Processing, Multilayer Capacitors, Polymers, Composites, Variable Frequency

53. Chemically Specific Coatings FY 1993
$450,000

DOE Contact: Charles A. Sorrell, (202) 586-1514
Sandia National Laboratories contact: Mark Phillips, (505) 844-8969

Inorganic films of controlled porosity are of considerable interest as selective coatings that can act as discriminating elements when deposited on membrane or sensor substrates. The objective of this project is to develop a new class of chemical sensors through sol-gel processing that can be used as process monitors to improve process energy efficiency. Current efforts are focused on optimizing the procedures for synthesizing hydrous metal oxide (HMO) films with controlled physical properties (thickness, porosity, surface area, and refractive index) on planar substrates, and investigating techniques for characterizing film interaction with ions in aqueous solution. Current results indicate that control over film porosity can be attained through solution aging and that certain films increased the acoustic plate mode device sensitivity relative to an uncoated acoustic plate mode device by two orders of magnitude.

Keywords: Coatings, Sol-Gel Processing

OFFICE OF TRANSPORTATION TECHNOLOGIES

	FY 1993
Office of Transportation Technologies - Grand Total	$32,000,000
Office of Transportation Materials	$16,984,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 7,265,000
High Temperature SX Silicon Carbide (WBS No. 1113)	0
Powder Characterization (WBS No. 1118)	110,000
Sintered Silicon Nitride (WBS No. 1121)	0
Microwave Sintering (WBS No. 1124)	400,000
Cost-Effective Silicon Nitride Powder (WBS No. 1125)	825,000
Novel Si_3N_4 Processing (WBS No. 1126)	0
Cost-Effective Sintering of Silicon Nitride Ceramics (WBS No. 1127)	183,000
Cost-Effective Manufacture of Silicon Nitride Components (WBS No. 1128)	0
Advanced Processing (WBS No. 1141)	243,000
Improved Processing (WBS No. 1142)	650,000
Processing Science for Reliable Structural Ceramics Based on Silicon Nitride (WBS No. 1144)	0
Advanced Composites (WBS No. 1225)	260,000
In-Situ-Toughened Silicon Nitride (WBS No.1226)	319,000
Dispersion Toughened Oxide Composites (WBS No. 1231)	350,000
Low Expansion Ceramics (WBS No. 1242)	0
Low Thermal Expansion Ceramics (WBS No. 1243)	100,000
Low Cost CTE Components (WBS No. 1245)	200,000
Low Cost CTE Components (WBS No. 1246)	0
Advanced Manufacturing (WBS No. 1520)	3,050,000
Alternative Fuel Lubricant Technology	50,000
Low-Wear Coatings for Transportation	275,000
HRRS Hard Coatings	0
IBAD of TiN and Cr_2O_3	0
Self-Lubricating Ceramic Surfaces	0
High-Current Ion Implantation	0
Lubricious Coatings for Transportation	250,000

OFFICE OF TRANSPORTATION TECHNOLOGIES

	FY 1993
Office of Transportation Materials (continued)	
Materials Properties, Behavior, Characterization or Testing	$5,460,000
Adherence of Coatings (WBS No. 2212)	0
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 Database (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)	317,000
Rotor Materials Database (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)	200,000
Standard Tensile Test Development (WBS No. 3413)	125,000
Non-Destructive Evaluation (WBS No. 3511)	430,000
Computed Tomography (WBS No. 3515)	100,000
Nuclear Magnetic Resonance Imaging (WBS No. 3516)	100,000
Additives for High-Temperature Liquid Lubricants	0
Friction & Wear Mechanisms in In-Situ-Reinforced Ceramics	125,000
Carbon-Based Materials for Engine Applications	125,000
Advanced Materials/Additive Interactions	150,000
Liquid Lubricants for Heat Engines	150,000
Advanced Lubricants for Engine Particulate Control	150,000
Lubricious Oxide Coatings	75,000
Alternative Fuels-Compatible Materials	800,000
Adhesive Bonding of Automotive Materials	200,000

OFFICE OF TRANSPORTATION TECHNOLOGIES

	FY 1993
Office of Transportation Materials (continued)	
Technology Transfer and Management Coordination	$1,675,000
Management and Coordination (WBS No. 111)	950,000
International Exchange Agreement (IEA) (WBS No. 4115)	400,000
Standard Reference Materials (WBS No. 4116)	150,000
Mechanical Property Standardization (WBS No. 4121)	100,000
Diamond Coatings for Tribology	75,000
Device or Component Fabrication, Behavior or Testing	$2,584,000
Advanced Coating Technology (WBS No. 1311)	175,000
Coatings to Reduce Contact Stress Damage of Ceramics (WBS No. 1313)	73,000
Wear Resistant Coatings (WBS No. 1331)	56,000
Wear Resistant Coatings (WBS No. 1332)	0
Thick Thermal Barrier Coating Systems for Low Heat Rejection Diesel Engines (WBS No. 1342)	175,000
Active Metal Brazing PSZ-Iron (WBS No. 1411)	220,000
Ceramic-Ceramic Joints AGT (WBS No. 1421)	0
Ceramic Machining (WBS No. 1500)	200,000
Next-Generation Grinding Wheel (WBS No. 1531)	430,000
High Speed Grinding (WBS No. 1532)	0
Chemically Assisted Grinding of Ceramics (WBS No. 1533)	150,000
Grindability Test (WBS No. 1542)	224,000
Grinding Consortium (WBS No. 1543)	150,000
Fluid-Film Bearings Model	69,000
Wear Mechanism Modeling	0
Instantaneous Friction Torque	25,000
Scale Effects in Friction Simulations	62,000
Thermomechanical Wear Model for Ceramics	0
Cylinder Kit Model Development	75,000
Advanced Metal Forming of Automotive Materials	500,000

OFFICE OF TRANSPORTATION TECHNOLOGIES

	FY 1993
Office of Propulsion Systems	$14,596,000
Advanced Propulsion Division	$10,933,000
Materials Properties, Behavior, Characterization or Testing	$ 235,000
Ceramic Durability Evaluation AGT	235,000
Device or Component Fabrication, Behavior or Testing	$10,698,000
Thick Thermal Barrier Coatings	25,000
Thick Thermal Barrier Coatings	25,000
Advanced Diesel Engine Component Development Project	1,098,000
Advanced Piston and Cylinder Component Development	1,200,000
Advanced Piston and Cylinder Component Development	1,200,000
High Temperature Solid Lubricant Coatings	50,000
Advanced Turbine Technology Applications Project (ATTAP, AGT-5)	4,800,000
Advanced Turbine Technology Applications Project (ATTAP, AGT-101)	2,300,000
Electric and Hybrid Propulsion Division	$ 3,663,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 105,000
Corrosion-Resistant Coatings for High-Temperature High-Sulfur Activity Applications	0
Improved Container Electrode Coating for Na/S Battery Systems	105,000
Materials Structure and Composition	$ 181,000
In situ Spectroscopic Applications to the Study of Rechargeable Lithium Batteries	86,000
Battery Materials: Structure and Characterization	95,000
Polymeric Electrolytes for Ambient-Temperature Lithium Batteries	0

OFFICE OF TRANSPORTATION TECHNOLOGIES

	FY 1993
Electric and Hybrid Propulsion Division (continued)	
Materials Properties, Behavior, Characterization or Testing	$ 219,000
Corrosion, Passivity, and Breakdown of Alloys Used in High-Efficiency-Density Batteries	0
Advanced Chemistry and Materials for Fuel Cells	94,000
Electrocatalysts for Oxygen Electrodes	0
Novel Concepts for Oxygen Electrodes in Secondary Metal/Air Battery	125,000
Device or Component Fabrication, Behavior or Testing	$3,158,000
Proton-Exchange-Membrane Fuel Cells for Vehicles	1,200,000
Electrochemical Energy Storage	1,765,000
Applied Research on Secondary Zn/NiOOH Cell Technology	193,000
Office of Alternative Fuels	$ 420,000
Materials Properties, Behavior, Characterization or Testing	$ 420,000
Cold-Start Assist Materials	120,000
CNG Adsorbents Demonstration	300,000

OFFICE OF TRANSPORTATION TECHNOLOGIES

The Office of Transportation Technologies seeks to develop, in cooperation with industry, technologies that are more energy-efficient and will enable the transportation sector to shift from near total dependence on petroleum to alternative fuels and electricity. Additional program goals are to increase the supply and availability of nonpetroleum fuels, and minimize the environmental impacts of transportation energy use. The Office of Transportation Technologies consists of the Office of Propulsion Systems, Office of Alternative Fuels, and Office of Transportation Materials, each having responsibility for specific technologies and program areas.

Office of Transportation Materials

The Office of Transportation Materials conducts research to develop an industrial technology base in transportation-related materials and materials processing in support of the Office of Transportation Technologies mission. R&D addresses materials needs for propulsion systems (heat engines, fuel cells, batteries, etc.); vehicle systems (chassis, body components) and fuel systems (fuel containment, emissions control, etc.). Materials development activities consist of four main programmatic elements: Ceramic Technology, Materials Technology (other than structural ceramics), Tribology, and the High Temperature Materials Laboratory.

The objective of the Ceramic Technology Program is to establish an industrial technology base for reliable structural ceramics and cost-effective manufacturing of ceramic components for high performance heat engines for transportation propulsion. A balanced program is conducted in the areas of materials processing, design methodology, and database and life prediction. A majority of the research is conducted by industry. The Ceramic Technology Project is managed by the Oak Ridge National Laboratory (ORNL). The DOE contact is Robert Schulz, (202) 586-8051.

The Materials Technology Program seeks to develop improved materials and the associated processing to make such materials cost-effective for various transportation applications. The program focuses on: materials for batteries and fuel cells that will make electric and hybrid vehicles cost-competitive with current production vehicles; high-strength, lightweight structural materials for more fuel-efficient, lightweight vehicles that do not compromise the safety and comfort of passengers; cost-effective materials compatible with alternative fuels (alcohol, natural gas) for fuel systems, engine components, and exhaust systems as well as new emission control system materials; and transportation infrastructure materials ranging from low cost corrosion resistant materials to reduce the capital cost of large-scale biofuels (alcohol) plants, to maglev guideways, to more durable, crack resistant road and bridge construction materials. The DOE contacts are: Sidney Diamond, (202) 586-8032, for lightweight transportation materials, and Joseph M. Perez, (202) 586-8060, for alternative fuels-compatible materials.

The Tribology Program seeks to develop high-temperature lubricants and lubricant delivery systems as well as surface engineering and coating techniques to improve friction and wear properties of engine parts, and to develop techniques to mitigate friction and wear of lubricated and unlubricated ceramics needed to commercialize advanced heat engine concepts. The Tribology Program is managed by Argonne National Laboratory (ANL). The DOE contact is Joseph M. Perez, (202) 586-8060.

The High Temperature Materials Laboratory (HTML) at Oak Ridge, Tennessee, is a state-of-the-art research and user facility which supports Government and industry efforts in high temperature materials research and serves as a unique technology transfer vehicle through its user program. The HTML comprises six user centers: materials analysis, high temperature mechanical properties, high temperature X-ray diffraction, physical properties, ceramic specimen preparation, and residual stress measurements. The DOE contact is Sidney Diamond, (202) 586-8032.

Materials Preparation, Synthesis, Deposition, Growth or Forming

54. High Temperature SX Silicon Carbide (WBS No. 1113) — FY 1993 $0

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: E. L. Long, Jr., (615) 574-5172
Carborundum Contact: Roger S. Storm, (716) 278-2544

The three major objectives for this program can be listed as follows: (1) to establish a mechanical property database for the current Hexoloy SX composition and (2) to further improve the mechanical properties via optimization of the composition, powder selection, dispersion/mixing conditions, and densification conditions.

Keywords: High Temperature Properties, Materials Processing, Silicon Carbide

55. Powder Characterization (WBS No. 1118) — FY 1993 $110,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. R. Johnson, (615) 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

56. Sintered Silicon Nitride (WBS No. 1121) FY 1993
$0

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. R. Johnson, (615) 576-6832
AMTL Contact: G. E. Gazza, (617) 923-5408

The overall objective of this effort is to develop scale up processing conditions for a silicon nitride having the general composition 85.8 mol % Si_3N_4-4.73 mol % Y_2O_3-9.47 mol % SiO_2-1.0 mol % Mo_2C and characterizing the properties of this composite with the goal of producing complex components for testing in related heat-engine programs. The first task of the program has concentrated on processing studies and database generation, while the second task will focus on producing and characterizing engine components. Ceradyne, Inc., is conducting this work, with support from AMTL.

Keywords: Sintering, Silicon Nitride, Testing

57. Microwave Sintering (WBS No. 1124) FY 1993
$400,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. R. Johnson, (615) 576-6832
ORNL Contact: T. N. Tiegs, (615) 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, or (4) produce unique microstructures.

The investigation of microstructure development is being done on dense silicon nitride materials annealed in the microwave furnace. The sintering of silicon nitride involves two approaches. In the first approach, silicon nitride and sialon powder compositions are heated in the 2.45- or 28-GHz units. The second approach deals with using reaction-bonded silicon nitride as the starting material and is done entirely in the 2.45-GHz microwave furnace.

Keywords: Microwave Sintering, Silicon Nitride

58. Cost Effective Silicon Nitride Powder (WBS No. 1125) FY 1993 $825,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: S. G. Winslow, (615) 574-0965
Dow Contact: G. A. Eisman, (517) 638-7864

The objective of this effort is to develop a commercial, domestic source of high-quality, low-cost ($10/lb sale price) silicon nitride powder with suitable properties for forming into components for heat engine applications. There are five technical tasks: (1) reference process flow sheet and cost estimate, (2) process development and scale up, (3) powder and sintered part characterization, (4) final process flow sheet and cost estimate, and (5) process demonstration.

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

59. Novel Si_3N_4 Processing (WBS No. 1126) FY 1993 $0

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: E. L. Long, Jr., (615) 574-5172
Sullivan Mining Corporation Contact: Thomas M. Sullivan, (317) 889-3855

The objective of this effort is to demonstrate the scalability of the Sullivan™ Process for making silicon nitride, to develop unique low- and high-temperature versions of the silicon nitride, to determine the net-shape capability of the process, and to characterize the microstructural, mechanical, tribological, and physical properties of the Sullivan™ Process silicon nitride. The intent of this project is to demonstrate that the Sullivan™ Process can be operated on a commercial scale to make significantly less costly net-shape ceramics with superior properties.

Keywords: Materials Processing, Silicon Nitride

60. Cost-Effective Sintering of Silicon Nitride Ceramics (WBS No. 1127) FY 1993 $183,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: T. N. Tiegs, (615) 574-5173
Southern Illinois University Contact: D. E. Wittmer, (618) 453-7006/7924

The objective of this effort is to investigate the potential of cost-effective sintering of Si_3N_4 through the development of continuous sintering techniques and the use of lower cost Si_3N_4 powders and sintering aids. The effect of heating rate on densification, microstructure, and properties will be investigated. The effects of using alternate materials for the furnace belt, and modifications in the furnace design to improve both furnace load and rate of throughput will also be determined.

Keywords: Cost-Effective Ceramics, Silicon Nitride, Sintering

61. Cost-Effective Manufacture of Silicon Nitride Components (WBS No. 1128) FY 1993 $0

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: R. L. Beatty, (615) 574-4536
Golden Technologies Contact: Jack Sibold, (303) 277-4441

The objective of this effort is to develop a low-cost process for manufacture of high quality ceramic engine components based on sintered reaction bonded silicon nitride technology. There are three technical tasks which address the areas of low-cost materials and processes and achievement of properties required for reliable performance. The material property goals for Phase I of this effort are a mean RT four-point flexure strength of 525 MPa and a Weibull modulus of 15.

Keywords: Cost Effective Ceramics, Silicon Nitride, SRBSN

62. Advanced Processing (WBS No. 1141) FY 1993 $243,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: R. L. Beatty, (615) 574-4536
Norton Contact: D. M. Tracey, (508) 393-5811

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

- reliability optimization of aqueous colloidal forming using highly loaded suspensions and glass encapsulated HIPing
- application of the high reliability colloidal processing technique to a gas pressure sinterable (GPS) composition
- demonstration of representative complex component fabrication in both the HIP and GPS systems.

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

63. Improved Processing (WBS No. 1142) — FY 1993 $650,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. R. Johnson, (615) 576-6832
ORNL Contact: S. D. Nunn, (615) 576-1668

The purpose of this work is to determine and develop the reliability of selected advanced ceramic processing methods. This program is being conducted on a scale that will permit the potential for manufacturing use of candidate processes to be evaluated. The principal material of interest is silicon nitride. Issues of practicality; safety, hygiene, and environmental issues; and in-process testing methods are to be addressed in addition to technical feasibility. The methodology includes selection of candidate processes and evaluation of their range of applicability to various kinds of commercially available ceramic powders.

Keywords: Powder Processing, Silicon Nitride

64. Processing Science for Reliable Structural Ceramics Based on Silicon Nitride (WBS No. 1144) — FY 1993 $0

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: R. L. Beatty, (615) 574-4536
University of California, Santa Barbara Contact: Fred F. Lange, (805) 893-8248

The current objective of this effort is to try to increase the understanding of the role of interparticle forces in the processing of ceramics. In particular, short-range repulsive forces are being created. Utilizing these forces, the rheological properties of dispersions, the kinetics of pressure filtration, and the mechanical properties and microstructure of the resulting bodies can be modified. Both aqueous and non-aqueous systems are being studied. For non-aqueous systems, the reaction of alcohol with the surface of silicon nitride is being explored. In aqueous systems, attempts are being made to make the surface of silicon nitride appear more alumina-like by coating it with an alumina layer.

Keywords: Alumina, Powder Processing, Silicon Nitride

65. Advanced Composites (WBS No. 1225) FY 1993
$260,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. R. Johnson, (615) 576-6832
University of Michigan Contact: T. Y. Tien, (313) 764-9449

The purpose of this effort is to optimize the properties of silicon nitride by microstructural design, specifically by developing fiber-like β-Si_3N_4 grains and control of the grain-boundary phase. Optimization of the silicon carbide ceramics will be accomplished by formation of composites containing AlN polytypoids.

Keywords: Composites, Physical/Mechanical Properties, Silicon Nitride, Silicon Carbide

66. In-Situ-Toughened Silicon Nitride (WBS No. 1226) FY 1993
$319,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: T. N. Tiegs, (615) 574-5173
Garrett 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. The work is divided into two stages. The first is a refinement stage focusing on the effects and interactions of the chemical composition and thermal processing variables on microstructure, mechanical behavior, and oxidation resistance. The second stage will be an optimization stage focusing on the development of in situ reinforced Si_3N_4 with optimized microstructure and properties which meet or exceed the property goals and on the establishment of composition-processing-property correlations. A simulated engine component will be fabricated in order to demonstrate process feasibility.

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

67. Dispersion Toughened Oxide Composites (WBS No. 1231) FY 1993 $350,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. R. Johnson, (615) 576-6832
ORNL Contact: T. N. Tiegs, (615) 574-5173

Initially this work involved development and characterization of SiC whisker-reinforced oxide composites for improved mechanical performance. To date most of the efforts involving SiC whisker-reinforced alumina, mullite, silicon nitride, and sialon have been completed. In addition, studies of whisker-growth processes were conducted to improve the mechanical properties of SiC whiskers by reducing their flaw sizes and, thereby, improving the mechanical properties of the composites. Currently, in situ acicular grain growth is being investigated to improve fracture toughness of silicon nitride materials. Microstructural development to promote this type of growth will be examined.

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

68. Low Expansion Ceramics (WBS No. 1242) FY 1993 $0

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: Victor J. Tennery, (615) 574-5123
VPI and SU Contact: J. J. Brown, (703) 961-6640

A major objective of this research is to investigate selected oxide systems for the development of a low expansion, high thermal shock resistant ceramic. Specifically, it is the goal of this study to develop an isotropic, ultra-low thermal expansion ceramic which can be used above 1200°C and which is relatively inexpensive, and to determine conditions necessary for synthesis, densification, and characterization of these systems. Two low thermal expansion compositions based on the zircon (NZP) and the β-eucryptite-$AlPO_4$ systems, respectively, have been selected for optimization. The major objective is to demonstrate fabricability and to promote commercialization of these ceramics.

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

69. Low Thermal Expansion Ceramics (WBS No. 1243)

FY 1993
$100,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. R. Johnson, (615) 576-6832
ORNL Contact: D. P. Stinton, (615) 574-4556

The objective of this effort is to develop a work plan and coordinate efforts regarding the application of low-expansion ceramics in advanced heat engines.

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

70. Low Cost CTE Components (WBS No. 1245)

FY 1993
$200,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. P. Stinton, (615) 574-4556
LoTEC, Inc. Contact: Santosh Limaye, (801) 277-6940

The purpose of this new effort is to scale up the work done at universities and develop materials that can be used as exhaust port liners in diesel engines and regenerators in automotive turbine engines. LoTEC will develop and scale up production of sodium-zirconium-phosphate (NZP) materials developed at Penn State University.

Keywords: Structural Ceramics, Ultra-low Expansion, Zirconia

71. Low Cost CTE Components (WBS No. 1246)

FY 1993
$0

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. P. Stinton, (615) 574-4556
Coors Contact: R. N. Kleiner, (303) 277-4739

The purpose of this new effort is to develop materials and fabrication technology for diesel engine exhaust port liners using their aluminum titanate material. In addition, Coors will scale up production of a unique NZP material developed at Virginia Polytechnic Institute and State University.

Keywords: Structural Ceramics, Ultra-low Expansion, Zirconia

72. Advanced Manufacturing (WBS No. 1520) FY 1993
$3,050,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. R. Johnson, (615) 576-6832
Industry Contact: TBD

The goal of this effort is to develop and demonstrate advanced manufacturing technology for the cost-effective production of ceramic heat engine components. The goal of this work is to focus on improvements in yield and quality by the use of production viable processes, statistical process control, and intelligent processing.

Keywords: Components, Cost-Effective Ceramics, Process Control

73. Alternative Fuel Lubricant Technology FY 1993
$50,000

DOE Contact: J. M. Perez, (202) 586-8060
ANL Contact: F. A. Nichols, (708) 252-8292
Penn State University Contact: E. E. Klaus, (814) 863-4804

Technological solutions aimed at reducing the environmental concerns of both automotive and diesel engines have resulted in the use of a variety of alternative fuels that are being researched by industry as relevant to future power plants to reduce emissions. However, major concerns over compatibility of the lubricants with the new fuels exist. The ability of the additives to remain soluble and perform their designed function is a problem with some of the leading alternative technologies. This activity will work cooperatively with industry in resolving the lubricant issues. The use of methanol and ethanol in automotive and diesel engines is a highly visible alternative to reducing atmospheric pollution in highly populated centers. The field testing of a number of diesel- and gasoline-powered vehicles is in progress in several areas of the U.S. and Canada. The lubricant problems are significant in a number of these studies and a timely solution is required.

Keywords: Coatings and Films, Chemical Vapor Deposition, Lubrication, Ceramics, Alternative Fuels

74. Low-Wear Coatings for Transportation FY 1993
$275,000

DOE Contact: J. M. Perez, (202) 586-8060
ANL Contact: Fred Nichols, (708) 252-8292

The recent reorganization of the Tribology Program from ECUT to the Office of Transportation Technologies places greater emphasis on working collaboratively with, and transferring technology and information obtained in this program, to industrial organizations that are involved in the development of advanced energy-conserving engines. The objective of this activity focuses on this aspect. Meetings will be held with industrial organizations that are either directly involved in the development of low-heat-rejection engines, advanced gas turbines, or associated with these projects by virtue of providing components for these engines. These meetings will focus on developing collaborative research programs to transfer the technologies developed under the ETI task to industry. Examples of these efforts include programs with Caterpillar Inc., Cummins Engine Company Inc., the Allison Gas Turbine Division of General Motors Corp., and a tentative program with Detroit Diesel Corp.

Keywords: Ion-Beam-Assisted Deposition, Coatings, Tribology, Friction, Wear, Heat Engines, Diesels, Gas Turbines

75. <u>HRRS Hard Coatings</u> <u>FY 1993</u> $0

DOE Contact: J. M. Perez, (202) 586-8060
ANL Contact: F. A. Nichols, (708) 252-8292
BIRL Contact: Raymond Fessler, (708) 491-4941

The high-rate reactive-sputtering (HRRS) process developed in the hard-coatings-for-cutting-tools program showed great promise for producing well-adherent, hard, wear-resistant coatings on steel substrates. Significant increases in the cutting lifetimes of coated inserts were observed; however, the wear mechanisms and in particular the effect of frictional heating on the coating failure are not fully understood. In the upcoming year, rolling-contact fatigue (RCF) samples will be coated with two reactively sputtered materials, TiN and TiC, and run in RCF and scuffing tests. The coatings will be characterized by scanning and transmission electron microscopy, Auger electron spectroscopy, X-ray diffraction, microhardness, and scratch-adhesion tests. Emphasis will be placed on understanding the failure mechanism in the coated RCF samples. Coated samples will also be supplied to ANL for high-temperature pin-on-disc tests to characterize their friction and wear performance during dry sliding.

Keywords: High-Rate Reactive Sputtering, Coatings, Friction, Wear

76. <u>IBAD of TiN and Cr_2O_3</u> <u>FY 1993</u> $0

DOE Contact: J. M. Perez, (202) 586-8060
ANL Contact: F. A. Nichols, (708) 252-8292
NRL Contact: Fred Smidt, (202) 767-4800

The objective of this project was to determine the mechanism by which ion-beam-assisted deposition (IBAD) produces beneficial modifications of tribological coatings and to establish the necessary correlations between processing parameters, microstructural features of the coating and tribological properties such as friction, wear and adhesion. General principles for producing the improved coatings were defined for the application of these coatings to advanced energy system requirements. This project has been completed and a final report has been prepared.

Keywords: Surface Modification, Coatings, Friction, Wear, Ion Assisted Deposition

77. Self-Lubricating Ceramic Surfaces — FY 1993 $0

DOE Contact: J. M. Perez, (202) 586-8060
ANL Contact: F. A. Nichols, (708) 252-8292
Universal Energy Systems Contact: Rabi Bhattacharya, (513) 426-6900

The objective of this project was to establish optimal conditions for ion implantation and ion-beam mixing of suitable additives into the surfaces of bulk ZrO_2, Al_2O_3, and hardened steel for obtaining self-lubricating, low friction-and-wear characteristics. The work focused on investigations of BaF_2/Ag coatings. Sputtering of a composite CaF_2 + Ag film was made to obtain a coating that was subsequently ion-mixed using MeV ions. Friction and wear of this coating was evaluated by ANL at room temperature and high temperature. This project has been completed and a final report has been prepared.

Keywords: Surface Modification, Coatings, Solid Lubricants, Friction, Wear, Ion Implantation, Ion Beam Mixing, Ceramics

78. High-Current Ion Implantation — FY 1993 $0

DOE Contact: J. M. Perez, (202) 586-8060
ANL Contact: F. A. Nichols, (708) 252-8292
CO State Univ Contact: Prof. Paul Wilbur (303) 491-8564

Ion implantation is a technology that has great potential for industrial applications in the field of tribology. One problem that is hindering wider acceptance of this technology is the long time it takes to implant surfaces due to low current densities of most commercial implanters. The objective of this program is to develop a high-current ion source in order to achieve low-cost, rapid ion implantation of surfaces. A unique broad beam (10 cm diameter) ultrahigh current density (1500 $\mu A/cm^2$) gas-ion implanter has been developed and successfully operated at Colorado State University using ion-rocket thruster technology. The research to be performed in this program will attempt to extend this ultrahigh-current-density technology to develop a unique high-current-density metal-ion implantation system. Another objective of this research is to investigate the effects of ultrahigh-current-density implantations on the tribological properties of the treated surfaces. These studies will establish permissible time-temperature relationships (during ion implantation) that do not cause deleterious changes.

Keywords: Surface Modification, Coatings, Solid Lubricants, Friction, Wear, Ion Implantation, Ion Beam Mixing, Ceramics

79. Lubricious Coatings for Transportation — FY 1993 $250,000

DOE Contact: J. M. Perez, (202) 586-8060
ANL Contact: F. A. Nichols, (708) 252-8292

This activity focuses on the development of low-friction coatings on engineering surfaces. The program involves efforts to develop processes, to characterize films by electron microscopy and mechanical-testing techniques, and to evaluate their tribological performance under different conditions. During FY92, tribological testing of IBAD Ag-coated ceramic substrates was continued to characterize the effects of processing parameters on tribological performance of coatings. Effects of load (stress), sliding velocity (particularly high speed) and sliding distance were investigated. The substrates selected will focus on advanced ceramics such as silicon nitride, silicon carbide, alumina, and zirconia. Other metals and coating processes will also be studied.

Keywords: Surface Modification, Coatings, Solid Lubricants, Friction, Lubricious Coatings

Materials Properties, Behavior, Characterization or Testing

80. Adherence of Coatings (WBS No. 2212) — FY 1993 $0

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. R. Johnson, (615) 576-6832
ORNL Contact: L. L. Horton, (615) 574-5081

Financial support is provided for a graduate research assistantship in the Department of Materials Science and Engineering at the University of Tennessee to conduct studies on the effects of ion bombardment on the structure of thin ceramic films on ceramic substrates.

Keywords: Adherence, Ion Beam, Coatings and Films, Structural Ceramics

81. Development of Standard Test Methods for Evaluating the Wear Performance of Ceramics (WBS No. 2222)

FY 1993
$30,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. R. Johnson, (615) 576-6832
ORNL Contact: P. J. Blau, (615) 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 ASTM to meet this objective.

Keywords: Structural Ceramics, Test Procedures, Wear

82. Advanced Statistics Calculations (WBS No. 2313)

FY 1993
$0

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. R. Johnson, (615) 576-6832
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 is 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, and confidence and tolerance bounds on predictions that use the Weibull distribution and function. The studies are being carried out largely by analytical and computer simulation techniques. Actual fracture data are 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

83. Microstructural Analysis (WBS No. 3111)

FY 1993
$50,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. R. Johnson, (615) 576-6832
NIST Contact: S. M. Wiederhorn, (301) 975-5772

The objective of this work is 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 to be studied include sialons, silicon nitride, and sintered silicon carbide.

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

84. Microstructural Characterization of Silicon Carbide and Silicon Nitride Ceramics for Advanced Heat Engines (WBS No. 3114) — FY 1993 $200,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. R. Johnson, (615) 576-6832
ORNL Contact: T. A. Nolan, (615) 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 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.

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

85. Project Database (WBS No. 3117) — FY 1993 $240,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. R. Johnson, (615) 576-6832
ORNL Contact: B. L. Keyes, (615) 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

86. Fracture Behavior of Toughened Ceramics (WBS No. 3213) FY 1993
$290,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. R. Johnson, (615) 576-6832
ORNL Contact: P. F. Becher, (615) 574-5157

The purpose of this work is to characterize the high-temperature strength, toughness, and creep response of advanced structural ceramics for heat engine applications. Studies will be aimed at providing fundamental insights into the processes responsible for toughness and time-dependent strength degradation of materials such as silicon carbide, silicon nitride, and dispersion-toughened and whisker-reinforced ceramics. Particular emphasis is given to understanding the effect of environment, temperature, and how these materials can be improved by systematic control of microstructure and composition.

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

87. Cyclic Fatigue of Toughened Ceramics (WBS No. 3214) FY 1993
$220,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. R. Johnson, (615) 576-6832
ORNL Contact: K. C. Liu, (615) 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

88. Tensile Stress Rupture Development (WBS No. 3215) FY 1993
$317,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. R. Johnson, (615) 576-6832
ORNL Contact: K. C. Liu, (615) 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 to 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

89. Rotor Materials Database (WBS No. 3216) FY 1993
$200,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. R. Johnson, (615) 576-6832
ORNL Contact: M. K. Ferber, (615) 576-0818

The goal of this research program is to systematically study the tensile strength of silicon nitride ceramics as a function of temperature and time in an air environment. Initial tests will be aimed at measuring the statistical parameters characterizing the strength distribution of three different sample types. The resulting data will be used to examine the applicability of different statistical models as well as sample geometries for determining the strength distribution. In the second phase, stress-rupture data will be generated for silicon nitride specimens by measuring fatigue life at constant stress. The time-dependent deformation will also be monitored during testing so that the extent of high-temperature creep may be ascertained. Tested samples will be thoroughly characterized using established ceramographic, SEM, and TEM techniques. A major goal of this effort will be to better understand the microstructural aspects of high-temperature failure including extent of slow crack growth, evolution of cavitation-induced damage and fracture, transition between brittle crack extension and cavitation-induced growth, and crack blunting. The resulting stress-rupture data will be used to examine the applicability of a generalized fatigue-life (slow crack growth) model.

Keywords: Alumina, Creep, Engines, High Temperature Service, Structural Ceramics, Tensile Testing, Predictive Behavior Modeling, Silicon Nitride, Scanning Electron Microscopy

90. Toughened Ceramics Life Prediction (WBS No. 3217) FY 1993 $200,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. R. Johnson, (615) 576-6832
NASA - Lewis Research Center Contact: Stanley R. Levine, (216) 433-3276

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

91. Life Prediction Methodology (WBS No. 3222) FY 1993 $0

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: C. R. Brinkman, (615) 574-5106
Allison Contact: N. J. Provenzano, (313) 230-3150

The objective of this effort is to develop and demonstrate the necessary nondestructive examination (NDE) technology, material database, and design methodology for predicting the useful life of structural ceramic components of advanced heat engines. The analytical methodology will be demonstrated through confirmatory testing of ceramic components subjected to thermal-mechanical loading conditions similar to those anticipated to occur in actual vehicular service. The project addresses fast fracture, slow crack growth, creep, and oxidation failure modes.

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

92. Life Prediction Methodology (WBS No. 3223) FY 1993
$600,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: C. R. Brinkman, (615) 574-5106
Garrett Contact: John Cuccio, (602) 220-3600

The objective of this effort is to develop the methodology required to adequately predict the useful life of ceramic components used in advanced heat engines. Various specimen geometries will undergo comprehensive testing under both uniaxial and multiaxial loads at different environmental conditions to determine the strength-controlling flaw distributions and to identify various failure mechanisms. NDE techniques will be correlated with failure analyses of the test specimens to help determine the flaw distributions. This information will be used to develop the flaw distribution statistical model and material behavior models for fast fracture, slow crack growth, creep deformation, and oxidation. As subroutines, these models will be integrated with stress and thermal analyses into a failure risk integration analytical tool to predict the life of ceramic components. The methodology developed will be verified by analytically predicting the life of several ceramic components and testing these components under stress and temperature conditions encountered in ceramic turbine engines. Correlation of the NDE data will be used to predict the flaw populations/sizes in the verification components.

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

93. Environmental Effects in Toughened Ceramics (WBS No. 3314) FY 1993
$383,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: Victor J. Tennery, (615) 574-5123
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

94. High Temperature Tensile Testing (WBS No. 3412) FY 1993
$200,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. R. Johnson, (615) 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 a sintered and HIPed Si_3N_4 at temperatures up to 1300°C. Currently, the emphasis is on analyzing the effect of thermal soaking and fatigue on the residual tensile strength of GTE's PY6 material. Microstructural/microchemical analysis of the fracture surfaces using scanning electron microscopy (SEM), transmission election microscopy (TEM), and energy-dispersive spectral analysis (EDS) is an integral part of this effort.

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

95. Standard Tensile Test Development (WBS No. 3413) FY 1993
$125,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. R. Johnson, (615) 576-6832
NIST Contact: S. M. Wiederhorn, (301) 975-5772

This project is 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 database for use in the structural design of heat engines for vehicular applications.

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

96. Non-Destructive Evaluation (WBS No. 3511) FY 1993
$430,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. R. Johnson, (615) 576-6832
ORNL Contact: D. J. McGuire, (615) 574-4835

The purpose of this program is to develop nondestructive evaluation (NDE) techniques in order to identify approaches for quantitative determination of conditions (including both properties and flaws) in ceramics that affect the structural performance. Initial emphasis will be on high-frequency ultrasonics and radiography. Materials to be incorporated include monolithic ceramics such as Si_3N_4 and SiC as well as ceramic composites and the studies will address problems unique to various fabrication techniques such as sintering, hot isostatic pressing, gel casting, etc.

Keywords: NDE, Radiography, Structural Ceramics, Ultrasonics

97. Computed Tomography (WBS No. 3515) FY 1993 $100,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. R. Johnson, (615) 576-6832
Argonne National Lab Contact: W. A. Ellingson, (312) 972-5068

The overall purpose of this program is to develop X-ray computed tomographic (XCT) imaging for characterizing structural ceramic materials relative to density distributions and the presence of voids, inclusions, and cracks and, further, to relate the detected variations to performance of processing variations. Currently, this technique is being used to study density distributions in composite green-state (as-cast) pressure slip-cast ATTAP rotors supplied by Garrett Ceramic Components Division of Allied-Signal Aerospace Company. Garrett will then perform destructive analysis of the as-cast rotors and their findings will be correlated with the 3D X-ray microtomography data.

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

98. Nuclear Magnetic Resonance Imaging (WBS No. 3516) FY 1993 $100,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. R. Johnson, (615) 576-6832
Argonne National Laboratory 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

99. Additives for High-Temperature Liquid Lubricants — FY 1993 $0

DOE Contact: J. M. Perez, (202) 586-8060
ANL Contact: F. A. Nichols, (708) 252-8292
JPL Contact: C. M. Moran, (818) 354-2982

Current additive technology is inadequate in that the additives generally available are designed to be effective at temperatures well below those encountered in the LHRE. They perform well at temperatures below 200°C. Volatility as well as both thermal and oxidative stability are some of the areas requiring improvement. Dinitrile compounds are in one chemical family that possesses the potential of meeting some of the desired properties. This project was initiated at JPL during the second quarter of FY 1991. The purpose of this research is to synthesize and characterize unique additives for liquid lubricants. The additives selected should lead to significant improvements in the major tribology task areas related to the reduction of friction and wear at high temperatures.

Keywords: Lubricants, Additives, Oils, Friction, Wear, Engines, High Temperature

100. Friction & Wear Mechanisms in In-Situ-Reinforced Ceramics — FY 1993 $125,000

DOE Contact: J. M. Perez, (202) 586-8060
ORNL Contact: Peter Blau, (615) 574-1514

Previous work has identified the friction and wear mechanisms of silicon nitride- and alumina-based whisker composites. This new effort extends this analysis to a new class of in-situ-toughened ceramics developed by subcontractors in the OTM Ceramics Technology for Advanced Heat Engines Program. Tests and analysis will be performed to compare their high-temperature friction and wear behavior with that of other ceramics and to identify the dominant friction and wear mechanisms that control that behavior. During the year, a CRADA will be instituted between ORNL and the developer of these materials.

Keywords: Lubrication, Ceramic Composites, Wear, Friction, Wear Transitions, Design Guidelines

101. Carbon-Based Materials for Engine Applications FY 1993 $125,000

DOE Contact: J. M. Perez, (202) 586-8060
ORNL Contact: Peter Blau, (615) 574-1514

Carbon-based materials offer a number of attractive advantages for friction and wear applications, having been used for many years in such applications as pumps, seals, and bearings. However, their introduction into advanced automotive and truck technology has been relatively slow. Part of the reason for this is a lack of focused R&D into the elevated-temperature tribological properties of carbon-based materials. We propose developing baseline data to explore the tribological potential of these materials under temperatures and lubricated environments typical of advanced transportation applications.

Keywords: Ceramics, Carbon, Graphite, Engines, Friction, Wear

102. Advanced Materials/Additive Interactions FY 1993 $150,000

DOE Contact: J. M. Perez, (202) 586-8060
NIST Contact: Stephen Hsu, (301) 921-2113

Ceramic materials are being used increasingly in various applications requiring superior tribological properties related to wear resistance under severe environmental conditions. Data obtained at NIST and those reported in the literature indicate that the wear rate and the friction coefficient of ceramics are generally too high to achieve material conservation or energy conservation. Thus, to successfully utilize ceramics, lubricants must be developed to control friction and wear in these systems. Interactions between various synthetic base oils, additive and ceramics will be studied at ambient and elevated temperatures using various testing and analytical resources. Specifically, the role of the ceramic surfaces on the tribochemical reactions leading to the formation of lubricating films, the effect of the substrate on the thermo-oxidative chemistry of the lubricant, and the effect of lubricant chemical structure will be determined and the competitive or additive interactions established. Analytical techniques considered will include SEM, EDX, FTIR, GPC, TEM and NMR.

Keywords: Ceramics, Ceramic Coatings, Lubrication, Friction, Wear

103. Liquid Lubricants for Heat Engines FY 1993 $150,000

DOE Contact: J. M. Perez, (202) 586-8060
NIST Contact: Stephen Hsu, (301) 921-2113

Successful implementation of advanced heat engines, such as the low-heat-rejection engine (LHRE), is hindered by the lack of stable lubricants and additives for high-temperature applications. Current engine technology is the result of years of materials and lubricants research and development. Extensive experience on metals, alloys, lubricants and additives has evolved from this process. However, extension of this experience to new technological areas has been slow and at times Edisonian. A major factor is that most conventional lubricant applications involve regimes of 200°C or lower and the extension of the knowledge gained to the temperature requirements for future advanced systems is lacking. The LHRE may have a top-ring-reversal temperature as high as 425°C. The need is for lubricants with the capability to effectively survive the severe thermo-oxidative environment, minimize deposit formation and still control friction and wear. A critical component to success in this area is the development of information and an understanding of high-temperature science involving new chemical additives and lubricants.

Keywords: High Temperature Liquid Lubricants, Tribology, Friction, Wear

104. Advanced Lubricants for Engine Particulate Control FY 1993
$150,000

DOE Contact: J. M. Perez, (202) 586-8060
NIST Contact: Stephen Hsu, (301) 921-2113

The U.S. Environmental Protection Agency (USEPA), starting in 1968 as part of its overall strategy to improve air quality, has reduced the contribution of diesel-engine emissions to the atmosphere through the implementation of increasingly more stringent regulations with time. The scenario has been well-documented in numerous publications. The regulations invoked for 1991 and 1994 reflect reductions in both the gaseous and particulate emissions, with the latter more difficult to achieve. In engines of the 1970's, the fuel was a major contributor to the particulates under many operating conditions. As the efficiency of the engines has improved through the use of electronic fuel injection and design changes, the contribution of the fuels to the particulate chemistry has diminished. Therefore, the lubricant and its additive components have become the major contributor to the organic fraction of particulates. Reduction or elimination of this fraction will significantly improve engine emissions. It is the objective of this project to explore concepts that would enable a two-thirds reduction in the organic fraction of diesel particulates.

Keywords: High Temperature Liquid Lubricants, Tribology, Emissions

105. Lubricious Oxide Coatings FY 1993
$75,000

DOE Contact: J. M. Perez, (202) 586-8060
ANL Contact: F. A. Nichols, (708)252-8292
Wear Sciences Contact: M. Peterson, (301) 261-2342

This project will attempt to define the principles of wear protection of sliding surfaces through the formation, in situ, of durable, hard but lubricious oxide films. Binary alloys will be prepared with solute elements which could form protective oxides based on several different approaches: (1) formation of a hard, compacted, wear-debris layer, (2) internal oxidation, (3) stress-free films, (4) increased oxidation, and (5) spall inhibition. Binary alloys of nickel, iron, copper, and titanium with selected additions of hard oxide formers (e.g. Si, Be, Ti, Ta, Zr, Nb, Al, In, Ge, V, and Cr) will be fabricated and evaluated in terms of their tribological performance and microstructural behavior. This research will involve a collaborative effort between WSC, ANL, CSU, and the Institute of Metal Research (Shenyang, China).

Keywords: Surface Modification, Coatings, Solid Lubricants, Friction, Lubricious Coatings

106. Alternative Fuels-Compatible Materials FY 1993
$800,000

DOE Contact: J. M. Perez, (202) 586-8060
ORNL Contact: Ralph McGill, (615) 574-4077

A new Alternative Fuels-Compatible Materials Program is being initiated. The objective of this program is to develop an industrial technology base in advanced materials for engines and vehicles to enable the optimization of the use of alternative fuels and to ensure that the infrastructure necessary to utilize these vehicles might be realized. Improved materials of all types, when available, should be exploited so that their inherently superior properties would make the greatest contribution to improved energy efficiency, reduced environmental degradation, and greater utilization of alternative fuels. A tentative program addressing the need for materials that are compatible with alternative fuels has been defined through several workshops conducted by DOE and ORNL with industry. Some of the critical needs identified at these workshops are for lean-burn catalysts, fuel system durability, reduction of emissions, lubrication of engine components, and materials compatibility. At the workshops, various alternative fuels were considered, but the focus of the program would primarily be on alcohol and natural gas fuels.

Keywords: Alternative Fuel Vehicles, Fuels/Materials Compatibility, Fuels/Lubricant Compatibility

107. Adhesive Bonding of Automotive Materials FY 1993
$200,000

DOE Contact: S. Diamond, (202) 586-8032
ORNL Contact: G. M. Wood, (615) 574-9693

The objective of this work is to establish reliable, relatively simple, and industry acceptable tests for adhesives intended for automotive applications. The experimental work is being coordinated with the Automotive Composites Consortium, a consortium consisting of technical representatives of the three American automobile manufacturers, and is intended to develop qualifying criteria that can be used to evaluate and rank candidate adhesives for rapidly, cost-effectively, and reliably bonding automotive polymer matrix composite components.

Keywords: Polymer Composites, Adhesive Bonding, Adhesive Properties, Polymers, Bonding

Technology Transfer and Management Coordination

108. Management and Coordination (WBS No. 111) FY 1993
$950,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. R. Johnson, (615) 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

109. International Exchange Agreement (IEA) (WBS No. 4115) FY 1993
$400,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. R. Johnson, (615) 576-6832
ORNL Contact: Victor J. Tennery, (615) 574-5123

The purpose of this effort is to organize, assist, and facilitate international research cooperation on the characterization of advanced structural ceramic materials. A major objective of this research is the evolution of measurement standards. Participants in Annex II are the United States, Federal Republic of Germany, Sweden, and Japan.

Keywords: IEA, Powder Characterization, Mechanical Properties

110. Standard Reference Materials (WBS No. 4116) FY 1993 $150,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. R. Johnson, (615) 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. There are three areas of emphasis: (1) to divide, certify, and distribute five ceramic powders for an international round-robin on powder characterization; (2) to provide reliable data on physical (dimensional), chemical, and phase characteristics of two silicon nitride powders (a reference powder and a test powder); and (3) to conduct a statistical assessment and modeling of round-robin data. The round-robin is to be conducted through the auspices of the International Energy Agency (IEA).

Keywords: IEA, Reference Material, Powder Characterization

111. Mechanical Property Standardization (WBS No. 4121) FY 1993 $100,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. R. Johnson, (615) 576-6832
NIST Contact: G. Quinn, (301) 975-5765

The purpose of this effort is to develop test methods in support of the Materials Development and the Advanced Turbine Technology Applications Programs.

Keywords: Mechanical Properties, Test Procedures

112. Diamond Coatings for Tribology FY 1993 $75,000

DOE Contact: J. M. Perez, (202) 586-8060
ANL Contact: Fred Nichols, (708) 252-8292

Much progress has been made in depositing hard diamond and diamond-like-carbon (DLC) films. Existing diamond-coating processes, while capable of producing true diamond films with hardness comparable to that of natural diamonds, result in films which are quite rough and too abrasive to be utilized in sliding- and rolling- contact applications. It is apparent that the production of diamond films suitable for tribological applications will require a thorough assessment of the deposition technology. ANL will organize and conduct a workshop which will bring together the leading researchers and potential users of thin diamond films, especially in applications relevant to transportation technologies. It is expected that, following the workshop, the program will be initiated by means of an RFP.

Keywords: Surface Modification, Coatings, Friction, Wear, Ion Assisted Deposition, Diamond Films, Hard Coatings

Device or Component Fabrication, Behavior or Testing

113. Advanced Coating Technology (WBS No. 1311) FY 1993 $175,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. R. Johnson, (615) 576-6832
ORNL Contact: D. P. Stinton, (615) 574-4556

The objective of this project is to develop an adherent coating that will prevent sodium corrosion of silicon nitride, silicon carbide, or other ceramics used as components in gas turbine engines. The specific coating composition must be compatible with these materials during both coating application and in the operating environment of a gas turbine engine. The effects of the combustion environment on the microstructure, wear, strength, and adherence of these coatings must be minimal.

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

114. Coatings to Reduce Contact Stress Damage of Ceramics (WBS No. 1313) FY 1993 $73,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. R. Johnson, (615) 576-6832
Boston University Contact: V. K. Sarin, (617) 353-2842

The objective of this effort is 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, Structural Ceramics

115. Wear Resistant Coatings (WBS No. 1331)

FY 1993
$56,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. P. Stinton, (615) 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

116. Wear Resistant Coatings (WBS No. 1332)

FY 1993
$0

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. P. Stinton, (615) 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
- good thermal shock resistance
- high uniformity and reproducibility

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

117. Thick Thermal Barrier Coating Systems for Low Heat Rejection Diesel Engines (WBS No. 1342)

FY 1993
$175,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. P. Stinton, (615) 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

118. Active Metal Brazing PSZ-Iron (WBS No. 1411)

FY 1993
$220,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. R. Johnson, (615) 576-6832
ORNL Contact: M. L. Santella, (615) 574-4805

The objective of this task is to develop strong, reliable joints containing ceramic components for applications in advanced heat engines. The emphasis is on studying general brazing characteristics of structural ceramics, assessing joint mechanical properties, relating properties to microstructure, and brazing process development.

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

119. Ceramic-Ceramic Joints AGT (WBS No. 1421)

FY 1993
$0

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: M. L. Santella, (615) 574-4805
Norton Contact: G. J. Sundberg, (508) 351-7908

The purpose of this program is to develop techniques for producing reliable ceramic-ceramic joints and analytical modeling to predict the performance of the joints under a variety of environmental and mechanical loading conditions. The purpose of the Phase II effort is to develop joining technologies for HIPed Si_3N_4 with 4 wt % Y_2O_3 and for a siliconized SiC (NT-230) for various geometries including butt joins, curved joins, and shaft-to-disk joins. In addition, more extensive mechanical characterization (MOR at 22°C and 1370°C, stress rupture at 1370°C, high-temperature creep, tensile tests at 22°C, and spin tests) of silicon nitride joins will be performed to enhance the predictive capabilities of the analytical/numerical models for structural components in advanced heat engines.

Keywords: Engines, Joining/Welding, Metals, Silicon Carbide, Silicon Nitride

120. Ceramic Machining (WBS No. 1500) FY 1993 $200,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. R. Johnson, (615) 576-6832
ORNL Contact: P. J. Blau, (615) 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.

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

121. Next-Generation Grinding Wheel (WBS No. 1531) FY 1993 $430,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: P. J. Blau, (615) 574-5377
Norton Contact: Robert H. Licht, (508) 351-7815

This new 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.

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

122. High Speed Grinding (WBS No. 1532) FY 1993
$0

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: P. J. Blau, (615) 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

123. Chemically Assisted Grinding of Ceramics (WBS No. 1533) FY 1993
$150,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: P. J. Blau, (615) 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 chemical reactions at the tips of the asperities produce a softer reaction layer which reduces contact stresses and, therefore, the extent of surface damage. Si_3N_4 is the material of focus, even though other material such as SiAlON and SiC may be examined for comparison.

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

124. Grindability Test (WBS No. 1542) FY 1993
$224,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: P. J. Blau, (615) 574-5377
Chand Kare Contact: Ronald H. Chand, (508) 793-9814

The objective of this new effort is to develop and validate an inexpensive, bench-top method to assess the relative grindability of ceramics in a manner that can help manufacturers define, in advance, the operations necessary to grind and finish newly developed ceramics for automotive and truck engine applications.

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

125. Grinding Consortium (WBS No. 1543) FY 1993
$150,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: P. J. Blau, (615) 574-5377
NIST Contact: Said Jahanmir, (301) 975-6871

The purpose of this new effort is to develop guidelines and recommendations for grinding optimization of advanced structural ceramics to achieve minimum cost and maximum reliability. The following steps are being 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

126. Fluid-Film Bearings Model FY 1993
$69,000

DOE Contact: J. M. Perez, (202) 586-8060
ANL Contact: F. A. Nichols, (708) 252-8292
Univ of Pittsburgh Contact: A. Z. Szeri (412) 624-9775

This subcontract consists of a three-year project to develop a simplified, yet accurate model of fluid-film lubrication under thermohydrodynamic conditions, with significant elastic and thermal distortion. The end product will include two user-friendly, comprehensive computer programs, one for journal bearings and one for thrust bearings, to be utilized interactively by designers on a personal computer such as the IBM PC/AT or IBM/PS2, or compatibles. The journal-bearing problem will include multiple-pad bearings, either fixed or pivoted, and the thrust-bearing code will cover sector-shaped pads. In addition to static performance parameters, the programs will also calculate linearized stiffness and damping coefficients in a form suitable for rotor-stability analyses. Continual liaison will be maintained with ACTIS, Inc., to insure compatibility for incorporation of these codes into the ACTIS family.

Keywords: Tribology, Bearings, Computer Models, Hydrodynamic Lubrication, Lubrication

127. Wear Mechanism Modeling | FY 1993 $0

DOE Contact: J. M. Perez, (202) 586-8060
ANL Contact: F. A. Nichols, (708) 252-8292
Cambridge Univ Contact: M. F. Ashby, 0-223-33-2-2622

The rate of wear when two surfaces slide, and the mechanisms responsible for it, depend on bearing pressure and sliding velocity, and on numerous bulk and surface properties of the mating materials. Frictional heating is an important factor in determining the mechanism of wear, and—unlike the wear rate itself—it is relatively easy to calculate. The unified approach to this problem previously developed in this activity and published as the user friendly, PC-based computer software T-MAPS will be further analyzed and applied to various sliding pairs utilized in the tribology program at ANL. As new insight and new questions are generated, these are fed back for incorporation into revision of the T-MAPS software at Cambridge. Currently, the lifetime for contact of one asperity with sliding-partner surface is being further refined due to feedback from ANL and other investigators. A final report will be prepared.

Keywords: Metals, Ceramics, Friction, Wear, Engines

128. Instantaneous Friction Torque | FY 1993 $25,000

DOE Contact: J. M. Perez, (202) 586-8060
ANL Contact: F. A. Nichols, (708) 252-8292
Wayne State Univ Contact: Naeim Henein, (313) 577-3887

A three-year project involving a new technique to evaluate instantaneous friction torque (IFT) in an operating, reciprocating internal-combustion engine, is in its third year at Wayne State University (WSU). This Pressure-Angular Velocity (P-ω) technique is based on in situ measurements of combustion pressure (P) and shaft angular velocity (ω) during both steady-state and transient operation of the engine. It is the only currently known method for measuring IFT under actual operating conditions. The final phase of the work will consist of in situ operating-engine tests of solid-lubricant-coated components. Experiments will be conducted in a single-cylinder gasoline engine where cycle-to-cycle variations are often significant. The goal is to determine the effect on engine friction and wear of low-friction, high-temperature, self-lubricating coatings prepared by Ion-Beam-Assisted Deposition (IBAD).

Keywords: Friction, Torque, Engines, Combustion, Modeling

129. Scale Effects in Friction Simulations — FY 1993 $62,000

DOE Contact: J. M. Perez, (202) 586-8060
ORNL Contact: Peter Blau, (615) 574-1514

Friction simulations for accurate screening of advanced materials requires attention to such details as contact-stress history, thermal history, contact arrangement, chemical environment, surface preparation, sliding velocity, and more. Previous work demonstrated how important testing-machine characteristics can be and how wear particles can sometimes accommodate interfacial shears so as to dominate frictional behavior. The project will study effects of contact aspect ratio and pressure distribution, to determine sensitivity of frictional behavior (including running-in) to macro-contact geometry, and strategies for selection of testing procedures (or equipment design) for effective simulations. In addition, more attention will be paid to vibrational characteristics of friction-testing machines and how these need to be characterized to better simulate the behavior of actual components.

Keywords: Friction, Friction Models, Scale Effects, Friction Mechanisms, Ceramics, Composites

130. Thermomechanical Wear Model for Ceramics — FY 1993 $0

DOE Contact: J. M. Perez, (202) 586-8060
ORNL Contact: P. J. Blau (615) 574-1514
GA Institute of Technology Contact: Ward Winer, (404) 894-3270

This project has resulted in the development of a thermomechanical model for wear and surface damage of ceramics. The initial model is being extended to permit lubrication effects to be incorporated. The final product of this work will be a series of thermomechanical wear maps for engineering ceramics (alumina, silicon nitride, zirconia, and silicon carbide) which identify combinations of contact pressure, velocity (thermal parameter), and time for satisfactory wear performance. This project has been completed.

Keywords: Ceramics, Wear, Friction, Lubrication

131. Cylinder Kit Model Development FY 1993
$75,000

DOE Contact: J. M. Perez, (202) 586-8060
ANL Contact: F. A. Nichols (708) 252-8292
Compu-Tec Eng Contact: L. J. Brombolich, (314) 532-4062

The research will be divided into three areas of effort. Phase I will consist of the analytical development of the RING and PISTON programs. Phase II will include a literature search to obtain any data that may be pertinent to the verification of the RING program. In addition, any algorithms that may be used in RING will be investigated. A database of cylinder-kit parameters will be assembled to provide guidelines for future analyses. Data previously developed as well as data generated during this subcontract will be obtained from piston and piston-ring manufacturers, oil companies, liner manufacturers and engine manufacturers. Phase III will consist of engine testing and verification of the RING computer program. Ford Motor Co. is supporting Compu-Tec in this phase of the work. It is anticipated that the three phases will be conducted essentially concurrently.

Keywords: Engines, Diesels, Cylinder Kit, Friction, Piston Rings, Lubrication

132. Advanced Metal Forming of Automotive Materials FY 1993
$500,000

DOE Contact: S. Diamond, (202) 586-8032
ORNL Contact: R.E. Zeigler, (615) 576-0285, (202) 586-2325

The purpose of this effort is to determine the applicability of certain advanced metal forming methods to the rapid production of automotive components and to ascertain the cost-effectiveness of these methods vis-a-vis conventional ones. This is proprietary work being conducted with one of the automotive companies. The effort is being funded by the Office of Transportation Materials in OTT with additional support from the Office of Industrial Technologies (OIT).

Keywords: Metals, Metal Forming, Advanced Metal Forming

Office of Propulsion Systems

The Office of Propulsion Systems is comprised of the Advanced Propulsion Division and the Electric and Hybrid Propulsion Division. Programs supported by this office are focused on developing, with industry through cost-shared contracts, 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. 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 has two major programs: Light Duty Engine Development focused on gas turbines through the Advanced Turbine Technology Applications Project (ATTAP) and Heavy Duty Engine Development focused on diesel engines through the Heavy Duty Transport Technology (HDTT) project. Materials activities supported by this office and managed through the NASA Lewis Research Center for component and coating applications are included in this report. The DOE contacts are: Thomas Sebestyen, (202) 586-9727 for ATTAP and John Fairbanks, (202) 586-8012 for the HDTT project.

Materials Properties, Behavior, Characterization or Testing

133. Ceramic Durability Evaluation AGT — FY 1993 $235,000

DOE Contact: Thomas Sebestyen, (202) 586-9727
NASA Contact: Sunil Dutta, (216) 433-3282
Garrett Turbine Engine Contact: Nancy Campbell, (602) 220-7006

The objective of the 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. In 1989, Kyocera SN-251 silicon nitride and Carborundum TiB_2 and silicon carbide were tested.

Keywords: Silicon Carbide, Silicon Nitride, Erosion, Corrosion, High Temperature, Long Life, Automobile Engine Environment, Gas Turbines

Device or Component Fabrication, Behavior or Testing

134. Thick Thermal Barrier Coatings — FY 1993 $25,000

DOE Contact: John W. Fairbanks, (202) 586-8066
NASA Contact: M. Murray Bailey, (216) 433-3416
Cummins Contact: Thomas M. Yonushonis, (812) 377-7078

Design and demonstration of the durability of thick thermal barrier coatings with low thermal conductance for use in low heat rejection diesel engines is the objective of the project. Zirconia-based coating systems will be developed and applied to metal engine parts for evaluation in a single cylinder engine rig. Completed 100 hours of engine testing and final report in process. No improvement in performance because duration of combustion was extended.

Keywords: Coatings, Oxide Ceramics, Diesel Engines

135. Thick Thermal Barrier Coatings FY 1993 $25,000

DOE Contact: John W. Fairbanks, (202) 586-8066
NASA Contact: M. Murray Bailey, (816) 433-3416
Caterpillar Contact: H. J. Larson, (309) 578-6549

Zirconia thermal barrier coating (TBC) systems are being developed and applied to diesel engine parts for evaluation in a single cylinder engine rig. Initial evaluation of engine tests indicated deterioration by combustion possibly attributed to TBC porosity and surface roughness. Impermeable sealing outerlayers that are aerodynamically smooth, coupled with combustion parameters modified for hot wall effects, produced a four percent fuel economy gain. Final report has been produced.

Keywords: Coatings, Oxide Ceramics, Diesel Engines

136. Advanced Diesel Engine Component Development Project FY 1993 $1,098,000

DOE Contact: John W. Fairbanks, (202) 586-8066
NASA Contact: Richard Barrows, (216) 433-3388
Detroit Diesel Corporation Contact: Theodore Freiheit, (313) 592-7224

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. 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

137. Advanced Piston and Cylinder Component Development FY 1993 $1,200,000

DOE Contact: John W. Fairbanks, (202) 586-8066
NASA Contact: J. J. Notardonato, (216) 433-3908
Caterpillar Inc. Contact: H. J. Larson, (309) 578-6549

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. 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

138. Advanced Piston and Cylinder Component Development FY 1993 $1,200,000

DOE Contact: John W. Fairbanks, (202) 586-8066
NASA Contact: J. J. Notardonato, (216) 433-3908
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. 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

139. High Temperature Solid Lubricant Coatings FY 1993 $50,000

DOE Contact: John W. Fairbanks, (202) 586-8066
NASA Contact: Hal Sliney, (216) 433-6055
Case Western Reserve University Contact: Joseph Prahl, (216) 368-2000

High temperature wear resistant sleeve bearing systems for use at operating temperatures of up to 500°C in diesel engines are being developed and evaluated. Powder metallurgy forms of wear resistant coatings containing solid lubricants for reduced friction are being developed. Current efforts involve development consistent with the process steps that are commercially competitive.

Keywords: Wear, Coatings, Diesel Engines, Tribology

140. Advanced Turbine Technology Applications Project (ATTAP, AGT-5) FY 1993 $4,800,000

DOE Contact: Thomas Sebestyen, (202) 586-9727
NASA Contact: Paul Kerwin, (216) 433-3409
General Motors, Allison Gas Turbine Division, Contact: Phil Haley, (317) 230-2272

Advanced structural ceramic materials are being developed for hot flow path components of an automotive gas turbine engine designed for operation at 2500°F. Efforts include material characterization, process development, and component design and test. In 1989, design of a 2500°F axial turbine stage was completed. Prototype ceramic components have been fabricated for dimensional and properties characterization.

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

141. Advanced Turbine Technology Applications Project (ATTAP, AGT-101) FY 1993
$2,300,000

DOE Contact: Thomas Sebestyen, (202) 586-9727
NASA Contact: Thomas N. Strom, (216) 433-3408
Allied Signal Engines Contact: Jay Smyth, (602) 220-3360

Advanced structural ceramic materials are being developed for hot flow path components for an automotive gas turbine engine designed for operation at 2500°F. The project combines an integrated design, fabrication, and test approach with component technology to be verified in an engine environment. Fabrication of prototype components is underway. A study to quantify rotor impact damage has been completed, which has led to a new mixed flow rotor design. This strengthens the (new) rotor and eliminates particle traps.

Keywords: Structural Ceramics, Component Design, Fabrication, Component Test, Gas Turbine 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; Pandit Patil, (202) 586-8055 for Fuel Cells Development; and Albert Landgrebe, (202) 586-1483 for Exploratory Research in support of Batteries and Fuel Cells.

Materials Preparation, Synthesis, Deposition, Growth or Forming

142. Corrosion-Resistant Coatings for High-Temperature High-Sulfur Activity Applications FY 1993
$0

DOE Contact: A. Landgrebe, (202) 586-1483
Illinois Institute of Technology Contact: J. R. Selman, (312) 567-3037

This research project explores electrodeposition and chemical vapor deposition techniques used to prepare corrosion-resistant coatings for high-temperature batteries. The deposition of molybdenum and Mo_2-C by electrochemical deposition in molten salt was optimized in order to obtain reproducible thicknesses and smooth surface morphology. Researchers observed that complete removal of moisture from the electrolysis bath is necessary to obtain a reproducible, high quality coating. Coatings of an even better quality were obtained with a bath containing non-Li alkali molybdates and carbonates. Through utilizing these coatings, researchers hope to obtain long-term endurance in Na/S cells. X-ray photoelectron spectroscopy (XPS) analysis indicates that the film deposited on a glass or steel substrate contains a significant fraction of oxygen. The use of hydrogen and methane as a carrier gas is being evaluated to minimize the oxygen activity in the reaction chamber. This project has been completed.

Keywords: Electrodeposition, Chemical Vapor Deposition, Corrosion, Coatings and Films

143. Improved Container Electrode Coating for Na/S Battery Systems — FY 1993 — $105,000

DOE Contact: A. Landgrebe, (202) 586-1483
Environmental Research Institute of Michigan Contact: T. Hunt, (313) 677-2113

The objective of this new project is to develop improved corrosion-resistant coatings for high-temperature secondary batteries by sputter-deposition techniques. Studies at Ford Motor Company indicated that sputter-coated TiN on Al was resistant to attack in a polysulfide melt. After three weeks of submersion, a conductive surface film was still present on the TiN coated sample. Final analyses of the physicochemical properties of the coating have not been completed. Reactive-sputtering will be used for the preparation of the majority of coatings that are being examined. However, experiments also will be conducted to understand the stress regimes on coatings obtained by radio frequency sputtering, because control of the deposition parameters for reactive sputtering appears to be more demanding. A reactive-sputtering system has been assembled at ERIM to duplicate the quality of coatings obtained at Ford, and to evaluate the corrosion-resistant properties of TiN for extended periods in polysulfide melts.

Keywords: Sputter-Deposition, Corrosion, Coatings and Films

Materials Structure and Composition

144. *In situ* Spectroscopic Applications to the Study of Rechargeable Lithium Batteries — FY 1993 — $86,000

DOE Contact: A. Landgrebe, (202) 586-1483
Case Western Reserve University Contact: D. A. Scherson, (216) 368-5186

Initiated in 1991, this project uses *in situ* spectroscopic techniques to investigate charge/discharge reactions of Li at Li/SPE interfaces. Techniques have been developed and implemented to investigate the Li electrode in PEO electrolytes under conditions of direct relevance to rechargeable Li/polymer battery technology. Preliminary cyclic voltammetry studies of Au in contact with $LiClO_4$- poly(ethylene oxide) electrolyte at 55°C showed evidence for underpotential deposition (UPD) of Li.

Keywords: Lithium, Batteries, Polymers, Electrodes

145. Battery Materials: Structure and Characterization FY 1993
$95,000

DOE Contact: A. Landgrebe, (202) 586-1483
Brookhaven National Laboratory Contact: J. McBreen, (516) 282-4513

This project attempts to elucidate the molecular aspects of materials and electrode processes in batteries and to use this information to develop electrode and electrolyte structures with improved performance and extended life. Work during the year included extended X-ray absorption fine structure (EXAFS) and X-ray absorption near-edge spectroscopy (XANES) studies of manganese oxides compounds, Bi-doped manganese oxide and Li_xMnO_2. EXAFS data were obtained at both the Mn K edge and the Bi L_3 edge for Bi-doped manganese oxide that was discharged in 9M KOH. At the end of the one-electron discharge, the manganese oxide is highly disordered, while on completion of the two-electron discharge, the product reverts back to an ordered phase.

Keywords: Electrodes, Morphology

146. Polymeric Electrolytes for Ambient-Temperature Lithium Batteries FY 1993
$0

DOE Contact: A. Landgrebe, (202) 586-1483
University of Pennsylvania Contact: G. Farrington, (215) 898-6642

University of Pennsylvania researchers have investigated polymeric electrolytes formed by radiation-polymerization of various oligomers that contain different compositions of plasticizer (ethylene carbonate, EC and propylene carbonate, PC) and 1 M $LiAsF_6$. Polymeric electrolytes with greater than or equal to 50 wt% PC in mixtures with Ec appear to exhibit acceptable electrochemical (reversible Li redox process) and physicochemical properties (ionic conductivity greater than 8 x 10^4 at room temperature, glass-transition temperature of -94°C, amorphous structure from -90 to 150°C) for use in rechargeable Li cells. This project has been completed.

Keywords: Polymers, Batteries

Materials Properties, Behavior, Characterization or Testing

147. Corrosion, Passivity, and Breakdown of Alloys Used in High-Energy-Density Batteries — FY 1993 $0

DOE Contact: A. Landgrebe, (202) 586-1483
Johns Hopkins University Contact: J. Kruger, (301) 338-8937

The objective of this project is to investigate the phenomena of passivation and its breakdown on metals and alloys in nonaqueous solvents for rechargeable Li batteries. The formation and the stability of passive films are important for the sustained integrity of construction materials used in high-energy batteries. This study is specifically concerned with the nature, formation mechanisms, and the mechanism of breakdown of passive films that exist on alloys in nonaqueous solvents. Researchers have observed that iron and 1018 carbon steel display an extensive and stable passive region in $LiAsF_6$/dimethoxyethane (DME). In a nominally dry $LiAsF_6$/DME solution (less than 100-ppm H_2O), the breakdown potentials of iron and carbon steel are 1300 mV (*vs* saturated calomel electrode, SCE) and 1050 mV, respectively. The adsorption of DME and the formation of carbon-based polymer film are believed to be responsible for passivation. This project has been completed.

Keywords: Passivation, Metals: Ferrous, Batteries

148. Advanced Chemistry and Materials for Fuel Cells — FY 1993 $94,000

DOE Contact: A. Landgrebe, (202) 586-1483
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 fuel cells. Researchers are utilizing X-ray absorption spectroscopy (XAS) to study the correlation between the electronic properties of carbon supported Pt/Cr, Pt/Co, and Pt/Ni alloy catalysts and their electrocatalytic activity for oxygen reduction.

Keywords: Fuel Cells, Catalysts, Oxygen Reduction

149. Electrocatalysts for Oxygen Electrodes FY 1993
$0

DOE Contact: A. Landgrebe, (202) 586-1483
Case Western Reserve University Contact: E. Yeager, (216) 386-3626

The objective of this research is to develop more effective electrocatalysts for O_2 reduction and generation which have high activity and long-term stability. Various electrocatalysts, including the transition-metal macrocycles and oxide catalysts, were evaluated to identify stable catalysts with much higher activity for both monofunctional and bifunctional air electrodes. Researchers observed that the catalytic activity for the reduction of O_2 at cobalt tetrasulfonated phthalocyanine (CoTsPc) adsorbed on ordinary pyrolytic graphite (OPG) in alkaline solution is enhanced by approximately 60 mV in the presence of alcohols. Further, the presence of methanol has no short-term deleterious effect on the kinetics for O_2 reduction on CoTsPc/OPG, which also exhibits negligible catalytic activity for methanol oxidation. This project has been completed.

Keywords: Catalysts, Polymers, Metals Surface, Composites, Batteries

150. Novel Concepts for Oxygen Electrodes in Secondary Metal/Air Battery FY 1993
$125,000

DOE Contact: A. Landgrebe, (202) 586-1483
Eltech Research Corporation Contact: E. Rudd, (216) 357-4073

Researchers are investigating the viability of graphitized carbon blacks and metal oxides as electrocatalyst supports in bifunctional air electrodes for electrically rechargeable Zn/air cells. Graphitized carbon blacks of Monarch 120 and Shawinigan acetylene black appear to be suitable electrocatalyst supports. Electrochemical tests of $NiCo_2O_4$/Monarch 120 in small cells at Metal Air Technology Systems International (MATSI) have achieved over 350 cycles (discharge 4h at $10mA/cm^2$, charge 8h at $5mA/cm^2$).

Keywords: Electrodes, Electrocatalysts, Batteries

Device or Component Fabrication, Behavior, or Testing

151. Proton-Exchange-Membrane Fuel Cells for Vehicles FY 1993
$1,200,000

DOE Contact: A. Landgrebe, (202) 586-1483
Los Alamos National Laboratory Contact: S. Gottesfeld, (505) 667-0853

Los Alamos National Laboratory conducts three major proton-exchange-membrane (PEM) fuel cell projects. These projects seek to: (1) develop better gas diffusion electrodes,

(2) measure and model the mass transport properties and conductivity of proton-conducting membranes, and (3) measure the operating characteristics of single PEM fuel cells and determine the conditions providing optimal performance. Researchers have found that processing membrane-electrode assemblies (MEA) with Nafion membranes that contain tetrabutyl ammonium are more robust than those obtained from the Na^+ and H^+ forms. Researchers have also characterized some of the H_2O-management properties of Nafion 117, membrane C, and an experimental Dow membrane. In addition, researchers have resolved the problem of membrane puncture that was observed in small fuel cells that contain thin membranes such as the 2-mil thick Nafion membrane by using thin Teflon gasket in the membrane/electrode/gasket assembly.

Keywords: Fuel Cells, Separators, Electrodes

152. Electrochemical Energy Storage FY 1993
$1,765,000

DOE Contact: A. Landgrebe, (202) 586-1483
Lawrence Berkeley Laboratory Contact: F. McLarnon, (510) 486-4636

The major thrust of this program is to evaluate promising electrochemical couples for advanced batteries for electric vehicles. Exploratory research was carried out on Zn/NiOOH and Na/metal oxide polymerization cells. Novel components for various versions of rechargeable Li, Na, and Zn cells were also investigated. Research topics include: Zn/KOH/NiOOH cells studies; electrochemical properties of solid-state sodium/polymer cells; surface morphology of metals in electrodeposition; high-temperature cell research; analysis and simulation of electrochemical systems; surface layers on batteries; application of photothermal deflection spectroscopy to electrochemical interfaces; electrode kinetics and electrocatalysis of methanol electrooxidation; effect of electrocatalyst and electrolyte composition on methanol/air fuel cell performance; transport in zinc-air cells and mathematical modeling; and development of electrically rechargeable zinc/air cells.

Keywords: Electrocatalyst, Batteries, Fuel Cells, Polymers

153. Applied Research on Secondary Zn/NiOOH Cell Technology FY 1993
$193,000

DOE Contact: A. Landgrebe, (202) 586-1483
Acme Electric Corporation Contact: M. Anderman, (602) 894-6864

The objectives of this project are to evaluate the Lawrence Berkeley Laboratory electrolyte composition for extending the cycle life of Zn/NiOOH cells, and to develop

Zn/NiOOH battery technology for EV applications. The project was initiated as a result of an award from a Request-for-Proposal that was issued by Lawrence Berkeley in 1992.

Keywords: Electrocatalyst, Batteries, Fuel Cells, Polymers

Office of Alternative Fuels

The Office of Alternative Fuels has three major programs: Biofuels Production, Alternative Fuels Utilization, and the Alternative Motor Fuels Act (AMFA) fleet test program. Materials technologies for alternative fuels are being addressed by the Office of Transportation Materials and other DOE offices. The DOE contact for biomass is Richard Moorer, (202) 586-5350, and the DOE contacts for alternative fuels are John Russell, Richard Wares, or Steve Goguen, (202) 586-8053.

Materials Properties, Behavior, Characterization or Testing

154. Cold-start Assist Materials — FY 1993 $120,000

DOE Contract: S. Goguen, (202) 586-8053
Oak Ridge National Laboratory Contact: R. Graves, (615) 574-2036

This project examines a wide variety of materials to determine their exothermic properties during phase change. The heat released would be utilized to vaporize alcohol automotive fuels to enhance their cold-starting characteristics.

Keywords: Phase-Change Materials, Alcohol Fuels

155. CNG Adsorbents Demonstration — FY 1993 $300,000

DOE Contact: M. Gurevich, (202) 586-8053

This project screens and evaluates materials for their effectiveness in adsorbing natural gas. An adsorbent placed in a storage vessel could hold sufficient CNG to reduce working pressure to 500 psi. This would permit introduction of complex geometry (shaped) automotive tanks configured to take advantage of interior vehicle "dead space" as well as reducing overall weight requirements. Net result would be increased range.

Keywords: Natural Gas Adsorbent Materials, Alternative Fuels

OFFICE OF UTILITY TECHNOLOGIES

	FY 1993
Office of Utility Technologies - Grand Total	$37,650,000
Office of Solar Energy Conversion	$19,400,000
Photovoltaic Energy Technology Division	$19,400,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$14,000,000
Amorphous Silicon for Solar Cells	4,900,000
Polycrystalline Thin Film Materials for Solar Cells	7,100,000
Deposition of III-V Semiconductors for High-Efficiency Solar Cells	2,000,000
Materials Properties, Behavior, Characterization or Testing	$ 3,000,000
Materials and Device Characterization	3,000,000
Device or Component Fabrication, Behavior or Testing	$ 2,400,000
High-Efficiency Crystal Silicon Solar Cells	2,400,000
Office of Renewable Energy Conversion	$ 687,000
Geothermal Division	$ 687,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 100,000
Thermally Conductive Composites for Heat Exchangers	100,000
Materials Properties, Behavior, Characterization or Testing	$ 587,000
Advanced High Temperature Geothermal Well Cements	310,000
Advanced High Temperature Chemical Systems for for Lost Circulation Control	100,000
Corrosion Mitigation in Highly Acidic Steam Condensates	100,000
High Temperature Chemical Bonding Systems	77,000

OFFICE OF UTILITY TECHNOLOGIES

	FY 1993
Office of Energy Management	$17,563,000
Advanced Utility Concepts Division	$17,563,000
Superconductivity Systems Program (National Laboratory Projects)	$16,820,000
Device or Component Fabrication, Behavior or Testing	$16,820,000
High-Temperature Superconductor Development for Electric Power Applications	4,600,000
Characterization and Development of High-Temperature Superconductors	600,000
Electrodeposition of High-Temperature Superconductors	750,000
Bulk and Thin-Film Materials Process Research for Practical High-Temperature Superconductor Development	1,100,000
High-Temperature Superconductor Wire and Component Development for Electric Power Applications	4,670,000
Conductor Development, Processing of Wires and Tapes, Magnet Design and Testing, and Applications Development for High-Temperature Superconductors	5,100,000
Thermal Energy Storage Program	$ 743,000
Materials Properties, Behavior, Characterization or Testing	$ 231,000
High Temperature Composite Phase Change Material	131,000
Geochemistry Dynamics Associated with Ground Water Heating	100,000
Device or Component Fabrication, Behavior or Testing	$ 512,000
Phase Change Thermal Storage for Domestic Water Heating	71,000
Phase Change Thermal Storage in Building Materials	74,000
Complex Compound Thermal Energy Storage System	367,000

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

156. Amorphous Silicon for Solar Cells — FY 1993 $4,900,000

DOE Contact: Richard King, (202) 586-1693
NREL Contact: Werner Luft, (303) 384-6452

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 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

157. Polycrystalline Thin Film Materials for Solar Cells FY 1993
$7,100,000

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

158. Deposition of III-V Semiconductors for High-Efficiency Solar Cells FY 1993
$2,000,000

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 (Liquid Phase Epitaxial Growth, Molecular Beam Epitaxial Growth)

Materials Properties, Behavior, Characterization or Testing

159. Materials and Device Characterization | FY 1993 $3,000,000

DOE Contact: Richard King, (202) 586-1693
NREL Contact: Larry Kazmerski, (303) 231-1115

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

160. High-Efficiency Crystal Silicon Solar Cells | FY 1993 $2,400,000

DOE Contact: Richard King, (202) 586-1693
NREL Contact: John Benner, (303) 384-6496
SNLA Contact: David Hasti, (505) 844-8161

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

161. Thermally Conductive Composites for Heat Exchangers FY 1993
$100,000

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 for 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 antioxidant additives on the fouling coefficient and scale adherence are also being evaluated.

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

Materials Properties, Behavior, Characterization or Testing

162. Advanced High Temperature Geothermal Well Cements FY 1993
$310,000

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

163. Advanced High Temperature Chemical Systems for Lost Circulation Control FY 1993 $100,000

DOE Contact: R. LaSala, (202) 586-4198
BNL Contact: L. E. Kukacka, (516) 282-3065

The cost of correcting lost circulation problems occurring during well drilling and completion operations constitutes 20 to 30 percent of the cost of a geothermal well. The objective of the program is to develop advanced high temperature chemical systems which are pumpable at high temperature and which upon curing will yield an expandable, high strength, brine-resistant, cementitious material. Emphasis is being placed upon high temperature rheology, phase chemistry, and the mechanical, physical and chemical resistance properties of the cured material. Optimization of the formulations with respect to various placement technologies is also being conducted. To date, formulations containing calcium phosphate cements have been optimized for placement at temperatures <100°C. Engineering-scale placement and downhole testing is scheduled for FY 1994.

Keywords: Cement, Pumpable Slurries, Strength, Transformation, Bulk Characterization

164. Corrosion Mitigation in Highly Acidic Steam Condensates FY 1993 $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

165. High Temperature Chemical Bonding Systems — FY 1993 $77,000

DOE Contact: R. LaSala, (202) 586-4198
BNL Contact: L. E. Kukacka, (516) 282-3065

The unavailability of hydrolytically (300°C) stable chemical coupling systems that will bond high temperature elastomers to metal reinforcing substrates is constraining the development of high temperature tools needed for the drilling and completion of geothermal wells. The objective of this program is to develop advanced bonding systems consisting of elementally modified metal surfaces, elastomers and hydrothermally stable polyaryl-type polymeric adhesives which will chemically bond with each to form stable interfaces. Specific end-use applications include drillpipe protectors, rotating head seals, blow-out preventors, and downhole drillmotors.

Keywords: Elastomers, Chemical Bonding, Metals, Interfacial Characteristics, Hydrothermal Stability

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 (National Laboratory Projects)

Device or Component Fabrication, Behavior or Testing

166. High-Temperature Superconductor Development for Electric Power Applications — FY 1993 $4,600,000

DOE Contact: J. Daley, (202) 586-1165
Argonne National Laboratory Contact: R. Poeppel, (708) 252-5118

The work consists of parallel efforts in research of fabrication methods for reliable high-temperature superconducting (HTS) wires and electric power devices. Conductor development efforts include microstructure control via powder synthesis, consolidation, and heat treatment, and share the goals of improving J_cs and mechanical properties. From this work came a novel two-powder processing method that produces high-quality Bi-2223 in as few as 50 hours; tapes from this process have achieved J_c values of up to 7 x 10^4 A/cm^2 at 77K in self-field. In addition, researchers' efforts to provide more intimate mixing of precursor powders via cryoprocessing will lead to better microstructures and properties. Device technology development includes wire and coil development for application at temperatures to 77K. The effort includes design/development of current leads, fault-current limiters, magnetic bearings, and flywheels. With 100-A current lead testing proceeding satisfactorily, the design of a >1000-A commercial scale current lead is underway. Collaborations with private industry included efforts with Intermagnetics General Corp., Superconductivity, Inc., Commonwealth Research Corp., General Electric, TRW, American Superconductor Corp., and Superconducting Products Co.

Keywords: Two-Powder, Microstructure, Cryoprocessing, Current Leads, Fault-Current Limiters, Magnetic Bearings, Flywheels

167. Characterization and Development of High-Temperature Superconductors

FY 1993
$600,000

DOE Contact: J. Daley, (202) 586-1165
Brookhaven National Laboratory Contact: D. Welch, (516) 282-3517

The work includes efforts that support development of scalable fabrication methods for composite conductors for electric power systems applications, and analytical and experimental studies of design and operation of HTS magnets. Through detailed measurements/modeling of superconducting microstructures and properties, researchers study factors that limit current carrying ability. BNL and collaborating universities conduct much of the characterization; industrial collaborators and subcontractors conduct most of the processing R&D. Characterization of Bi-2223/Ag tapes showed that vortex pinning in highly connected grains controls J_c. Multiple pressing and annealing achieved significant improvements in both J_c and mechanical properties of Bi-2223 mono- and multi-filament conductors. Study of the stability and protection of HTS devices showed that nearly uniform dissipation of stored electromagnetic energy during a quench is necessary to make HTS magnets self-protecting. Collaborative efforts include projects with MIT, Intermagnetics General Corp., Oxford Superconducting Technology, Grumman Electronics Systems, and American Superconductor Corp.

Keywords: Scalable Fabrication, Composite Conductors, HTS Magnets, Characterization, Stability, Protection

168. Electrodeposition of High-Temperature Superconductors FY 1993
$750,000

DOE Contact: J. Daley, (202) 586-1165
National Renewable Energy Laboratory Contact: R. McConnell, (303) 231-1019

This project supports development of HTS oxide materials for conductors that can operate at liquid nitrogen temperatures. The primary materials under investigation are Tl-oxide superconductors that offer T_cs up to 127K and magnetic properties at 77K that should be useful for wire or tape. Through electrodeposition or other novel thick-film deposition techniques, researchers are attempting to form polycrystalline Tl-compound conductors that do not exhibit the weak-link degradation that is evident in YBCO materials. The electrodeposition process is economical and scalable. The research includes study of electrodeposition parameters and control of reaction conditions to synthesize Tl-compounds. The efforts center on demonstration of electrical transport current in a mechanically rugged and flexible conductor suitable for electric power applications. Collaborations include projects with General Electric, General Dynamics, and Power Superconductor Applications.

Keywords: Thallium, Magnetic Properties, Electrodeposition, Weak-Link Behavior, Process Parameters

169. Bulk and Thin-Film Materials Process Research for Practical High-Temperature Superconductor Development FY 1993
$1,100,000

DOE Contact: J. Daley, (202) 586-1165
Sandia National Laboratories: T. Bickel, (505) 844-9301

The research includes four interrelated efforts: (1) processes for synthesis of HTS materials, (2) processes for synthesizing Tl-based thick-films, (3) processes for synthesis and characterization of HTS wire and tape, and (4) cryogenic design of an HTS motor. These efforts interactively support development of HTS wires and tapes that can carry high currents in the presence of magnetic fields at liquid nitrogen temperatures. Materials synthesis research has developed processes that produce Tl-based powders with controlled stoichiometry, phase composition, and homogeneity; wire and tape fabrication efforts have employed these powders to study the effects of composition and thermal processing on transport properties of the composite conductors; Tl-film efforts have developed processes to make thick-film conductors from these materials; cryogenic design of an HTS motor has employed measured properties of these HTS materials, and has also identified operating regions in which HTS materials need optimization. Industrial collaborators include Nuclear Metals Incorporated, AT&T, and Intermagnetics General.

Keywords: HTS Synthesis, Characterization, Cryogenic Design, HTS Motor, Tl-Films

170. High-Temperature Superconductor Wire and Component Development for Electric Power Applications

FY 1993
$4,670,000

DOE Contact: J. Daley, (202) 586-1165
Los Alamos National Laboratory: D. Peterson, (505) 665-3030

Research includes three related efforts: (1) powder synthesis and characterization, (2) bulk conductor processing and characterization, and (3) power systems design, prototyping, and testing. Each area supports development of HTS wires and components for electric power applications. Powder synthesis work generated methods that improve reproducibility, phase content, grain size, and homogeneity of Bi- and Tl-based materials. Bulk conductor efforts successfully generated 30-meter lengths of Bi-2223 tapes; the effort also included initiation of a 10-parameter statistical study of Bi-2223. System design, prototyping and, testing included engineering analysis of bulk conductor applications and fabrication and testing of prototype components for electric power applications. The efforts improved the accuracy of characterization tools for measurement of critical currents in magnetic fields, texture, and particle size. Industry collaborations include projects with American Superconductor Corp., Intermagnetics General Corp., Nuclear Metals, AT&T, Reliance Electric, and General Dynamics.

Keywords: Powder Synthesis, Characterization, Bulk Conductors, System Design, Prototype

171. Conductor Development, Processing of Wires and Tapes, Magnet Design and Testing, and Applications Development for High-Temperature Superconductors

FY 1993
$5,100,000

DOE Contact: J. Daley, (202) 586-1165
Oak Ridge National Laboratory: R. Hawsey, (615)574-8057

Research includes conductor and electric power applications development that supports a technology base for commercial development of HTS electric power applications. Thermomechanical processing of BSCCO conductors includes activities associated with the industry-led Wire Development Group; the study examined effects of fabrication variables on the quality of the conductor. Thallium conductor efforts examined Tl-films prepared by industry; the effort found that intra-granular properties limit high-field conduction. Critical current and microstructure studies examined the flux-pinning structures of YBCO, BSCCO, and TBCCO materials; the efforts identified an upper limit to loss-free conduction in YBCO. Coil development efforts obtained measurements that indicate that useful temperatures for Bi-2223 coils may be as high as 50K. Magnetic refrigeration work initiated fabrication of a 50W/40K magnetic refrigerator. Industrial collaborations include projects with American Superconductor

Corp., Intermagnetics General Corp., General Electric, Superconductive Components, Inc., IAP Research, and IBM.

Keywords: Thermomechanical Processing, BSCCO, Tl-Films, Coils, Magnetic Refrigerator

Thermal Energy Storage Program

Materials Properties, Behavior, Characterization or Testing

172. High Temperature Composite Phase Change Material FY 1993 $131,000

DOE Contact: Dr. Eberhart Reimers, (202) 586-4563
PNL Contact: Dr. W. Kevin Winegardner, (509) 375-3839
Mississippi State University Contact: Professor G. A. Adebiyi, (601) 325-3260

The objective of the work is to develop high temperature sensible/latent heat storage media for use in a packed bed regenerator for the capture and reuse of waste heat. The near-term application of this technology is recovery of heat currently exhausted into the air by flue gases in high-temperature industrial processes. The composite material consists of a ceramic matrix (sponge) in which a phase change material (salt eutectic) is imbibed forming a composite phase change material (CPCM). When the salt melts, capillary forces retain the salt in the ceramic matrix, providing form-stability to the PCM. Samples of conventional sensible storage material and the CPCM have been prepared and testing of the sensible material in a packed bed configuration has been undertaken. Testing with the CPCM will follow.

Keywords: Heat Storage, Phase Change Materials, Composites

173. Geochemistry Dynamics Associated with Ground Water Heating FY 1993 $100,000

DOE Contact: Dr. Eberhart Reimers, (202) 586-4563
PNL Contact: Dr. W. Kevin Winegardner, (509) 375-3839
PNL Technical Contact: Dr. E. A. Jenne, (509) 376-4412

The objective of this effort is to obtain the equilibrium and kinetic data required to accurately predict important geochemical reactions and permeability reduction in an aquifer during thermal energy injection, storage and recovery. Geochemical studies were used to acquire the former equilibrium data. Computer software has been developed to reliably identify the need for water treatment to avoid carbonate scaling and clogging and to calculate the portion of the water that must be treated at any given temperature, and the capacity requirements of various treatments. A study, near completion, is evaluating the importance of dissolved organic carbon in ground water in preventing carbonate precipitation although kinetic data may also be needed. An outline has been developed for preparation of a comprehensive users guide for ATES.

Keywords: Minerals, Permeability, Aquifer

Device or Component Fabrication, Behavior or Testing

174. Phase Change Thermal Storage for Domestic Water Heating FY 1993
$71,000

DOE Contact: Dr. Eberhart Reimers, (202) 586-4563
PNL Contact: Dr. W. Kevin Winegardner, (509) 375-3839
University of Florida - Gainsville Contact: Professor D. Yogi Goswami, (904) 392-0851

The objective of this work is to develop new thermal energy storage prototypes that double the energy density of conventional electrically heated storage water heaters. The development effort includes the identification and development of phase change materials (PCM) and their encapsulating materials where appropriate. Several concepts are under development including use of cross-linked polyethylene and pentaerythritol as solid-solid PCMs. Encapsulation in lined and unlined pouches are being studied, including sealing methods such as ultrasonic welding, adhesives, and thermal welding. Corrosion studies will be conducted on encapsulated materials. Theoretical models will be used to design prototype units that will then be constructed and tested.

Keywords: Phase Change Materials, Encapsulation, Corrosion

175. Phase Change Thermal Storage in Building Materials FY 1993
$74,000

DOE Contact: Dr. Eberhart Reimers, (202) 586-4563
PNL Contact: Dr. W. Kevin Winegardner, (509) 375-3839
University of Dayton Contact: Dr. I. O. Salyer, (513) 229-2213

The objective of this effort is to develop and adapt low-cost, effective phase change systems that melt and freeze in the temperature range 23-25°C for building materials. The near-term emphasis is on incorporating these materials in plasterboard. Crystalline alkyl hydrocarbon materials (paraffin) have been identified as promising PCMs for wallboard applications. The paraffin is imbibed into interstices of the gypsum. Evaluation of critical performance factors includes characterization of the quantities of paraffin that can be imbibed, internal distribution of paraffin, effect of thermal cycling, propensity for leakage, combustibility, and smoke evolution during combustion. Alternative methods for introducing the PCM into the plasterboard production process have been investigated, including imbibition in high-density polyethylene and dry mixing with high-surface-area silica. Performance has been sufficiently promising to persuade U.S. Gypsum to try a short plant production run with this material.

Keywords: Building Materials, Phase Change Materials, Paraffin

176. Complex Compound Thermal Energy Storage System FY 1993 $367,000

DOE Contact: Dr. Eberhart Reimers, (202) 586-4563
PNL Contact: Dr. W. Kevin Winegardner, (509) 375-3839
Rocky Research Contact: Dr. Uwe Rockenfeller, (702) 293-0851

The objective of this work is to develop an advanced chill storage system using ammoniated complex compounds. The application for this technology is for load shifting and peak load reduction in industrial refrigeration and residential and commercial air conditioning systems. The storage concept uses the chemical adsorption of ammonia vapor on an inorganic metal salt. Suitable media for the application will be identified and the performance of the media, in terms of amount and rate of adsorption and desorption, will be characterized. A full-scale prototype chemical reactor will be designed, fabricated, and tested.

Keywords: Adsorption Refrigeration, Adsorbing Materials, Complex Compound

OFFICE OF ENERGY RESEARCH

	FY 1993
Office of Energy Research - Grand Total	$324,512,190
Office of Basic Energy Sciences	$285,128,044
Division of Materials Sciences	$267,140,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 31,500,000
Materials Structure and Composition	$ 33,000,000
Materials Properties, Behavior, Characterization or Testing	$ 98,140,000
Facilities	$104,500,000
Division of Chemical Sciences	$ 5,320,000
Heterogeneous Catalysis	$ 870,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 200,000
Materials Structure and Composition	$ 670,000
Advanced Battery Research and Development	$ 2,700,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 1,300,000
Materials Structure and Composition	$ 120,000
Materials Properties, Behavior, Characterization or Testing	$ 850,000
Device or Component Fabrication, Behavior or Testing	$ 430,000

OFFICE OF ENERGY RESEARCH (Continued)

	FY 1993
Office of Basic Energy Sciences (continued)	
Division of Materials Sciences (continued)	
Materials Precursor Chemistry	$ 1,750,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 1,000,000
Materials Structure and Composition	$ 750,000
Division of Engineering and Geosciences	$ 7,228,044
Engineering Sciences Research	$ 5,278,392
Materials Properties, Behavior, Characterization or Testing	$ 5,278,392
Bounds on Dynamic Plastic Deformation	137,000
In-Flight Measurement of the Temperature of Small, High Velocity Particles	493,000
Intelligent Control of Thermal Processes	530,000
Multivariable Control of the Gas-Metal/Arc Welding Process	158,000
Metal Transfer in Gas-Metal Arc Welding	122,300
Modeling and Analysis of Surface Cracks	196,000
Thermal Plasma Processing of Materials	141,928
Transport Properties of Disordered Porous Media from the Microstructure	205,892
Inelastic Deformation and Damage at High Temperature	134,000
Energy Changes in Transforming Solids	175,000
Stress Induced Phase Transformations	66,169
Optical Techniques for Superconductor Characterization	285,500
Effective Elastic Properties and Constitutive Equations for Brittle Solids Under Compression	59,798
Investigation of PACVD Protective Coating Process Using Advanced Diagnostic Techniques	0
Elastic-Plastic Fracture Analysis Emphasis on Surface Flaws	430,000

OFFICE OF ENERGY RESEARCH (Continued)

	FY 1993
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)	
Continuous Damage Mechanics - Critical States	60,000
Thin Film Characterization and Flaw Detection	89,450
Development of Measurement Capabilities for the Thermophysical Properties of Energy-Related Fluids	551,000
Flux Flow, Pinning and Resistive Behavior in Superconducting Networks	69,500
An Investigation of the Effects of History Dependent Damage in Time Dependent Fracture Mechanics	94,027
Mixing and Settling in Continuous Metal Production	135,000
Application of Magnetomechanical Hysteresis Modelling to Magnetic Techniques for Monitoring Neutron Embrittlement and Biaxial Stress	99,912
Stability and Stress Analysis of Surface Morphology of Elastic and Piezoelectric Materials	96,665
Micromechanical Viscoplastic Stress-Strain Model with Grain Boundary Sliding	50,000
Micromechanical Viscoplastic Stress-Strain Model with Grain Boundary Sliding	48,000
Modeling of Thermal Plasma Processes	232,000
Nondestructive Evaluation of Superconductors	200,000
Heat Transfer to Viscoelastic Fluids	79,980
Pulse Propagation in Inhomogeneous Optical Waveguides	83,537
Low Resistivity Ohmic Contacts Between Semiconductors and High-T_c Superconductors	0
The Evolution of a Hele-Shaw Interface and Related Problems in Dendritic Crystal Growth	66,116

OFFICE OF ENERGY RESEARCH (Continued)

		FY 1993
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)		
Degenerate Four-Wave Mixing as a Diagnostic of Plasma Chemistry		95,328
Effect of Forced and Natural Convection on Solidification of Binary Mixtures		93,290
Geosciences Research	$	1,949,642
Materials Preparation, Synthesis, Deposition, Growth or Testing	$	327,209
An Investigation of Mineral Hydrolysis Kinetics		226,000
Transition Metal Catalysis in the Generation of Petroleum and Natural Gas		101,209
Materials Structure and Composition	$	351,025
Infrared Spectroscopy and Hydrogen Isotope Geochemistry of Hydrous Silicate Glass		104,517
Crystal Chemistry of Hydroxyl and Water in Silicate Minerals		80,448
Zircons and Fluids: An Experimental Investigation with Applications for Radioactive Waste Storage		28,167

OFFICE OF ENERGY RESEARCH (Continued)

	FY 1993
Office of Basic Energy Sciences (continued)	
Division of Materials Sciences (continued)	
Division of Engineering and Geosciences (continued)	
Engineering Research (continued)	
Geosciences Research (continued)	
Materials Structure and Composition (continued)	
High-Resolution Transmission Electron Microscopy/ Analytical Electron Microscopy and Scanning Electron Microscopy Study of Fluid-Rock Interactions: Interaction of Copper-, Silver-, Selenium-, Chromium-, and Cadmium-Bearing Solutions with Geological Materials at Near-Surface Conditions, with an Emphasis on Phyllosilicates	137,893
Materials Properties, Behavior, Characterization or Testing	$1,271,418
Cation Diffusion Rates in Selected Silicate Minerals	174,000
Shear Strain Localization and Fracture Evolution in Rocks	75,443
Poroelasticity of Rock	250,406
Oxygen and Cation Diffusion in Oxide Materials	150,000
Modification of Fracture Transport Properties of Rocks by Mechanical and Chemical Processes	180,000
Grain Boundary Transport and Related Processes in Natural Fine-Grained Aggregates	146,285
New Method for Determining Thermodynamic Properties of Carbonate Solid-Solution Minerals	76,926
Investigation of Ultrasonic Wave Interactions with Fluid-Saturated Porous Rocks	61,895
Three-Dimensional Imaging of Drill Core Samples Using Synchrotron-Computed Microtomography	21,463
Thermodynamics of Minerals Stable Near the Earth's Surface	135,000

OFFICE OF ENERGY RESEARCH (Continued)

	FY 1993
Division of Advanced Energy Projects	$ 5,440,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 3,708,000
Metallic Multilayer and Thin Film Fabrication	270,000
Synthesis of New High Performance Lubricants and Solid Lubricants	218,000
Combustion Synthesis and Engineering of Nanoparticles for Electronic, Structural and Superconductor Applications	225,000
Creation and Destruction of C_{60} and Other Fullerene Solids	302,000
Synthesis and Properties of High Strength Nanolayered Composites	150,000
Optimally Controlled Interior Manipulation of Solids	329,000
Design of Materials with Photonic Band Gaps	314,000
High-Flux, Large-Area Carbon-Cluster Beams for Thin Film Deposition and Surface Modification	400,000
Novel Composite Coatings for High Temperature Friction and Wear Control	250,000
Synthesis of Advanced Composite Ceramic Precursor Powders by the Electric Dispersion Reactor	365,000
New Ion Exchange Materials for Environmental Restoration and Waste Management	435,000
Development of an Ion Replacement Electrorefining Method	450,000
Materials Properties, Behavior, Characterization or Test	$ 836,000
A Study of Potential High Band-Gap Photovoltaic Materials for a Two Step Photon Intermediate Technique in Fission Energy Conversion	317,000
Nonlinear Optics in Doped Fibers	363,000
Feasibility of a Novel Approach for Fast, Economical Determination of Radiation Damage in Nuclear Reactor Cores	156,000

OFFICE OF ENERGY RESEARCH (Continued)

	FY 1993
Division of Advanced Energy Projects (continued)	
Device or Component Fabrication, Behavior or Testing	$ 896,000
Ultrafast Molecular Electronic Devices	425,000
Photo-Induced Electron Transfer From a Conducting Polymer to Buckminsterfullerene: A Molecular Approach to High Efficiency Photovoltaic Cells	171,000
Superconducting Bitter Magnets	300,000
Office of Fusion Energy	$13,980,000
Materials Properties, Behavior, Characterization or Testing	$13,980,000
Structural Materials Development	545,000
Repair Welding of Fusion Reactor Components	98,000
Insulating Ceramics for Fusion	400,000
Modeling Irradiation Effects in Solids	66,000
Fusion Systems Materials	2,186,000
Structural Materials for Fusion Systems	1,991,000
Development of Radiation-Hardened Ceramic Composites for Fusion Applications	80,000
Radiation Effects and Micromechanics of SiC/SiC Composites	110,000
Damage Analysis and Fundamental Studies for Fusion Reactor Materials Development	199,000
Development of Lithium-Bearing Ceramic Materials for Tritium Breeding in Fusion Reactors	300,000
Post-Irradiation Examination of Lithium-Bearing Ceramic Materials for Tritium Breeding in Fusion Reactors	500,000
ITER Materials Development for Plasma Facing Components	2,200,000
ITER Structural Materials Development	750,000
ITER Ceramic Materials	530,000
Radiation Hardened Fiber Optics for ITER Fusion Diagnostic Systems	125,000
ITER Materials Evaluation	1,510,000

OFFICE OF ENERGY RESEARCH (Continued)

	FY 1993
Office of Fusion Energy (continued)	
Materials Properties, Behavior, Characterization or Testing (continued)	
ITER Structural Materials Evaluation	910,000
Development of Nb_3Sn Superconducting Wire for the ITER Magnet Program	500,000
Structural Materials Development for the Conduit of ITER Cable-in-Conduit-Conductors	980,000
Small Business Innovation Research Program	$25,404,146*
Materials Preparation, Synthesis, Deposition, Growth, or Forming	$9,577,109
Phase I Projects:	
Multi Layer, Quantum Well Layer Film Thermoelectrics	75,000
Indium Gallium Arsenide Thermophotovoltaic Energy Converters	67,820
Production of Carbon Materials from Biomass	74,929
Oxide Dispersion Strengthened Silver for Use in High-Temperature Superconductor Composite Wires	75,000
Lubricious-Surface Silicon-Nitride Rings for High-Temperature Tribological Applications	74,898
Room Temperature Photoluminescence of Germanium Nanostructures by High Energy Implantation of Germanium into a Buried Oxide of Silicon	74,927
Nanoscale Processing for Ternary Semiconductors	75,000
Low Temperature Deposition of Titanium Nitride	74,599

*Includes 64 new Phase I and 22 new Phase II projects initiated in FY 1993 and 20 Phase II projects initiated in FY 1992. The funding shown for each Phase II project is the total allocated for the duration of the project (up to two years).

OFFICE OF ENERGY RESEARCH (Continued)

	FY 1993
Small Business Innovation Research Program (continued)	
Materials Preparation, Synthesis, Deposition, Growth, or Forming (continued)	
Phase I Projects: (continued)	
Quantum Confinement Effects in Heteroepitaxial Silicon/Zinc Sulfide Nanostructures Produced by Metallo-Organic Chemical Vapor Deposition	74,788
Coated Micrograin Carbides for Wear Resistance	69,781
Composite Plasma-Polymer Membranes	74,969
Solid Polymer Electrolyte Membranes for Olefin Separation	75,000
Improved Coated-Metal Hydrogen Extraction Membranes	72,912
Zeolite Membranes for Gas Separations	75,000
A Vapor-Grown, Carbon Fiber-Reinforced Beryllium Composite for Plasma Facing Material	74,853
Methods of Improving Internal-Tin Niobium-Tin for Fusion Applications	74,982
Advanced Ultrasonic Methods for the Nondestructive Evaluation of Bond Quality in Brazed Composite-Metal Joints	74,974
High Thermal Conductivity Graphite for the International Thermonuclear Experimental Reactor First Wall	75,000
Highly Efficient, Heat-Dissipating, Functionally Gradient Plasma Facing Materials	74,936
Development of a Novel Brazing Material to Join Carbon-Carbon to Metals	74,999
Development of an Electrochemical Infiltration Method for Carbon-Carbon Composite Surface Preparation	74,998
Thermo-Mechanical Processing of Niobium Titanium Based Superconductors	75,000
Flexible Electrochromic Window Materials Based on Poly (Diphenyl Amine) and Related Conducting Polymers	74,976
Electrochromic Glazings Deposited by High Rate Processes	$75,000
Development of Advanced Window Materials Based on Conducting Polymer/Sol-Gel Ceramic Composites	75,000

OFFICE OF ENERGY RESEARCH (Continued)

	FY 1993
Small Business Innovation Research Program (continued)	
Materials Preparation, Synthesis, Deposition, Growth, or Forming (continued)	
Phase I Projects: (continued)	
Liquid Crystal Smart Windows	74,780
An Innovative Approach for the Formation of Silicon Carbide/Silicon Carbide Composites	74,959
Doping of Chemically Vapor Infiltrated Silicon Carbide to Enhance Thermal Conductivity	74,883
Phase II Projects: (First Year)	
Development of a Novel Reverse-Osmosis Membrane with High Rejections for Organic Compounds	499,911
Development of a Process to Synthesize Tubular Fullerenes	500,000
Continuous Production of Fullerenes from Hydrocarbon Precursors	500,000
Preparation of Low-Density Microcellular Materials from Fullerenes	500,000
New Gadolinium-Boron Compounds for Neutron Capture Therapy	500,000
Refractory Metal Coatings on Carbon/Carbon Composites for First Wall Applications	500,000
A Thermal Composite Plasma Facing Material	500,000
A Niobium-Tin Multifilamentary Composite Superconductor with Artificial Copper (Bronze) Inclusions	499,848
A Porous Metal Heat Exchanger Cooled Microwave Cavity	499,794
Development of Silicon Carbide Ceramic Composites for Fusion Reactor Applications	500,000
Radiation Damage Resistant Silicon for Particle Physics Detectors	500,000

OFFICE OF ENERGY RESEARCH (Continued)

	FY 1993
Small Business Innovation Research Program (continued)	
Phase II Projects: (Second Year)	
Graphite and Metal Oxide Catalyst Supports for Rechargeable Oxygen Electrodes	500,000
Development of Hollow-Fiber Modules for the Purification of Natural Gas	493,602
Inexpensive Pathways for the Synthesis of p-Boronophenylalanine and New Boron Containing Agents	500,000
An Improved Method of Introducing Additional Alloying Elements into Nb_3Sn in Internal-Tin Processes	499,991
Materials Properties, Behavior, Characterization or Testing	$4,644,510
Phase I Projects:	
In Situ Electrical Testing of Multicell Thermionic Fuel Elements	74,552
A Testing Process to Define Electrode Current Wear Mechanisms and Develop Improved Electrodes	75,000
Phase II Projects: (First Year)	
A Novel Energy-Efficient Membrane System for the Recovery of Volatile Organic Contaminants from Industrial Process Gases	499,931
Phase II Projects: (Second Year)	
Thermophotovoltaic Cogenerators for Advanced Integrated Appliances	499,737
Spontaneous Natural Gas Oxidative Dimerization Across Mixed Conducting Ceramic Membranes	499,996
A Membrane Process for Hot-Gas Cleanup and Decomposition of H_2S to Elemental Sulfur	499,425

OFFICE OF ENERGY RESEARCH (Continued)

	FY 1993
Small Business Innovation Research Program (continued)	
Materials Properties, Behavior, Characterization or Testing (continued)	
Phase II Projects: (Second Year) (continued)	
In Situ FT-IR Diagnostics for Coal Liquefaction Processes	499,675
Deep Hole Drilling in Refractory Metals Using Abrasive Waterjets	497,035
Improved Properties in Nb 46.5 Weight % Ti Materials for the SSC by Reducing the Separation Between Filaments	499,988
Multifilamentary Nb_3Sn Superconducting Wire Using APC, Composite Filaments with Improved High Field Performance	499,905
A Novel Joining Method for Graphite and Carbon-Carbon Composites	499,266
Device or Component Fabrication, Behavior, or Testing	$11,182,527
Phase I Projects:	
Glass-Ceramic Construction Tiles from Coal-Fired Boiler Flyash	74,886
Precision Machining of Integral Fast Reactor Metal Fuel Pins with Argon Cutting Jets	68,952
A High Repetition-Rate, High Power, All-Solid-State Pulsed Driver for Electrodeless Inductive Thrusters	74,940
Low Bandgap Thermophotovoltaic Devices for a General Purpose Heat Source	74,822
An Improved Carbonate Fuel Cell Design	74,972
On-Chip Ferroelectric Energy Storage Capacitors for Silicon Solar Cells	74,573
Porous Aluminum Nitride Part Fabrication to Support Advanced Battery Development	74,878
Capacitive Energy Storage Using High Surface Area Transition Metal Compounds	75,000
Molded Titanium Carbide Bipolar Plates for High Voltage Battery and Fuel Power Sources	74,978

OFFICE OF ENERGY RESEARCH (Continued)

	FY 1993
Small Business Innovation Research Program (continued)	
Device or Component Fabrication, Behavior, or Testing (continued)	
Phase I Projects: (continued)	
Jet Vapor Deposition of Ultra-thin Platinum Catalyst Loadings Directly on Polymer Ion-Exchange Membranes for Fuel Cell Applications	75,000
A Direct Thermal to Optical Energy Converter	74,918
Advanced Ceramic Fibers for a Carbonate Fuel Cell Matrix	74,960
A Novel Detector for X-ray Absorption Spectroscopy	75,000
An In Situ Particle Sensor for Metal Forming Processes	74,957
A High Count Rate Two-Dimensional Neutron Detector	74,639
A Wavelength Dispersive Spectrometer for Analytical Electron Microscopy	75,000
Development of a High Spatial Resolution Neutron Detector	75,000
A High Resolution Scintillator-Based Neutron Detector	75,000
High Energy Density Ceramic Capacitors for Uranium Atomic Vapor Laser Isotope Separation	75,000
Aluminum Nitride Copper Laser Tubes	75,000
On-Chip Infrared-Spectral Sensors by Superconducting Detector Arrays	74,717
On-Line Micro-Sensors for Analytical Chemical Measurement	74,949
Radiation Resistant Radio Frequency Feedthrough Insulators for Fusion Applications	75,000
Helium-Cooled Divertors with Low-Activation Materials and Simple Fabrication Techniques	74,990
Niobium-Tin Superconducting Wire with a Built-in Niobium Surface Coating to Limit Inter-Strand Eddy Currents in Cables	74,990
An Extended Interdigital Niobium Superconducting Linac Structure for Low Velocity Heavy Ions	74,925
Monolithically Integrated Detector Arrays	75,000
Diamond-Based Photomultipliers	75,000
Gallium Arsenide Pixel and Microstrip Detectors	69,755
Oxide-Based Ceramic Composite Hot Gas Filter Development	74,715

OFFICE OF ENERGY RESEARCH (Continued)

	FY 1993
Small Business Innovation Research Program (continued)	
Device or Component Fabrication, Behavior, or Testing (continued)	
Phase I Projects: (continued)	
Innovative Silicon Carbide Fiber Composite Filters	75,000
A Carbonate Fuel Cell Monolith for Low-Cost and High Power Density Operation	74,976
Fabrication of a Superconducting Super Collider Dipole Magnet Bore Tube Liner from Copper-Niobium Nanocomposite Produced by Mechanical Alloying	74,984
Phase II Projects: (First Year)	
Digital Processing Electronics for X-ray Detector Arrays	500,000
A Cold/Thermal Beam Bender Using Capillary Optics to Increase the Number of End-Guide Instrument Positions	474,458
A Thomson-Scattering Plasma Diagnostic for Materials Testing and Divertor Concept Testing	500,000
Eddy-Current Nondestructive Testing Methods for On-Line Detection of Cable Manufacturing Defects	499,996
Low-Cost Microstrip Detectors on Conductivity-Modified Polyimide	499,938
High Strength Mono- and Multi-filament High Temperature Superconductors for High Field Applications	499,988
Fabrication of Niobium-Aluminum Superconducting Strands Using Mechanical Alloying and Other Techniques	499,962
Durable, Low Cost Ceramic Materials for Use in Hot Gas Filtration Equipment	493,071
High Cation Mobility Lithium Polymer Batteries	499,968
A Real-Time X-ray Detector	500,000

OFFICE OF ENERGY RESEARCH (Continued)

	FY 1993
Small Business Innovation Research Program (continued)	
Device or Component Fabrication, Behavior, or Testing (continued)	
Phase II Projects: (Second Year)	
Metal Hydride Refrigerators	499,935
A Catalytic Membrane Reactor for Facilitating the Water-Gas Shift Reaction at High Temperature	492,117
A Single Manifold, Radial Flow, Solid Oxide Fuel Cell	499,402
Ceramic/Metal Elements for MHD Sidewalls	499,991
Fabrication of Tungsten and Tungsten-Molybdenum Alloy Tubing	498,555
A Distributed Fiber Optic Sensor for Reversible Detection of Atmospheric CO_2	499,954
An Electron Bombarded Semiconductor Device	499,756
Silicon Junction Diode Absolute Radiometers for Plasma Diagnostics in the Soft X-ray and Vacuum Ultraviolet Spectral Region	263,960

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; Division of Advanced Energy Projects; and Division of Chemical Sciences

- **Office of Health and Environmental Research**: Division of Physical and Technology Research

- **Office of Fusion Energy**

Materials research is carried out through the DOE national laboratories, other federal laboratories, grants to universities, and grants to 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 strategic materials research 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 Laboratory, Lawrence Livermore National Laboratory, Los Alamos National Laboratory, Pacific Northwest Laboratory and the Sandia 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, 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. Ames Laboratory and the Stanford Synchrotron Radiation Laboratory are funded by the Division of Materials Sciences and the Division of Chemical Sciences.

In addition, the Division of Materials Sciences also funds a program, which consisted of 45 investigators in FY 1993, at the Frederick Seitz Materials Research Laboratory at the University of Illinois. The Laboratory is also funded by the National Science Foundation and the State of Illinois.

Advanced materials preparation and characterization capabilities are available to academic and industrial researchers at 14 major user centers located at several of the multipurpose and special purpose laboratories. These user facilities are funded by the Division of Materials Sciences and the Division of Chemical Sciences.

Basic Energy Sciences contributes to the advancement of economic and competitive U.S. industry through Cooperative Research and Development Agreements (CRADAs), Small Business Innovation Research awards (SBIRs), use of the major user centers by industrial researchers, informal collaborations, direct research grants, and training of students. As of March 1994, 96 CRADAs involving about 60 companies originated in work sponsored by the Office of Basic Energy Sciences at the national laboratories. Industrial researchers are among the major users of advanced characterization facilities. During FY 1993, among the 4,367 scientists who conducted X-ray and neutron beam experiments at Basic Energy Sciences-supported user facilities, there were 597 industrial scientists from 89 U.S. companies. Support for research and development on new energy-related materials, processes and instrumentation by small businesses is funded through the Small Business Innovation Research Program, which is administered through the Division of Advanced Energy Projects. This program funded 168 Phase I projects in FY 1993.

Division of Materials Sciences

The largest portion of the strategic, materials-related research program in DOE is located in the Division of Materials Sciences. The program incorporates the full range of materials science, including efforts in high-temperature superconductors, radiation effects, synthesis and processing, computation and theory, nonequilibrium and artificially structured materials, interfacial structure and dynamics, materials reliability and life prediction, semiconducting and photovoltaic materials, polymeric materials, magnetic materials, ceramic materials, and metals and alloys. The operating funds for FY 1993 for the Division of Materials Sciences were $267,140,000. These funds were allocated to 472 projects.

A goal of the program is to increase the understanding of materials properties, behavior, and phenomena in those classes of materials that are or might be important to the mission of the Department of Energy. Research sponsored by the Division of Materials Sciences is conducted by metallurgists, ceramists, solid state physicists, and materials chemists in 127 different institutions, including DOE laboratories, universities, and to a lesser extent at industrial laboratories. Some of the materials research has a specific relationship to identified energy technologies (e.g., photovoltaic phenomena for solar energy conversion, fast-ion diffusion for solid electrolytes in fuel cells and batteries); some is related to many energy technologies simultaneously (e.g., hydrogen embrittlement, corrosion, intermetallic alloys, high temperature structural metals and ceramics); and some is important to fundamental understanding of new experimental or theoretical research tools. Finally, through a substantial number (237 in FY 1993) of research grants to universities, the Division of Materials Sciences fosters the training of new scientific and technical personnel for academia, national laboratories, and industry.

A collaborative thrust on critical problems relevant to the synthesis and processing of advanced materials is fostered through the Center for Excellence in Synthesis and Processing of Advanced Materials. The Center consists of 12 Department of Energy Laboratories encompassing a diversity of unique and highly relevant professional skills, facilities, and instruments. The management of the Center has focussed on multi-institutional interaction and collaboration amongst its member institutions as well as numerous partnerships with industry and academia. Special objectives of the Center are: (1) to develop synthesis and processing methodologies to control structure, and thereby materials properties, from atomic to the macroscopic scale; (2) to discover and develop high-payoff, advanced materials; and (3) to reduce the time span and cost, with attention to environmental and energy concerns, for materials commercialization by integrating synthesis and processing collaboration between the Department of Energy technologists and industry.

A second goal of the program is the development of new forefront analytical instruments and facilities that are used to probe the structure and behavior of matter. Through the operation of 13 major user centers, this program carries a major responsibility for many of the nation's premier research facilities. These facilities include three neutron sources, two synchrotron radiation sources, processing facilities, and four centers for electron beam microcharacterization.

A new synchrotron source, the 1-2 GeV Advanced Light Source (ALS) at Lawrence Berkeley Laboratory, was commissioned in FY 1993. A second major synchrotron radiation facility is under construction, the 6-7 GeV Advanced Photo Source (APS) at Argonne National Laboratory. The APS is scheduled for completion in FY 1997. This machine will provide the brightest source of photons in the hard X-ray region.

The material sciences research of the Division of Materials Sciences is grouped into three subprograms:

- Metallurgy and Ceramics seeks to understand the synergistic relationship between synthesis, processing, structure, properties, and behavioral parameters of materials.

- Solid State Physics is concerned with understanding the interactions of electrons, atoms, and defects and their role in determining the structure and properties of condensed matter.

- Materials Chemistry focuses on understanding the chemical properties of materials and their relationship to composition, structure, and specimen environment.

For information about specific programs the appropriate DOE staff listed below may be contacted by calling (301) 903-3427. The reader also is referred to DOE publication Materials Sciences Programs Fiscal Year 1993 (DOE/ER-0612P dated February 1994). This publication contains summaries of all funded programs, summaries of Small Business Innovation Research programs; and descriptions of major user facilities and other user facilities. Limited copies may be obtained by calling (301) 903-3427.

NAME	PROGRAM AREA
Iran L. Thomas	Director, ER-13
Environment, Safety and Health, ER-13	
Albert E. Evans	
Michael F. Teresinski	
Metallurgy and Ceramics Branch, ER-131	
Robert J. Gottschall	Electron Beam, Microcharacterization, Facilities
Otto Buck	Mechanical Behavior, NDE
Alan L. Dragoo	Ceramics
Joseph B. Darby, Jr.*	Physical Metallurgy
John N. Mundy	Physical Behavior, Irradiation Effects

*Retired as of December 30, 1993

NAME	PROGRAM AREA
Yok Chen	Physical Behavior, Irradiation Effects
Michael E. Kassner	Mechanical Behavior
Helen M. Kerch	Microstructure, Processing
Solid State Physics and Materials Chemistry Branch, ER-132	
William T. Oosterhuis	Neutron and X-ray Facilities
Richard D. Kelley	Materials Chemistry, Polymers, Surface Science
Jerry J. Smith	Solid State Physics, Surface Science
Manfred Leiser	Solid State Theory
Harold L. Davis	Solid State and Surface Theory
Douglas K. Finnemore	Solid State Physics, Superconductivity, Magnetism

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 1993 for materials-related programs was $5,320,000 and was allocated to 41 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. 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, bifunctional air electrodes, 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, zinc 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 appropriate DOE staff listed below may be contacted by calling (301) 903-5904. The reader also is referred to DOE publication Summaries of FY 1993 Research in the Chemical Sciences (DOE/ER-0411/11 dated August 1993) 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 the telephone number given above.

NAME	PROGRAM AREA
Robert S. Marianelli	Director, Facilities Operations
Steven G. Barnhart	Advanced Battery Program
Environmental Safety and Health	
Sat Goel	
Ted Tomczak	
Fundamental Interactions	
Allan H. Laufer	Chief
Mary E. Gress	Photochemical and Radiation Sources
William H. Kirchhoff	Chemical Physics
J. V. Martinez	Atomic Physics
Processes and Techniques	
F. Dee Stevenson	Chief, Chemical Engineering
Stephen A. Butter	Chemical Energy
William S. Millman	Chemical Energy
John L. Burnett	Separations and Analysis
Harry J. Dewey	Separations and Analysis
John L. Burnett	Heavy Element Chemistry

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

177. Bounds on Dynamic Plastic Deformation — FY 1993 $137,000

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

178. In-Flight Measurement of the Temperature of Small, High Velocity Particles

FY 1993
$493,000

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, Idaho National Engineering Lab).

Keywords: Plasma Processing, Particle/Plasma Interaction

179. Intelligent Control of Thermal Processes

FY 1993
$530,000

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

180. Multivariable Control of the Gas-Metal/Arc Welding Process | FY 1993 | $158,000

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

181. Metal Transfer in Gas-Metal Arc Welding FY 1993
$122,300

DOE Contact: Oscar P. Manley, (301) 903-5822
MIT Contact: 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

182. Modeling and Analysis of Surface Cracks FY 1993
$196,000

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

183. Thermal Plasma Processing of Materials

FY 1993
$141,928

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

184. Transport Properties of Disordered Porous Media from the Microstructure

FY 1993
$205,892

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

185. Inelastic Deformation and Damage at High Temperature FY 1993 $134,000

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

186. Energy Changes in Transforming Solids FY 1993 $175,000

DOE Contact: Oscar P. Manley, (301) 903-5822
Stanford University Contacts: George Herrmann, David M. Barnett, (415) 723-4143

Heterogenization techniques developed with DOE support. The methods have been extended to provide a number of universal formulae valid for the average stresses between two holes or inclusions, for inclusions with imperfect interfaces, and for stresses in cylindrical and plane layered media. A new methodology to establish conservation laws for dissipative systems has been advanced, and a theory of stressed solids prone to damage has been formulated based on the Gibbs free energy.

Another portion of our research has as its objective the development of further understanding of subsonic and supersonic surface waves and interfacial and bulk waves in anisotropic linear elastic solids. New investigations of so-called "generalized surface waves" and Stoneley waves in pre-stressed anisotropic bimaterials have also been undertaken.

Keywords: Stress Analysis, Materials Science

187. Stress Induced Phase Transformations

FY 1993
$66,169

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

188. Optical Techniques for Superconductor Characterization

FY 1993
$285,500

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

189. Effective Elastic Properties and Constitutive Equations for Brittle Solids Under Compression

FY 1993
$59,798

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 cracks 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

190. Investigation of PACVD Protective Coating Process Using Advanced Diagnostic Techniques

FY 1993
$0

DOE Contact: Oscar P. Manley, (301) 903-5822
United Technologies Research Center Contact: W. C. Roman, (203) 727-7590

The research objective is the comprehensive experimental investigation of the fundamental nonequilibrium reactive plasma assisted chemical vapor deposition (PACVD) process as applied to hard face coatings (e.g., TiB_2 or diamond). Nonintrusive laser diagnostics (e.g., laser induced fluorescence (LIF) and coherent anti-Stokes Raman spectroscopy (CARS) are being used to probe gas phase species, concentrations and rotational temperatures *in situ*. Detailed coating characterization is accomplished using Auger, Ion Scattering and secondary ion mass spectroscopies (AES, ISS and SIMS) and complementary techniques. In addition, coating characteristics such as smoothness, adhesion (UTRC custom built pin-on-disc apparatus) and hardness (state-of-the-art nanoindenter apparatus) are measured. Gas phase spectroscopy is interpreted through chemical kinetic modelling and will be correlated to coating characteristics thus providing a predictive capability that is severely lacking in the present science base of advanced protective coatings.

Keywords: Coatings, Plasma Diagnostics

191. Elastic-Plastic Fracture Analysis Emphasis on Surface Flaws FY 1993 $430,000

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

192. Continuous Damage Mechanics - Critical States

FY 1993
$60,000

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: (a) response of microcrack weakened solids in the vicinity of the critical state, and (b) 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

193. Thin Film Characterization and Flaw Detection

FY 1993
$89,450

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

194. Development of Measurement Capabilities for the Thermophysical Properties of Energy-Related Fluids

FY 1993
$551,000

DOE Contact: Oscar P. Manley, (301) 903-5822
National Institute of Standards and Technology Contact: 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

195. Flux Flow, Pinning and Resistive Behavior in Superconducting Networks

FY 1993
$69,500

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

196. An Investigation of the Effects of History Dependent Damage in Time Dependent Fracture Mechanics — FY 1993 $94,027

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

197. Mixing and Settling in Continuous Metal Production FY 1993 $135,000

DOE Contact: Oscar P. Manley, (301) 903-5822
Dartmouth College Contact: H. Richter, (603) 646-2707

For reasons of both energy conservation and environmental protection, tonnage oxygen has become an essential component in many ferrous and nonferrous smelting and refining operations. Innovative reactors such as the QSL converter for direct lead bullion production are also suitable for direct coppermaking and a modification of the reactor is also very attractive for steelmaking.

The research objectives of the work are, to learn about the behavior of gas and particulate matter in turbulent liquids, the nature and paths of liquids and particulate entrainment into the plumes, and separation phenomena including travel to and behavior in the settling zones. Such knowledge is of fundamental value in designing reactors for continuous, direct metalmaking.

The new information will predict bath mixing, heat and mass transfer and settling parameters under the variety of operating conditions which will prevail in continuous, direct metalmaking oxygen reactors of the future. Therefore, it is proposed to study gas injection through submerged injectors, and also particulate addition from above, into a liquid bath consisting of two immiscible layers of liquids having roughly the same viscosities as slag and matte or metal and with roughly comparable density ratios.

Keywords: Bath Mixing, Heat and Mass Transfer, Settling

198. Application of Magnetomechanical Hysteresis Modelling to Magnetic Techniques for Monitoring Neutron Embrittlement and Biaxial Stress FY 1993 $99,912

DOE Contact: Oscar P. Manley, (301) 903-5822
Southwest Research Institute Contact: M. Sablik, (512) 522-3342

The project objective is to study the effects of neutron embrittlement and biaxial stress on signals from various magnetic measurement techniques in steels. It is expected that interaction between experiment and modeling will lead to design of efficient magnetic measurement procedures for monitoring neutron embrittlement and biaxial stress. Project research is important for safety monitoring in the nuclear power and gas industries.

Magnetic measurement techniques to be assessed are: (1) magnetic hysteresis loop measurement of properties like coercivity and permeability; (2) magabsorption, which measures the impedance of an rf coil brought close to a magnetic sample; (3) Barkhausen noise analysis; (4) magnetically induced velocity change (MIVC) of an ultrasonic wave; and (5) harmonic analysis of an ac magnetic hysteresis loon. The model of Sablik *et al* for magnetic hysteresis and uniaxial stress effects on magnetic properties will be extended to conditions of biaxial stress and neutron embrittlement. The effects of these conditions on magnetic probe signals (1)-(5) will be modeled and compared to experiment. In the case of neutron embrittlement, measurements will be made on steel samples characterized by Charpy tests after previous exposure to various neutron fluences.

Keywords: Magnetic NDE Techniques, Neutron Embrittlement, Biaxial Stress

199. <u>Stability and Stress Analysis of Surface Morphology of Elastic and Piezoelectric Materials</u> <u>FY 1993</u>
$96,665

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

200. Micromechanical Viscoplastic Stress-Strain Model with Grain Boundary Sliding

FY 1993
$50,000

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 also 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

201. Micromechanical Viscoplastic Stress-Strain Model with Grain Boundary Sliding

FY 1993
$48,000

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

202. Modeling of Thermal Plasma Processes FY 1993
$232,000

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

203. Nondestructive Evaluation of Superconductors FY 1993
$200,000

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

204. Heat Transfer to Viscoelastic Fluids FY 1993
$79,980

DOE Contact: Oscar P. Manley, (301) 903-5822
University of Illinois at Chicago Contact: J. P. Hartnett, (312) 966-4490

The goal of the research is to study the fluid mechanical and heat transfer behavior of viscoelastic aqueous polymer solutions. The ultimate objective is to provide a basis for predicting the performance of such fluids.

Recent studies of the heat transfer performance of viscoelastic aqueous polymer solutions have been directed to the pool boiling behavior of such solutions. The heat transfer coefficients of aqueous hydroxyethy cellulose (Natrosol) solution boiling on horizontal wires were found to be considerably higher than the values found for water alone, whereas the pool boiling performance of other polymer solutions (including polyacrylamide solutions) was inferior to that of water. A distinguishing characteristic of the Natrosol solutions is their lower surface tension values. Accordingly an investigation of the influence of two different surfactants (i.e., agents which reduce surface tension) on the pool boiling behavior of aqueous polyacrylide solutions was carried out. When the surfactant polyoxyethylene sorbitan monoleate (Tween 80) was added to the aqueous polyacrylamide solution the surface tension decreased by 10 to 20 percent but the boiling performance was not affected. In contrast, the presence of sodium lauryl sulfate (SLS) resulted in a similar decrease in surface tension but a significant increase in the boiling heat transfer coefficient was recorded relative to the pool boiling performance of deionized water. On the basis of these experimental results it can be concluded that lowering the surface tension of an aqueous polymer solution does not guarantee enhancement of the boiling heat transfer performance.

Keywords: Heat Transfer, Aqueous Polymer Solutions

205. Pulse Propagation in Inhomogeneous Optical Waveguides FY 1993 $83,537

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

206. Low Resistivity Ohmic Contacts Between Semiconductors and High-T_c Superconductors FY 1993 $0

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

207. The Evolution of a Hele-Shaw Interface and Related Problems in Dendritic Crystal Growth

FY 1993
$66,116

DOE Contact: Oscar P. Manley, (301) 903-5822
Ohio State University Contact: S. Tanveer, (614) 292-4972

A cell consisting of two parallel plates separated by a thin layer of liquid, the so-called Hele-Shaw cell, serves as a model of a porous medium. For example, one can readily observe the displacement of a more viscous fluid by a less viscous one, such as is taken advantage of in secondary oil recovery methods.

Most mathematical models of the displacement process studied to date have dealt with steady states and their stability. Under those conditions solutions can be obtained even if the surface tension at the interface between the two fluids is ignored. As to the initial value problem, it has been found that ignoring surface tension leads to an ill-posed problem in the sense that nonphysical cusps form at the interface in a finite time. Experimentally it is found that when the surface tension is small no steady state is reached and the interface continues to deform into a finer and finer fractal-like structure.

Recent work by the proposer has revealed that it is possible to imbed the ill-posed problem into a well-posed one so as to clarify what happens when the surface tension tends to zero. For the proposed research detailed calculations will be carried out to examine how the singularities in the model equations are related to the evolution of the shape of the interface. Second, the results obtained for the Hele-Shaw cell will be extended to study the time evolution of the surface of a growing crystal with dendrites. Third, statistics of the observed patterns will be related to the statistical distribution of singularities in the model equations. Next, more general boundary conditions will be considered to conform to a broader class of physically realistic situations. Finally, some intrinsically nonlinear aspects of dendritic growth will be examined.

Keywords: Crystal Growth, Dendrites

208. Degenerate Four-Wave Mixing as a Diagnostic of Plasma Chemistry FY 1993 $95,328

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

209. Effect of Forced and Natural Convection on Solidification of Binary Mixtures FY 1993 $93,290

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_4 Cl-H_2O) systems.

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

Geosciences Research

Materials Preparation, Synthesis, Deposition, Growth or Forming

210. An Investigation of Mineral Hydrolysis Kinetics — FY 1993 $226,000

DOE Contact: W. C. Luth, (301) 903-5822
SNL Contact: Henry R. Westrich, (505) 844-9092, R. T. Cygan, G. W. Arnold and W. H. Casey

Objectives of this research are to provide a fundamental understanding of aqueous dissolution of simple silicate minerals by measurement of their dissolution kinetics, chemical and structural characterization of their reacted surfaces, and simulation of the mineral-surface interface. Dissolution rates of end member and mixed-cation orthosilicate minerals were examined as a function of pH and temperature. Dissolution rates of compositionally distinct orthosilicates correlate well with water exchange rates around the corresponding divalent cation. Structural and chemical characterization of acid-reacted single crystals and powders was done with electron (SEM/TEM) and ion beam (ERD/RBS) techniques, as well as with vibrational (Raman) spectroscopy demonstrate dissolution of intact silicate tetrahedra. Protonation and hydration of metal-oxygen bonds on the acid-reacted mineral surface apparently control both the pH- and temperature- dependencies of mineral dissolution rates.

Keywords: Dissolution Kinetics, Orthosilicate Minerals

211. Transition Metal Catalysis in the Generation of Petroleum and Natural Gas

FY 1993
$101,209

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 digenesis, can be proposed as catalysts in the generation of light hydrocarbons. Transition metal-rich kerogeneous sedimentary rocks were reacted under reducing conditions at temperatures for which the substrates alone, *N*-octadecene + hydrogen, are stable indefinitely. Catalytic activity was measured to be on the order of 10^{-7} g CH_4/d/g kerogen, suggesting robust catalytic activity over geologic time at moderate sedimentary temperatures.

Keywords: Transition Metals, Catalysis, Petroleum

Materials Structure and Composition

212. Infrared Spectroscopy and Hydrogen Isotope Geochemistry of Hydrous Silicate Glasses

FY 1993
$104,517

DOE Contact: W. C. Luth, (301) 903-5822
Caltech Contact: 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, Hydrogen Isotopes, Silicate Glasses, Oxygen Diffusion

213. Crystal Chemistry of Hydroxyl and Water in Silicate Minerals — FY 1993 $80,448

DOE Contact: W. C. Luth, (301) 903-5822
University of Colorado Contact: Joseph R. Smyth, (303) 492-5521

Hydrogen in the form of hydroxyl and molecular water plays an important role in the chemical and physical properties of silicate minerals. The stability of hydroxyl-bearing silicates such as omphacite, wadsleyite (beta-Mg_2SiO_4), rutile, and stishovite may control magma generation in the mantle; the hydration and cation exchange kinetics of various cation-substituted zeolites may control sorption and migration of cations and radionuclides. Mechanisms of hydroxyl incorporation in these phases are being investigated with IR, X-ray and neutron crystallographic methods. Experiments on natural zeolites show that alkalis Na, K, and Cs exchange much faster than the alkaline earths Ca, Sr and Ba. These data are being incorporated in calculations of electrostatic site potentials to generate a predictive model for temperature-dependence of hydrogen and oxygen isotope substitution.

Keywords: Silicate Minerals, Hydroxyl, Water, Infrared Spectroscopy, Crystal Chemistry, Isotopic Substitution

214. Zircons and Fluids: An Experimental Investigation with Applications for Radioactive Waste Storage — FY 1993 $28,167

DOE Contact: W. C. Luth, (301) 903-5822
VPI Contact: A. K. Sinha, (703) 231-5580

The research objective is to develop a predictive correlation between the physical and chemical (including uranium-lead isotopic studies) stability of ZrSiO4 (zircon) and metamictization (alpha damage) for its consideration as a host for high-level radioactive waste. A model was developed from elasticity theory to describe the state of stress in idealized metamict zircons. For a zircon with a metamict core and undamaged outer shells, the model predicts that the normal stresses will be compressional and tangential stresses will be extensional in the outer shells, potentially resulting in radial fractures. Alternatively, zircon with a metamict rim and an undamaged core may develop concentric fractures. Stress gradients across damaged and undamaged areas may be sufficient to cause both radial and concentric fractures. Such potential fracture mechanisms would provide easy pathways for fluids and increase the surface area for fluid-solid reactions. Natural zircons are being analyzed for such stress-induced fractures and the enhanced permeability and porosity that may accompany such a process.

Keywords: Zircon, Metamict Behavior, Irradiation Damage

215. High-Resolution Transmission Electron Microscopy/Analytical Electron Microscopy and Scanning Electron Microscopy Study of Fluid-Rock Interactions: Interaction of Copper-, Silver-, Selenium-, Chromium-, and Cadmium-Bearing Solutions with Geological Materials at Near-Surface Conditions, with an Emphasis on Phyllosilicates

FY 1993
$137,893

DOE Contact: W. C. Luth, (301) 903-5822
Johns Hopkins University Contact: D. R. Veblen, (410) 516-8487
Lehigh University Contact: E. S. Ilton, (215) 758-5834

Oxidation-reduction reactions at the mineral-fluid interface can be responsible for the attenuation or mobilization of multivalent elements in the near-surface environment. This project involves investigation of the interaction of silver-, copper-, selenium (Se^{4+} and Se^{6+})-, and chromium (Cr^{6+})-bearing solutions with ferrous phyllosilicates such as biotite, a potential reducing agent, under both oxic and anoxic conditions. The objectives of the experimental work are to examine the surfaces and interior portions of the reacted phyllosilicates with TEM, analytical electron microscopy, scanning electron microscopy, and X-ray photoelectron spectroscopy (XPS). The combination of these techniques will help to determine the oxidation state and form of the sorbed species. This information provides constraints on the physical and chemical conditions that are required for mobilization or attenuation of these elements by or from phyllosilicates.

Keywords: Surface Reactions, High-Resolution Transmission Electron Microscopy, Oxidation-Reduction, Phyllosilicates

Materials Properties, Behavior, Characterization or Testing

216. Cation Diffusion Rates in Selected Silicate Minerals

FY 1993
$174,000

DOE Contact: W. C. Luth, (301) 903-5822
Sandia National Laboratory Contact: Randall T. Cygan, (505) 844-7216; H. R. Westreich, (505) 844-9092 and Craig S. Schwandt, (505) 844-7216

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 pyrone for relatively reducing conditions.

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

217. Shear Strain Localization and Fracture Evolution in Rocks — FY 1993 $75,443

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 the evolution of typical fault zones.

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

218. Poroelasticity of Rock — FY 1993 $250,406

DOE contact: W. C. Luth, (301) 903-5822
LLNL contact: B. P. Bonner, (510) 422-7080
University of Wisconsin contact: H. F. Wang, (608) 262-5932

The objective of this project is to improve treatment of poroelastic problems involving the coupled processes of deformation and fluid flow by obtaining improved theoretical estimates of the poroelastic coefficients and by performing experiments designed to test and extend the theory. The dynamic elastic constants, pore pressure buildup (Skemptons) coefficient, permeability, and low-frequency shear modulus and attenuation have all been measured for synthetic sandstones (prepared from glass beads) for comparison with natural sandstones. The theoretical component of the project led to an extension of the effective pressure law for permeability. By combining theoretical estimates and experimental data for the bulk modulus of the synthetic sandstones, it was demonstrated that a theory sensitive to microstructure can predict the modulus reduction to porosities of 40 percent.

Keywords: Poroelasticity, Coupled Processes, Deformation, Fluid Flow, Permeability

219. Oxygen and Cation Diffusion in Oxide Materials — FY 1993 $150,000

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

220. Modification of Fracture Transport Properties of Rocks by Mechanical and Chemical Processes — FY 1993 $180,000

DOE Contact: W. C. Luth, (301) 903-5822
LLNL Contact: W. B. Durham, (510) 422-7046 and B. P. Bonner, (510) 422-7080

This project aims to understand the hydraulic and mechanical properties of individual fractures in crustal rock and identify processes by which joints are modified or resist modification over long time scales. Detailed study of Westerly granite show that when joints are well mated, the application of confining pressures to 160 MPa is sufficient to close the joint hydraulically; however if there is a small lateral offset across the joint, it remains open. For both kinds of joints, increasing pressure reduces permeability more than expected because increasing wall-to-wall contacts lead to more tortuous flow paths and lower flow rates. Existing models have been unsatisfactory in fitting the observations, especially at low values of mean aperture. A modified effective medium theory model is being formulated that will allow percolation (i.e., water flow through the joint) where wall-to-wall contact areas exceed 50 percent of the total area, the upper limit for flow predicted by conventional models.

Keywords: Fluid Flow, Fractures

221. Grain Boundary Transport and Related Processes in Natural Fine-Grained Aggregates

FY 1993
$146,285

DOE Contact: W. C. Luth, (301) 903-5822
Brown University Contact: R. A. Yund, (401) 863-1931 and J. R. Farver, (401) 863-1931

The objective of this study is the direct measure of diffusional transport rates in rocks and how the rates vary with mineralogy and microstructure, as well as temperature and pressure. The results provide much needed data on the nature of grain boundaries in rocks and the rate of transport of chemical components through rocks. Grain boundary diffusion of oxygen and cations in monomineralic aggregates of feldspar and of calcite, and aggregates of feldspar plus quartz were determined with the ion microprobe (SIMS). Calcium grain boundary diffusion rates in Ca-rich feldspar aggregates are several orders of magnitude slower than oxygen, and than potassium in K-rich feldspar. This suggests that differences in size and formal charge of chemical species may play an important role in their relative grain boundary diffusion rates. TEM analysis of microstructures suggests that the equilibrium distribution of water in feldspar aggregates is that of isolated pockets. Studies continue in order to evaluate the role of pressure and nonhydrostatic stresses on fluid-feldspar interfacial energies and microstructures.

Keywords: Diffusion, Rocks, Quartz, Feldspar, Microstructures

222. New Method for Determining Thermodynamic Properties of Carbonate Solid-Solution Minerals

FY 1993
$76,926

DOE Contact: W. C. Luth, (301) 803-5822
UC Davis Contact: P. A. Rock, (916) 752-0940 and W. E. Casey, (916) 752-3211

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

Keywords: Carbonate Minerals, Solubility, Electrochemical Cell, Infrared Spectroscopy, Silicate Minerals, Glasses, Silicate Liquids, Speciation

223. Investigation of Ultrasonic Wave Interactions with Fluid-Saturated Porous Rocks

FY 1993
$61,895

DOE Contact: W. C. Luth, (301) 903-5822
Ohio State University Contact: L. Adler and P.B. Nagy, (614) 292-1974

The research involves the investigation of ultrasonic wave propagation over a wide frequency range in fluid-saturated porous materials. Two new techniques, based on direct generation of surface waves by edge excitation, are being developed for the inspection of highly permeable natural rocks:

(1) Low-frequency (100 to 500 kHz) shear transducers were used to launch and receive the ultrasonic surface wave. With this technique, Rayleigh-type surface modes were generated on the free surface of both dry and water-saturated specimens.

(2) Ultrasonic waves transmitted through air-filled porous plates were used to study the frequency-dependent propagation of slow compressional waves in porous materials.

An interferometric technique for noncontact detection of ultrasonic vibrations on diffusely reflecting rough surfaces provides clear evidence of propagation of the new slow surface mode on the free surface of a fluid-saturated porous solid when the pores are closed at the surface by capillary forces.

Keywords: Porous Materials, Surface Waves, Ultrasonic Wave Propagation

224. Three-Dimensional Imaging of Drill Core Samples Using Synchrotron-Computed Microtomography

FY 1993
$21,463

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

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

225. Thermodynamics of Minerals Stable Near the Earth's Surface — FY 1993 $135,000

DOE Contact: W. C. Luth, (301) 903-5822
Princeton University: A. Navrotsky, (609) 258-4674

The purpose of this work is to expand our database 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

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 definition and, therefore, beyond the scope of ongoing 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 have applications that may span several disciplines or technical areas.

The Division provides a mechanism for converting basic research findings to applications that eventually 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

226. Metallic Multilayer and Thin Film Fabrication

FY 1993
$270,000

DOE Contact: Walter M. Polansky, (301) 903-5995
Lawrence Berkeley Laboratory Contact: Ian G. Brown, (415) 486-4174

The application of pulsed metal plasma gun techniques to the fabrication of metallic superlattices, multilayers and thin films will be investigated. Multilayer structures will be synthesized that are of relevance to X-ray optical devices, to magnetic and magneto-optical recording media, and to the fabrication of high temperature superconducting thin films. The quality and characteristics of the thin film structures formed in this way will be explored. This means of fabrication of metallic multilayer systems is new and has not yet been examined except in preliminary testing at this laboratory. At the same time, interest in artificial metallic superlattices from a fundamental scientific perspective, and in metallic multilayer structures from the standpoint of applied technology, is growing rapidly. It is important to explore and develop the application of this new technique to these fields. The proposed program will make immediate application of the method within the three fields mentioned above (X-ray optics, magneto-optics and superconducting thin films) via collaborations with materials science research groups at this laboratory.

Keywords: Thin Films, Plasma Gun

227. Synthesis of New High Performance Lubricants and Solid Lubricants

FY 1993
$218,000

DOE Contact: Walter M. Polansky, (301) 903-5995
University of Texas Contact: Richard J. Lagow, (512) 471-1032

Work will be conducted on the synthesis and characterization of perfluoropolyethers, an extraordinary class of high performance lubricants, by a relatively new technique, direct fluorination, which is emerging as the best way to prepare perfluoropolyethers. Many new and important classes of perfluoropolyethers will be prepared with very significant potential as lubricants. Currently the highest obtainable molecular weight perfluoropolyether synthesized using conventional polymerization processes is 50,000. This fluid with a molecular weight of 50,000 has a viscous syrup-like consistency. High molecular weight solids with a perfluoropolyether backbone have not been attained using methods other than direct fluorination technology. There exists now the capability to synthesize perfluoropolyethers with molecular weights over 1,000,000. Thus solid perfluoropolyether lubricants are accessible for the first time. A feature of direct fluorination technology where hydrocarbon structures are converted to fluorocarbon structures is that the organic precursors are converted to fluorocarbon fluids and solids without substantial cross-linking and without increases or decreases in degree of polymerization. The synthesis of hydrocarbon polymers as starting materials has many other advantages and introduces great flexibility and capabilities not attainable using polymerization processes with various perfluorinated ethylene oxides. Work will be done on many generic classes of solid fluorocarbon lubricants. The capability to make perfluoropolyethers soluble (miscible) with less expensive hydrocarbon lubricants and poly alpha olefins has recently been developed. One of the most important and promising prospects of this research is the synthesis of chlorinated perfluoropolyether fluids which are very compatible and soluble in hydrocarbons offering potential as high performance lubrication additives.

Keywords: Lubricants, Fluorination

228. Combustion Synthesis and Engineering of Nanoparticles for Electronic, Structural and Superconductor Applications — FY 1993 $225,000

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

229. Creation and Destruction of C_{60} and Other Fullerene Solids — FY 1993 $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 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

230. Synthesis and Properties of High Strength Nanolayered Composites — FY 1993 $150,000

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

231. Optimally Controlled Interior Manipulation of Solids — FY 1993 $329,000

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

232. Design of Materials with Photonic Band Gaps — FY 1993 $314,000

DOE Contact: Walter M. Polansky, (301) 903-5995
Ames Laboratory Contact: Kai-Ming Ho, (515) 294-1960

This project is intended to design, fabricate and characterize a new class of composite materials which possess forbidden ranges of frequencies, in which electromagnetic waves cannot propagate in any direction. These materials are called "photonic crystals" and the forbidden frequencies are called "photonic gaps" and they can be regarded as photonic analogues of electronic semiconductors with electronic gaps. This class of material will exhibit many interesting physical properties and will find important practical applications in lasers, mirrors, resonators, filters, and quantum optical devices. Theory will be directed at designing periodic dielectric structures that give the optimal frequency gap for various applications with special emphasis on the fabricability of these structures, especially in the sub-micron length scale where these materials will find applications in optical measurements. Experimental effort will apply theoretical results to fabricate structures in the micron and sub-micron length scales, using micro-fabrication patterning and etching techniques. The effect of disorder, defects and structural imperfections on the propagation of electromagnetic waves through these photonic crystals will be studied.

Keywords: Patterning, Plutonics, Optical Devices

233. High Flux, Large-Area Carbon-Cluster Beams for Thin Film Deposition and Surface Modification — FY 1993 $400,000

DOE Contact: Walter M. Polansky, (301) 903-5995
Argonne National Laboratory Contact: Dieter M. Gruen, (708) 252-3513

Fullerenes, such as C_{60} or buckminsterfullerene, are kinetically stable carbon cluster molecules, but are thermodynamically unstable with respect to diamond and graphite by

~5 kcal/mol C. The fact that C_{60} has a vapor pressure of ~10^{-3} Torr at 500°C opens up the possibility of generating high-flux, high-energy carbon-cluster ion beams for thin-film deposition (including diamond films) and surface modification. A microwave-driven electron cyclotron resonance (ECR) plasma source will be used to generate the fullerene ion beams. The substrate impact energy will be controlled independently of the plasma parameters by biasing the substrate. End-Hall optics will be combined with the ECR plasma to provide additional control of beam characteristics. The ECR facility will be used to synthesize and characterize, by a variety of techniques, diamond films, diamond-like films, and carbon-implanted layers on large areas with high-deposition rates. The effort is directed toward producing high-quality films at low-substrate temperatures in a manner that can be adapted to industrial processes.

Keywords: Fullerenes, Ion Beams, Diamond, Diamond-like Carbon

234. Novel Composite Coatings for High Temperature Friction and Wear Control

FY 1993
$250,000

DOE Contact: Walter M. Polansky, (301) 903-5995
Oak Ridge National Laboratory Contact: Theodore M. Besmann, (615) 574-6852

Chemical vapor deposition (CVD) techniques offer the opportunity to create very uniform self-lubricating composites which slowly wear away to expose pockets of lubricants which then spread across the surface. In CVD gaseous reactants are allowed to flow over a heated substrate where they react and deposit a solid coating. Solid lubricants have higher use temperatures and higher load-bearing capacities than do liquid lubricants. Consequently, they find use in applications where liquid lubricants prove inadequate. It has been noted that because buckminsterfullerene (C_{60}) is a spherical macromolecule and is thought to be very stable and slow to react with other substances, it should make an excellent lubricant. This project utilizes the controlled wear of a hard matrix to reveal the embedded high-temperature, solid lubricant. Such a composite coating would be produced by CVD, which has been demonstrated capable of producing multiphase coatings of controlled composition and microstructure. The C_{60} phase cannot be simultaneously formed during deposition, as can other of the proposed lubricants. The material can be incorporated into a coating, however, by entrainment in the coating gases.

Keywords: Chemical Vapor Deposition, Fullerenes, Composites

235. Synthesis of Advanced Composite Ceramic Precursor Powders by the Electric Dispersion Reactor

FY 1993
$365,000

DOE Contact: Walter M. Polansky, (301) 903-5995
Oak Ridge National Laboratory Contact: Michael T. Harris, (615) 574-1275

The use of high-intensity-pulsed electric fields for droplet size control in dispersed liquid systems is being investigated. This technology has been utilized in a device called the electric dispersion reactor (EDR) to carry out the synthesis of micron-sized particles for the production of precursor powders of advanced ceramic materials. In this approach, pulsed electric fields are employed to create dispersions of microscopic conducting (aqueous-based) drops in nonconducting (organic) liquids. Each of these droplets becomes a localized microreactor where reactants in the organic phase diffuse into the aqueous droplets in which precipitation and gelation occur, while water and reaction products diffuse into the organic phase. The particle morphology is altered by varying reactant compositions in the liquid-liquid system while achieving intraparticle stoichiometric consistency. This leads to the production of high-quality precursor powders which, in turn, yields dense, consistent green-body material. Furthermore, this method requires far less energy expenditures than conventional approaches which rely on such inefficient operations as solids blending, mixing, and grinding to accomplish the formation of mixed-oxide precursor material.

Keywords: Ceramics, Ceramic Precursors

236. New Ion Exchange Materials for Environmental Restoration and Waste Management

FY 1993
$435,000

DOE Contact: Walter M. Polansky, (301) 903-5995
Argonne National Laboratory Contact: E. Philip Horwitz, (708) 972-3653

The objective of this program is to synthesize, characterize, and evaluate a new class of cation exchange resins. The new resins will contain the geminally substituted diphosphonic acid functional group. Ion exchange resins containing geminally substituted diphosphonic acid groups should have vastly superior properties compared to commercially available cation exchange resins and should find wide-scale applications in environmental restoration (e.g., groundwater cleanup) and in waste management (e.g., minimization of waste volume). Alkyl-1,1-diphosphonic acids are among the most powerful complexing agents for polyvalent metal ions in aqueous solution, particularly at $pH<2$. But, heretofore, it has not been possible to synthesize resins containing diphosphonic acid groups, because of the difficulty of introducing this group into a preformed polymer matrix. The synthesis of resins with the diphosphonic acid groups will be accomplished by the polymerization of vinylidene-1,1-diphosphonic acid (VDPA) or by the copolymerization of VDPA with suitable comonomers (e.g., acrylamide/bis-acrylamide or styrene/divinylbenzene). This approach represents a major departure from the traditional methods for preparing ion exchange materials whereby the exchangeable functional groups are introduced onto a preformed polymer matrix.

Keywords: Ion Exchange, Environmental Restoration

237. Development of an Ion Replacement Electrorefining Method | FY 1993 | $450,000

DOE Contact: Walter M. Polansky, (301) 903-5995
Argonne National Laboratory Contact: Zygmunt Tomczuk, (708) 252-7294

The objective of this project is to investigate promising methods for carrying out a new metal separation and purification process called ion replacement electrorefining. The challenge and program focus lies in developing a counter electrode that can serve in a sequential and, if possible, reversible manner as a cathode during metal dissolution and an anode during metal separation/deposition. The key goal is to produce a clean separation between actinide and non-actinide elements, such as required for the separation of spent nuclear reactor fuel. One potential use for the ion replacement electrorefining method is the reprocessing of spent metal fuel from an Integral Fast Reactor (IFR), but it is also adaptable to the separation of transuranic elements from spent fuel and waste generated by the light water nuclear reactor (LWR) industry and the defense nuclear programs. In the case of the IFR, the proposed process offers a simplification of the conventional pyrometallurgical electrorefining process under development within the IFR program. For LWR and defense waste applications, the ion replacement electrorefining method could be used in conjunction with processes that incorporate reduction of actinide element compounds (usually oxides) to a metallic form.

Keywords: Separations, Actinides, Electrorefining

Materials Properties, Behavior, Characterization or Testing

238. A Study of Potential High Band-Gap Photovoltaic Materials for a Two Step Photon Intermediate Technique in Fission Energy Conversion | FY 1993 | $317,000

DOE Contact: Walter M. Polansky, (301) 903-5995
University of Missouri Contact: Mark A. Prelas, (314) 882-3550

The efficiency of modern day power plants is limited by the steam cycle that they employ. Future power plants may be able to improve upon the efficiency of the steam cycle provided that other energy conversion techniques become available. One such energy conversion method is excimer channeling. Excimer channeling is a method of efficiently creating a narrow band photon spectrum directly from the products of nuclear reactions. This narrow band photon spectrum can be used in an energy conversion cycle based upon photovoltaic reactions. This project addresses the issue of photovoltaic materials that can interface with the narrow band photon spectrum in the excimer channeling energy conversion method. Photovoltaics are generally thought to be inefficient because of their association with solar cells. Solar cells are photovoltaic cells that convert the broad band photon spectrum of the sun directly into electricity at an efficiency of 10 percent to as much as 20 percent. Conversion of photons into electricity could be vary efficient (as high as 85 percent) if the photon spectrum were sufficiently narrow, such as that produced by excimer channeling, and matched to the bandgap of the photovoltaic material. Development of high bandgap photovoltaic materials that match the excimer channeling photon spectrum is the goal of this research program. This effort centers on materials with bandgaps exceeding 5 eV. High bandgap crystals will be synthesized, doped to form P-N junctions, characterized by various surface analysis methods, made into photovoltaic cells, the cells' characteristics tested, and the cells' tolerance to various types of electromagnetic radiation assessed.

Keywords: Photovoltaics, Nuclear Reactors

239. Nonlinear Optics in Doped Fibers FY 1993 $363,000

DOE Contact: Walter M. Polansky, (301) 903-5995
Stanford University Contact: Richard H. Pantell, (415) 723-2564

The objective of this project is to develop a novel and simple technology for optical, all-fiber switches based on the third order nonlinear effect in doped, single-mode fibers. The principle is that when exciting a transition near resonance the electronic distribution changes and so does the contribution of this transition to the refractive index of the material. In this novel approach, a fiber doped with an appropriate impurity, is excited optically near an absorption resonance of the impurity to produce strongly enhanced nonlinear susceptibilities. Modeling shows that it is then possible to reduce the pump and length requirements by several orders of magnitude each, and to produce a π phase shift in centimeter lengths with milliwatts of pump power. A variety of impurities will be investigated. For picosecond response times, the reduction in the pump power-fiber length product is predicted to be 7-8 orders of magnitude over undoped silica. Erbium and neodymium doped fibers will also be studied. This investigation is anticipated to open the door to the first low-power, ultra-short switches and modulators made with single-mode optical fibers, operated with a low-power, long-lifetime laser diode. There are a variety of energy applications for the proposed research, including oil exploration, control of power substations, and management of consumer distribution systems.

Keywords: Optical Switch, Nonlinear Optic, Optical Fibers

240. Feasibility of a Novel Approach for Fast, Economical Determination of Radiation Damage in Nuclear Reactor Cores FY 1993 $156,000

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

Device or Component Fabrication, Behavior or Testing

241. Ultrafast Molecular Electronic Devices FY 1993 $425,000

DOE Contact: Walter M. Polansky, (301) 903-5995
Argonne National Laboratory Contact: Michael R. Wasielewski, (708) 252-3538

The objective of this project is to apply the fundamental chemistry of ultra-fast photo-initiated electron transfer reactions to produce high speed, energy efficient molecular electronic devices. These molecules, designed around electron donor-acceptor molecules, will act as opto-electronic switches on a picosecond time scale. Photo-excitation of these molecules with visible light results in very efficient charge separation reactions that set the on or off state of the molecular switch. Two types of switches will be developed: (1) a bistable electron transfer switch that will use a light pulse of one color to store information in the solid state in the form of a long-lived charge separation, and a light pulse of a second color to recover it; and (2) a field effect switch that will use the electric field generated by one charge separated electron donor-acceptor pair to influence the on or off state of a second donor-acceptor pair. These electro-optic switch molecules will be assembled in ordered arrays on surfaces using self-assembled monolayer and liquid crystal polymer technology. Potential applications of this technology are optical computing, wavelength selective gates and switches, laser detectors, electro-optic devices, modulators, and memories.

Keywords: Opto-electronic Switches, Liquid Crystals, Photo-initiated Electron Transfer

242. Photo-Induced Electron Transfer From a Conducting Polymer to Buckminsterfullerene: A Molecular Approach to High Efficiency Photovoltaic Cells

FY 1993
$171,000

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 photoinduced 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

243. Superconducting Bitter Magnet

FY 1993
$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

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

244. Structural Materials Development

FY 1993
$545,000

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

245. Repair Welding of Fusion Reactor Components

FY 1993
$98,000

DOE Contact: F. W. Wiffen, (301) 903-4963
Auburn University Contact: B. A. Chin, (205) 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

246. Insulating Ceramics for Fusion

FY 1993
$400,000

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

247. Modeling Irradiation Effects in Solids FY 1993 $66,000

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

248. Fusion Systems Materials FY 1993 $2,186,000

DOE Contact: F. W. Wiffen, (301) 903-4963
ORNL Contacts: E. E. Bloom, (615) 574-5053 and A. F. Rowcliffe, (615) 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 martensitic/bainitic steels, vanadium alloys and SiC/SiC composites. Investigations focus on the most critical questions or limiting properties in each of these systems: martensitic/bainitic steels - DBTT transition shifts and fracture toughness, vanadium alloys - 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 two material classes involves irradiation in fission reactors, including HFIR, EBR-II, and HFBR, as partial simulation of the fusion environment.

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

249. Structural Materials for Fusion Systems

FY 1993
$1,991,000

DOE Contact: F. W. Wiffen, (301) 903-4963
PNL 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

250. Development of Radiation-Hardened Ceramic Composites for Fusion Applications

FY 1993
$80,000

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

251. Radiation Effects and Micromechanics of SiC/SiC Composites

FY 1993
$110,000

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

252. Damage Analysis and Fundamental Studies for Fusion Reactor Materials Development

FY 1993
$199,000

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 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 steels in ITER and other fusion systems.

Keywords: Steels, Irradiation Effects, Fracture

253. Development of Lithium-Bearing Ceramic Materials for Tritium Breeding in Fusion Reactors

FY 1993
$300,000

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

254. Post-Irradiation Examination of Lithium-Bearing Ceramic Materials for Tritium Breeding in Fusion Reactors

FY 1993
$500,000

DOE Contact: S. Berk, (301) 903-4171
PNL 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) have been mostly completed and PIE on the Phase 2 specimens (lithium-oxide and lithium-zirconate irradiated to 5 percent lithium atom burnup) has been initiated.

Keywords: Ceramics, Lithium Ceramics, Tritium Release

255. ITER Materials Development for Plasma Facing Components

FY 1993
$2,200,000

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 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 power 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. The ITER Industrial Partnership (McDonnell-Douglas, Westinghouse, Rocketdyne, General Atomics, and University of Illinois) is involved in the joining studies, erosion rate studies, and fatigue testing.

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

256. ITER Structural Materials Development FY 1993
$750,000

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 refractory metals, alloys based on vanadium and niobium. 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, Niobium, Irradiation Effects, Compatibility

257. ITER Ceramic Materials FY 1993
$530,000

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

258. Radiation Hardened Fiber Optics for ITER Fusion Diagnostic Systems
FY 1993
$125,000

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 optic 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

259. ITER Materials Evaluation FY 1993 $1,510,000

DOE Contact: F. W. Wiffen, (301) 903-4963
ORNL Contact: E. E. Bloom, (615) 574-5053, and A. F. Rowcliffe, (615) 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 on 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

260. ITER Structural Materials Evaluation FY 1993 $910,000

DOE Contact: F. W. Wiffen, (301) 903-4963
PNL 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 PNL 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 PNL also is examining hydrogen effects and compatibility with water cooling.

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

261. Development of Nb_3Sn Superconducting Wire for the ITER Magnet Program FY 1993 $500,000

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., Teledyne Wah Chang Albany, Oxford Superconducting Technologies, and Supercon. 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

262. Structural Materials Development for the Conduit of ITER Cable-in-Conduit-Conductors

FY 1993
$980,000

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 and awards prior to FY 1993 were limited to $50,000; in FY 1993 the award size was increased to $75,000. Phase II is the principal research or research and development effort, and awards have been as high as $500,000 for work to be performed in a period of up to two years. 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. Conclusions were reached on the basis of detailed reports returned by reviewers drawn from DOE laboratories, universities, private industry, and government. In the Phase II technical evaluation process, in the case in which two or more grant applications were judged to be of approximately equal scientific and technical merit, preference was given to those applications that had demonstrated third phase, non-Federal capital commitments.

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, 1993 (DOE/ER-0599), Abstracts of Phase II Awards, 1993 (DOE/ER-0600), and Abstracts of Phase II Awards, 1992 (DOE/ER-0561). Copies of these publications may be obtained by calling Mrs. Kay Etzler at (301) 903-5867.

Materials Preparation, Synthesis, Deposition, Growth, or Forming

Phase I Projects

Multi Layer, Quantum Well Layer Film Thermoelectrics - DOE Contact Chet Bigelow, (301) 903-4299; Hi-Z Technology, Inc. Contact Mr. Norbert B. Elsner, (619) 535-9343

Indium Gallium Arsenide Thermophotovoltaic Energy Converters - DOE Contact Chet Bigelow, (301) 903-4299; Spire Corporation Contact Mr. Patrick N. McDonnell, (617) 275-6000

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) 903-5995; American Superconductor Corporation Contact Mr. Edward P. Hamilton, (617) 923-1122

Lubricious-Surface Silicon-Nitride Rings for High-Temperature Tribological Applications - DOE Contact Cynthia Carter, (301) 903-5995; Colorado Engineering Research Laboratory, Inc. Contact Dr. Paul J. Wilbur, (303) 484-5940

Room Temperature Photoluminescence of Germanium Nanostructures by High Energy Implantation of Germanium into a Buried Oxide of Silicon - DOE Contact Cynthia Carter, (301) 903-5995; Ibis Technology Corporation Contact Dr. G. Ryding, (508) 777-4247

Nanoscale Processing for Ternary Semiconductors - DOE Contact Cynthia Carter, (301) 903-5995; Interphases Research Contact Mr. Leslie Affonso, (805) 493-2257

Low Temperature Deposition of Titanium Nitride - DOE Contact Cynthia Carter, (301) 903-5995; ISM Technologies, Inc. Contact Mr. Robert J. Stinner, (619) 530-2332

Quantum Confinement Effects in Heteroepitaxial Silicon/Zinc Sulfide Nanostructures Produced by Metallo-Organic Chemical Vapor Deposition - DOE Contact Cynthia Carter, (301) 903-5995; Spire Corporation Contact Mr. Patrick N. McDonnell, (617) 275-6000

Coated Micrograin Carbides for Wear Resistance - DOE Contact Cynthia Carter, (301) 903-5995; 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

Solid Polymer Electrolyte Membranes for Olefin Separation - DOE Contact Robert Marianelli, (301) 903-5804; Membrane Technology and Research, Inc. Contact Ms. Elizabeth Weiss, (415) 328-2228

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

Zeolite Membranes for Gas Separations - DOE Contact Robert Marianelli, (301) 903-5804; TDA Research, Inc. Contact Mr. Michael E. Karpuk, (303) 422-7819

A Vapor-Grown, Carbon Fiber-Reinforced Beryllium Composite for Plasma Facing Material - DOE Contact Warren Marton, (301) 903-4965; Applied Sciences, Inc. Contact Mr. Max L. Lake, (513) 766-2020

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 Ultrasonic Methods for the Nondestructive Evaluation of Bond Quality in Brazed Composite-Metal Joints - DOE Contact Warren Marton, (301) 903-4965; Karta Technology, Inc. Contact Dr. G. P. Singh, (210) 681-9102

High Thermal Conductivity Graphite for the International Thermonuclear Experimental Reactor First Wall - DOE Contact Warren Marton, (301) 903-4965; Nuclear and Aerospace Materials, Inc. Contact Dr. Glen B. Engle, (610) 487-0325

Highly Efficient, Heat-Dissipating, Functionally Gradient Plasma Facing Materials - DOE Contact Warren Marton, (301) 903-4965; Plasma Processes Contact Ms. Cheri M. McKechnie, (205) 881-7572

Development of a Novel Brazing Material to Join Carbon-Carbon to Metals - DOE Contact Warren Marton, (301) 903-4965; Surmet Corporation Contact Dr. Suri A. Sastri, (617) 272-3250

Development of an Electrochemical Infiltration Method for Carbon-Carbon Composite Surface Preparation - DOE Contact Warren Marton, (301) 903-4965; Surmet Corporation Contact Dr. Suri A. Sastri, (617) 272-3250

Thermo-Mechanical Processing of Niobium Titanium Based Superconductors - DOE Contact Jerry Peters, (301) 903-5228; IGC Advanced Superconductors, Inc. Contact Mr. Bruce A. Zeitlin, (203) 753-5215

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. Chandrasekhar, (908) 462-1270

Electrochromic Glazings Deposited by High Rate Processes - DOE Contact Sam Taylor, (202) 586-9214; EIC Laboratories, Inc. Contact Dr. A. C. Makrides, (617) 769-9450

Development of 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

Liquid Crystal Smart Windows - DOE Contact Sam Taylor, (202) 586-9214; Meyer and Lonberg Association Contact Dr. Franklin Lonberg, (617) 277-0394

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

Phase II Projects: (First Year)

Development of a Novel Reverse-Osmosis Membrane with High Rejections for Organic Compounds - DOE Contact Robert Marianelli, (301) 903-5804; Bend Research, Inc. Contact Dr. Scott B. McCray, (503) 382-4100

Development of a Process to Synthesize Tubular Fullerenes - DOE Contact Robert Marianelli, (301) 903-5804; Materials and Electrochemical Research Corporation Contact Dr. J. C. Withers, (602) 574-1980

Continuous Production of Fullerenes from Hydrocarbon Precursors - DOE Contact Robert Marianelli, (301) 903-5804; TDA Research, Inc. Contact Mr. John D. Wright, (303) 422-7918

Preparation of Low-Density Microcellular Materials from Fullerenes - DOE Contact Robert Marianelli, (301) 903-5804; TDA Research, Inc. Contact Dr. William L. Bell, (303) 420-4329

New Gadolinium-Boron Compounds for Neutron Capture Therapy - DOE Contact Gerald Goldstein, (301) 903-3213; Boron Biologicals, Inc. Contact Dr. Bernard F. Spielvogel, (919) 832-2044

Refractory Metal Coatings on Carbon/Carbon Composites for First Wall Applications - DOE Contact Marvin Cohen, (301) 903-4253; Applied Sciences, Inc. Contact Mr. Jyh-Ming Ting, (513) 766-2020

A Thermal Composite Plasma Facing Material - DOE Contact Marvin Cohen, (301) 903-4253; Energy Science Laboratories, Inc. Contact Dr. Timothy R. Knowles, (619) 552-2034

A Niobium-Tin Multifilamentary Composite Superconductor with Artificial Copper (Bronze) Inclusions - DOE Contact Marvin Cohen, (301) 903-4253; Supercon, Inc. Contact Dr. Dingan Yu, (508) 842-0174

A Porous Metal Heat Exchanger Cooled Microwave Cavity - DOE Contact T. V. George, (301) 903-4957; Thermacore, Inc. Contact Mr. John H. Rosenfeld, (717) 569-6551

Development of Silicon Carbide Ceramic Composites for Fusion Reactor Applications - DOE Contact F. W. Wiffen, (301) 903-4963; Materials and Electrochemical Research Corporation Contact Dr. J. C. Withers, (602) 574-1980

Radiation Damage Resistant Silicon for Particle Physics Detectors - DOE Contact William Watson, (214) 708-2417; IntraSpec, Inc. Contact Mr. John Walter, (615) 483-1859

Phase II Projects: (Second Year)

Graphite and Metal Oxide Catalyst Supports for Rechargeable Oxygen Electrodes - DOE Contact Ken Barber, (202) 586-2198; MATSI, Inc. Contact Mr. Ronald A. Putt, (404) 876-8009

Development of Hollow-Fiber Modules for the Purification of Natural Gas - DOE Contact Harold Shoemaker, (304) 291-4715; Bend Research, Inc. Contact Dr. Scott B. McCray, (503) 382-4100

Inexpensive Pathways for the Synthesis of p-Boronophenylalanine and New Boron Containing Agents - DOE Contact Donald W. Cole, (301) 903-3268; Boron Biologicals, Inc. Contact Dr. Bernard F. Spielvogel, (919) 832-2044

An Improved Method of Introducing Additional Alloying Elements into Nb_3Sn in Internal-Tin Processes - DOE Contact Warren Marton, (301) 903-4965; IGC Advanced Superconductors, Inc. Contact Dr. Eric Gregory, (203) 574-7988

Materials Properties, Behavior, Characterization or Testing

Phase I Projects:

In Situ Electrical Testing of Multicell Thermionic Fuel Elements - DOE Contact Chet Bigelow, (301) 903-4299; Space Exploration Associates, Inc. Contact Mr. Max L. Lake, (513) 766-2050

A Testing Process to Define Electrode Current Wear Mechanisms and Develop Improved Electrodes - DOE Contact Charles Thomas, (412) 892-5731; Montec Associates, Inc. Contact Mrs. Cynthia K. Farrar, (406) 494-2596

Phase II Projects: (First Year)

A Novel Energy-Efficient Membrane System for the Recovery of Volatile Organic Contaminants from Industrial Process Gases - DOE Contact Dan Kung, (708) 252-2023; Bend Research, Inc. Contact Dr. Scott B. McCray, (503) 382-4100

Phase II Projects: (Second Year)

Thermophotovoltaic Cogenerators for Advanced Integrated Appliances - DOE Contact Terry Statt, (202) 586-9169; Quantum Group, Inc. Contact Dr. Mark Goldstein, (619) 457-3048

Spontaneous Natural Gas Oxidative Dimerization Across Mixed Conducting Ceramic Membranes - DOE Contact Harold Shoemaker, (304) 291-4715; Eltron Research, Inc. Contact Dr. Anthony F. Sammells, (708) 898-1583

A Membrane Process for Hot-Gas Cleanup and Decomposition of H_2S to Elemental Sulfur - DOE Contact Thomas P. Dorchak, (304) 291-4305; Bend Research, Inc. Contact Dr. David J. Edlund, (503) 382-4100

In Situ FT-IR Diagnostics for Coal Liquefaction Processes - DOE Contact Dr. Shelby Rogers, (412) 892-6132; Advanced Fuel Research, Inc. Contact Dr. Michael A. Serio, (203) 528-9806

Deep Hole Drilling in Refractory Metals Using Abrasive Waterjets - DOE Contact Clint Bastin, (301) 903-5259; Quest Integrated, Inc. Contact Dr. Mohamed Hashish, (206) 872-9500

Improved Properties in Nb 46.5 Weight % Ti Materials for the SSC by Reducing the Separation Between Filaments - DOE Contact Gregory Haas, (214) 708-2510; IGC Advanced Superconductors, Inc. Contact Dr. Eric Gregory, (203) 574-7988

Multifilamentary Nb_3Sn Superconducting Wire Using APC, Composite Filaments with Improved High Field Performance - DOE Contact Gerald Peters, (301) 903-5228; Supercon, Inc. Contact Mr. Kenneth DeMoranville, (508) 842-0174

A Novel Joining Method for Graphite and Carbon-Carbon Composites - DOE Contact Warren Marton, (301) 903-4965; Materials and Electrochemical Research Corporation Contact Dr. Sumit Guha, (602) 574-1980

Device or Component Fabrication, Behavior, or Testing

Phase I Projects

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

Precision Machining of Integral Fast Reactor Metal Fuel Pins with Argon Cutting Jets - DOE Contact Clint Bastin, (301) 903-5259; Quest Integrated, Inc. Contact Ms. Diana J. Suzuki, (206) 872-9500

A High Repetition-Rate, High Power, All-Solid-State Pulsed Driver for Electrodeless Inductive Thrusters - DOE Contact Chet Bigelow, (301) 903-4299; Science Research Laboratory, Inc. Contact Dr. Jonah Jacob, (617) 547-1122

Low Bandgap Thermophotovoltaic Devices for a General Purpose Heat Source -DOE Contact Chet Bigelow, (301) 903-4299; United Solar Technologies, Inc. Contact Mr. Richard J. Kelley, (206) 705-2000

An Improved Carbonate Fuel Cell Design - DOE Contact Clifford Carpenter, (304) 291-4041; Energy Research Corporation Contact Dr. Hans Maru, (203) 792-1460

On-Chip Ferroelectric Energy Storage Capacitors for Silicon Solar Cells - DOE Contact Cynthia Carter, (301) 903-5995; Advanced Fuel Research, Inc. Contact Dr. David G. Hamblen, (203) 528-9806

Porous Aluminum Nitride Part Fabrication to Support Advanced Battery Development - DOE Contact Cynthia Carter, (301) 903-5995; 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) 903-5995; Chemat Technology, Inc. Contact Ms. Xin Qin, (818) 727-9786

Molded Titanium Carbide Bipolar Plates for High Voltage Battery and Fuel Power Sources - DOE Contact Cynthia Carter, (301) 903-5995; GINER, Inc. Contact Dr. Anthony B. LaConti, (617) 899-7270

Jet Vapor Deposition of Ultra-thin Platinum Catalyst Loadings Directly on Polymer Ion-Exchange Membranes for Fuel Cell Applications - DOE Contact Cynthia Carter, (301) 903-5995; Jet Process Corporation Contact Mr. Jerome J. Schmidt, (203) 786-5130

A Direct Thermal to Optical Energy Converter - DOE Contact Cynthia Carter, (301) 903-5995; New Material Concepts Contact Mr. R. G. Roy, (508) 851-2451

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

A Novel Detector for X-ray Absorption Spectroscopy - DOE Contact Roland Hirsch, (301) 903-2682; InterFET Corporation/RMD, Inc. Contact Dr. Gerald Entine, (617) 926-1167

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

A High Count Rate Two-Dimensional Neutron Detector - DOE Contact Manfred Leiser, (301) 903-3426; Advanced Optical Technologies, Inc. Contact Mrs. Feng Liu, (203) 657-2668

A Wavelength Dispersive Spectrometer for Analytical Electron Microscopy -DOE Contact Manfred Leiser, (301) 903-3426; Advanced Research and Applications Corporation Contact Mr. Ed LeBaker, (408) 733-7780

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. James K. Walker, (904) 378-6620

High Energy Density Ceramic Capacitors for Uranium Atomic Vapor Laser Isotope Separation - DOE Contact Arnold Litman, (301) 903-5777; Cape Cod Research, Inc. Contact Ms. Katherine D. Finnegan, (508) 540-4400

Aluminum Nitride Copper Laser Tubes - DOE Contact Arnold Litman, (301) 903-5777; Cercom, Inc. Contact Mr. Richard Palicka, (619) 727-6200

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

On-Line Micro-Sensors for Analytical Chemical Measurement - DOE Contact Robert Marianelli, (301) 903-5804; Ciencia, Inc. Contact Mr. Arturo O. Pilar, (203) 528-9737

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

<u>Helium-Cooled Divertors with Low-Activation Materials and Simple Fabrication Techniques</u> - DOE Contact Warren Marton, (301) 903-4965; Creare, Inc. Contact Mr. Robert A. Hicken, (603) 643-3800

<u>Niobium-Tin Superconducting Wire with a Built-in Niobium Surface Coating to Limit Inter-Strand Eddy Currents in Cables</u> - DOE Contact Warren Marton, (301) 903-4965; Supercon, Inc. Contact Ms. Elaine Drew, (508) 842-0174

<u>An Extended Interdigital Niobium Superconducting Linac Structure for Low Velocity Heavy Ions</u> - DOE Contact Richard Rinkenberger, (301) 903-3613; AccSys Technology, Inc. Contact Dr. Marianne E. Hamm, (510) 462-6949

<u>Monolithically Integrated Detector Arrays</u> - DOE Contact Richard Rinkenberger, (301) 903-3613; Advanced Research and Applications Corporation Contact Mr. Ed LeBaker, (408) 733-7780

<u>Diamond-Based Photomultipliers</u> - DOE Contact Richard Rinkenberger, (301) 903-3613; Advanced Technology Materials, Inc. Contact Mr. Daniel P. Sharkey, (203) 794-1100

<u>Gallium Arsenide Pixel and Microstrip Detectors</u> - DOE Contact Richard Rinkenberger, (301) 903-3613; Detectronics Contact Dr. Helen F. Wang, (510) 455-6520

<u>Oxide-Based Ceramic Composite Hot Gas Filter Development</u> - DOE Contact Richard Tischer, (412) 892-4891; Ceramic Composites, Inc. Contact Mrs. Sharon Fehrenbacher, (301) 261-8373

<u>Innovative Silicon Carbide Fiber Composite Filters</u> - DOE Contact Richard Tischer, (412) 892-4891; Materials and Electrochemical Research Corporation Contact Dr. J. C. Withers, (602) 574-1980

<u>A Carbonate Fuel Cell Monolith for Low-Cost and High Power Density Operation</u> - DOE Contact Venkat Venkataraman, (304) 291-4105; Energy Research Corporation Contact Dr. Hans Maru, (203) 792-1460

<u>Fabrication of a Superconducting Super Collider Dipole Magnet Bore Tube Liner from Copper-Niobium Nanocomposite Produced by Mechanical Alloying</u> -DOE Contact William Watson, (214) 708-2417; Supercon, Inc. Contact Ms. Elaine Drew, (508) 842-0174

Phase II Projects: (First Year)

Digital Processing Electronics for X-ray Detector Arrays - DOE Contact Manfred Leiser, (301) 903-3426; X-ray Instrumentation Associates Contact Dr. William K. Warburton, (415) 903-9980

A Cold/Thermal Beam Bender Using Capillary Optics to Increase the Number of End-Guide Instrument Positions - DOE Contact Manfred Leiser, (301) 903-3426; X-ray Optical Systems, Inc. Contact Dr. Qi-fan Xiao, (518) 442-5250

A Thomson-Scattering Plasma Diagnostic for Materials Testing and Divertor Concept Testing - DOE Contact Charles Finfgeld, (301) 903-3423; Princeton Scientific Instruments, Inc. Contact Dr. Dirck L. Dimock, (908) 274-0774

Eddy-Current Nondestructive Testing Methods for On-Line Detection of Cable Manufacturing Defects - DOE Contact William Watson, (214) 708-2417; SE Systems, Inc. Contact Dr. Duane P. Johnson, (510) 293-3000

Low-Cost Microstrip Detectors on Conductivity-Modified Polyimide - DOE Contact William Watson, (214) 708-2417; Spire Corporation Contact Dr. Anton C. Greenwald, (617) 275-6000

High Strength Mono- and Multi-filament High Temperature Superconductors for High Field Applications - DOE Contact Gerald Peters, (301) 903-5228; IGC Advanced Superconductors, Inc. Contact Dr. Leszek R. Motowidlo, (203) 753-5215

Fabrication of Niobium-Aluminum Superconducting Strands Using Mechanical Alloying and Other Techniques - DOE Contact Gerald Peters, (301) 903-5228; IGC Advanced Superconductors, Inc. Contact Mr. G. M. Ozeryansky, (203) 753-5215

Durable, Low Cost Ceramic Materials for Use in Hot Gas Filtration Equipment - DOE Contact Norman Holcombe, (304) 291-4829; Industrial Filter and Pump Manufacturing Company Contact Mr. Paul Eggerstedt, (708) 656-7800

High Cation Mobility Lithium Polymer Batteries - DOE Contact Al Landgrebe, (202) 586-1483; Covalent Associates, Inc. Contact Dr. Larry A. Dominey, (617) 938-1140

A Real-Time X-ray Detector - DOE Contact Stan Sobczynski, (202) 586-1878; Advanced Technology Materials, Inc. Contact Mr. David Kurtz, (203) 794-1100

Phase II Projects: (Second Year)

Metal Hydride Refrigerators - DOE Contact Terry Statt, (202) 586-9169; Thermal Electric Devices, Inc. Contact Dr. E.M. Redding, (505) 345-8668

A Catalytic Membrane Reactor for Facilitating the Water-Gas Shift Reaction at High Temperature - DOE Contact James R. Longanbach, (304) 291-4414; Bend Research, Inc. Contact Dr. David J. Edlund, (503) 382-4100

A Single Manifold, Radial Flow, Solid Oxide Fuel Cell - DOE Contact William Huber, (304) 291-4663; Technology Management, Inc. Contact Mr. Michael Petrik, (216) 541-1000

Ceramic/Metal Elements for MHD Sidewalls - DOE Contact Charles A. Thomas, (412) 892-5731; Busek Company, Inc. Contact Dr. V. Hruby, (617) 449-3929

Fabrication of Tungsten and Tungsten-Molybdenum Alloy Tubing - DOE Contact Clint Bastin, (301) 903-5259; Creare, Inc. Contact Dr. Thomas J. Jasinski, (603) 643-3800

A Distributed Fiber Optic Sensor for Reversible Detection of Atmospheric CO_2 - DOE Contact Robert Marianelli, (301) 903-5804; Eltron Research, Inc. Contact Dr. Ronald L. Cook, (708) 898-1583

An Electron Bombarded Semiconductor Device - DOE Contact Gerald Peters, (301) 903-5228; Advanced Technology Materials, Inc. Contact Dr. Charles P. Beetz, Jr., (203) 794-1100

Silicon Junction Diode Absolute Radiometers for Plasma Diagnostics in the Soft X-ray and Vacuum Ultraviolet Spectral Region - DOE Contact Charles Finfgeld, (301) 903-3423; International Radiation Detectors Contact Dr. Raj Korde, (213) 542-0041

OFFICE OF ENVIRONMENTAL MANAGEMENT

	FY 1993
Office of Environmental Management - Grand Total	$22,557,000
Office of Waste Management	$ 8,890,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 2,570,000
Technical Support West Valley Demonstration Project	2,570,000
Materials Properties, Behavior, Characterization or Testing	$ 6,320,000
Materials Characterization Center Testing of West Valley Formulation Glass	400,000
Development of Test Methods and Testing of West Valley Reference Formulation Glass	600,000
Process and Product Quality Optimization for the West Valley Waste Form	320,000
Waste Form Qualification	5,000,000
Office of Technology Development	$13,667,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$10,579,000
Polymers for Removal of Pu and Am from Wastewaters	50,000
Polymer Solidification National Effort	451,000
Polymer Solidification Development	1,209,000
Polyethylene Encapsulation	225,000
Low Level Mixed Waste (LLMW) Vitrification Process Limits	1,200,000
Vitrification of Rocky Flats Waste	274,000
Mixed Waste Destruction (Vitrification)	25,000
Vitrification of Controlled-Air Incinerator Ash	50,000
Microwave Solidification	1,302,000
Minimum Additive Waste Stabilization (MAWS) Program	1,575,000
Glass Compositional Envelope Study	1,400,000
Extension of MAWS Concept to Glass Ceramic Waste Forms	175,000
Plasma Centrifugal Furnace	175,000

OFFICE OF ENVIRONMENTAL MANAGEMENT

	FY 1993
Office of Technology Development (continued)	
Materials Preparation, Synthesis, Deposition, Growth or Forming (continued)	
Plasma Arc	300,000
Fixed Hearth Plasma Arc for Mixed Waste Treatment (RETECH)	1,968,000
Plasma Hearth Process (ANL-W) Radioactive Waste Test	200,000
Materials Properties, Behavior, Characterization or Testing	$ 3,088,000
Mixed Waste Program Support - Plasma Hearth Process	588,000
Waste Form Performance Criteria	100,000
Arc Melter Vitrification	650,000
Graphite DC Plasma Arc Melter	1,750,000

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. This new office combines nuclear waste management and the environmental clean-up elements that were spread across four offices. EM's goal is to insure that risks to human health and safety and to the environment from past, present, and future operations are either eliminated or reduced to prescribed, safe levels by the year 2019.

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 nonradioactive 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

263. Technical Support to West Valley Demonstration Project — FY 1993 $2,570,000

DOE Contact: W. S. Ketola, (716) 942-4314
PNL Contact: W. A. Ross, (509) 376-3644

Pacific Northwest Laboratory (PNL) provides technical assistance to the West Valley demonstration project in characterizing high-level waste samples taken from the West Valley tanks; characterizing operating conditions for ion exchange processes that remove cesium and plutonium from the high level supernate; developing an empirical model which relates borosilicate glass composition to the chemical durability of the final waste form (including both preparation and testing of materials and the statistical analysis of the results to allow modeling); and characterizing individual process operations to show overall control of the vitrification process and the final waste form.

Keywords: Ion Exchange, Borosilicate Glass, Process Control, Radioactive Waste Host

Materials Properties, Behavior, Characterization or Testing

264. Materials Characterization Center Testing of West Valley Formulation Glass

FY 1993
$400,000

DOE Contact: W. S. Ketola, (716) 942-4314
PNL Contact: S. C. Marschman, (509) 376-3569

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 began testing of a small sample of glass containing actual West Valley high-level waste. MCC continues to provide assistance to West Valley relative to enhancing the quality of their analytical data.

Keywords: Radioactive Waste Host

265. Development of Test Methods and Testing of West Valley Reference Formulation Glass

FY 1993
$600,000

DOE Contact: W. S. Ketola, (716) 942-3414
CUA Contact: P. B. Macedo, (202) 635-5327

Vitreous State Laboratory (VSL) of the Catholic University of America(CUA) continues to develop test methods for nonradioactive and radioactive borosilicate glass waste forms for the West Valley Demonstration Project and is studying means to maximize the region of acceptable quality around the point of optimal durability for the borosilicate waste form.

Keywords: Radioactive Waste Host

266. Process and Product Quality Optimization for the West Valley Waste Form

FY 1993
$320,000

DOE Contact: W. S. Ketola, (716) 942-4314
AU Contact: L. D. Pye, (607) 871-2432

Alfred University(AU) is studying properties and crystallization behavior of the West Valley borosilicate glass reference composition in anticipation of providing methods for control of product quality during routine manufacture of the West Valley Demonstration Project waste form.

Keywords: Radioactive Waste Host, Borosilicate Glass

267. Waste Form Qualification

FY 1993
$5,000,000

DOE Contact: W. Pearson, (803) 557-1066
WSRC Contact: M. J. Plondinec, (803) 725-2170

These studies provide fundamental data for start-up of the Defense Waste Process Facility, for waste compliance activities, and for acceptance of borosilicate glass at a repository. Site specific testing is included.

Keywords: Waste, Waste Form, Borosilicate Glass, Waste Acceptance Specifications

Office of Technology Development

The Office of Technology Development (TD) has the mission to facilitate EM's 30-year goal by developing and implementing new technologies to assist DOE in achieving compliance with all applicable statues and regulations. The TD program is designed to make new, innovative, and effective technology available for use and transfer it to the field offices.

Certain areas of TD's program focus on materials research in order to provide better, faster, safer and less expensive approaches to identify, characterize and clean up DOE's waste problem. In the area of soil and groundwater remediation, as well as waste retrieval processing, TD 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 are being pursued to better understand vitrification technologies, useful for containment of contaminated soils. New fibers and inorganic membranes are being tested for efficiency and reuse in HEPA filters that DOE uses for air cleaning in a wide variety of operations involving radioactive particulates. TD will continue to fund these materials research projects, as well as others, to provide the basis for other applied research in the TD program.

Materials Preparation, Synthesis, Deposition, Growth or Forming

268. Polymers for Removal of Pu and Am from Wastewaters FY 1993 $50,000

DOE Field Office Contact: Darrell Bandy, (505) 845-6101
DOE HQ Program Manager: Paul Hart, (301) 903-7456
Los Alamos National Laboratory Contact: Gordan Jarvinen, (505) 665-0822

The objective of this project is to remove actinide metal ions, plutonium and americium, from wastewater streams at the Waste Treatment Facility at Los Alamos through commercial and experimental polymer extraction systems. These systems will also be explored for removing hazardous wastes, such as chromium metal, from aqueous waste streams. The system will be developed for efficiency, capacity and selectivity so that it could be commercially developed by the private sector. Polymer extractions offer advantages in cost, handling benefits, recycle chemistry, reduced radiation exposure, and long term stability.

Keywords: Alternative Final Waste Form, Polymer Extraction, Radioactive and Metal Ion Wastes

269. Polymer Solidification National Effort FY 1993 $451,000

DOE Field Office Contact: Steve Webster, (708) 252-2822
DOE HQ Program Manager: Paul Hart, (301) 903-7456
Brookhaven National Laboratory Contact: Paul Kalb, (516) 282-7644

The objective of this project is to develop polyethylene encapsulation for nitrate salt waste present at many DOE sites. The process has been established at Brookhaven National Laboratory, from conception through parameter optimization, waste form testing and scale-up feasibility for concentrated salts and ion exchange resins. Brookhaven National Laboratory has been working with Rocky Flats to implement polymer solidification as a replacement for cement solidification because of improvements in waste form performance and increased encapsulation efficiency. The process will be demonstrated in the lab using Rocky Flats waste surrogate. National interest has been expressed in pursuing polymer solidification as an alternative to cement processes. Brookhaven National Laboratory will coordinate efforts to implement this program.

Keywords: Alternative Final Waste Form, Polymer Solidification, Nitrate Salt Wastes

270. <u>Polymer Solidification Development</u> <u>FY 1993</u>
$1,209,000

DOE Field Office Contact: Reginald Tyler, (303) 966-5927
DOE HQ Program Manager: Jim Taylor, (301) 903-7686
EG&G Rocky Flats Contact: A. M. Faucette, (303) 966-6420

The objective of this project is to develop and support implementation of polymer encapsulation technologies for Rocky Flats radioactive mixed waste streams. The development will demonstrate the ability of polymer encapsulation to meet applicable Nevada Test Site (NTS), Environmental Protection Agency (EPA) and Department of Transportation (DOT) criteria. Polymer solidification has been identified as viable treatment for many waste streams including nitrate salts, precipitated hydroxide sludge, soils, ground glass, beryllium dust, and lead metals. Initial activities will focus on nitrate salt surrogate waste drying and polymer extrusion including identification of existing production scale drying technologies, refinement of leachability model for heavy metals, evaluation of waste form durability and lab scale treatability studies. Other polymer processes will be evaluated at a later date because no single method will be successful with all waste streams. One advantage of the polymer process is the production of much less volume than conventional cement solidification technologies so cost benefits will occur in storage, transport and disposal.

Keywords: Alternative Final Waste Form, Polymer Solidification, Hydroxide Sludge

271. <u>Polyethylene Encapsulation</u> <u>FY 1993</u>
$225,000

DOE Field Office Contact: Joel Haugen, (708) 972-2093
DOE HQ Program Manager: Paul Hart, (301) 903-7456
Brookhaven National Laboratory Contact: Paul Kalb, (516) 282-7644

Many DOE sites contain underground storage tanks containing mixed waste. These tanks are intended for temporary storage. Stabilization technologies will be implemented to treat these wastes. The objective of the program at Brookhaven National Laboratory is to explore alternative waste stream stabilization methods for radionuclides and toxic metals. Polyethylene encapsulation is a thermoplastic method which can stabilize nitrate, mercury and chloride salts, and sludges, evaporator concentrates, and ion exchange resins. Previous studies show the polyethylene process to be cost saving due to low temperature processing and reduction in waste volume generated. Treatability studies on surrogate Hanford waste will examine waste loading potential and performance followed by scale up studies.

Keywords: Alternative Final Waste Form, Polyethylene Encapsulation, Radionuclides, Toxic Metals

272. Low Level Mixed Waste (LLMW) Vitrification Process Limits

FY 1993
$1,200,000

DOE Field Office Contact: M. G. O'Rear, (803) 725-5541
DOE HQ Program Manager: Paul Hart, (301) 903-7456
Westinghouse Savannah River Contact: Denny Bickford, (803) 725-3737

The objective of this project is to establish vitrification technology to dispose low-level mixed waste, "Vitrify to Delist to Dispose." The work will establish performance technology for specific waste sludges containing fly ash and homogeneous solid wastes, from Oak Ridge, Los Alamos and Rocky Flats. The goal is to bring lab scale treatments on surrogates up to full scale hot demonstrations.

Keywords: Vitrification, Low-Level Mixed Waste, Fly Ash

273. Vitrification of Rocky Flats Waste

FY 1993
$274,000

DOE Field Office Contact: Deborah Trader, (509) 376-1831
DOE HQ Program Manager: Paul Hart, (301) 903-7456
Pacific Northwest Laboratory Contact: Richard Peters, (509) 376-4579

The objective of this project is to develop pilot scale demonstrations of vitrification technologies for mixed low-level wastes. The plan describes the steps required to prepare a pilot scale vitrification system for mixed waste. The steps include waste characterization, bench scale crucible tests, treatability studies, pilot scale testing and off-gas characterization. Joule-heated melters will be evaluated for feedstock limitations with emphasis on the relationship between combustible materials, halides and the evolution of metal contaminants. From these results, manufacturers of vitrification units will be contacted regarding design strategies for glass melters to treat low-level mixed waste.

Keywords: Vitrification, Joule Heated Glass Melter, Low-Level Mixed Waste

274. Mixed Waste Destruction (Vitrification)

FY 1993
$25,000

DOE Field Office Contact: Reginald Tyler, (303) 966-5927
DOE HQ Program Manager: Paul Hart, (301) 903-7456
EG&G Contact: J. J. Lucerna, (303) 966-7229

The objective of this project is to develop and demonstrate vitrification treatment of low-level mixed waste using a joule heated glass melter. Vitrification has been established for high-level mixed waste but has not been demonstrated for low-level radioactive mixed waste. Cement solidification is typically used to stabilize low-level mixed waste. This work will focus on treating Rocky Flats surrogate for glass development and data collection. The data will be used to establish vitrification capabilities and life cycle cost improvements compared to cement baseline technology.

Keywords: Vitrification, Joule Heated Glass Melter, Low-Level Mixed Waste, Rocky Flats

275. Vitrification of Controlled-Air Incinerator Ash FY 1993
$50,000

DOE Field Office Contact: Darrell Bandy, (505) 845-6101
DOE HQ Program Manager: Paul Hart, (301) 903-7456
Los Alamos National Laboratory Contact: Ron Nakaoka, (505) 665-5971

Vitrification has been identified as a leading candidate for the processing of mixed wastes. The objective of this project will be to support vitrification projects in the Mixed Waste Integrated Program (MWIP) in the areas of performance standards development and vitrification specifications and procurement. The Final Waste Form Technical Support Group (TSG) has been created to review, prioritize, recommend and oversee activities associated with the production and performance evaluation of final waste forms. This project will provide technical support to the Final Waste Form Technical Support Group by evaluating testing and demonstration capabilities. These evaluations will include a review of DOE, university and industrial vitrification processes.

Keywords: Vitrification, Technical Support

276. Microwave Solidification FY 1993
$1,302,000

DOE Field Office Contact: J. Peterson, (303) 966-5349
DOE HQ Program Manager: Jim Taylor, (301) 903-7686
EG&G Rocky Flats Contact: G. Sprenger, (303) 345-3159

The objective of this project is to develop microwave melter technology for solidification of Rocky Flats waste streams containing precipitated hydroxide sludge, incinerator ash, slag crucibles and soil. Microwave technology offers many advantages over the current cement technology. It has a greater volume reduction and removes more water while immobilizing radionuclides and heavy metals. Also, the glass final waste form has better leachability, waste loading, product density, and life cycle costs. The goal of this project is to scale up laboratory and pilot scale demonstrations from cold surrogates to actual wastes. Optimum operating conditions will be determined by varying the power level, feed rate and glass additives.

Keywords: Microwave Solidification

277. Minimum Additive Waste Stabilization (MAWS) Program FY 1993
$1,575,000

DOE Field Office Contact: Rod Warner, (513) 648-3156
DOE HQ Program Manager: Grace Ordaz, (301) 903-7440
Catholic University Contact: Ian Pegg, (202) 319-6700

The MAWS technology development program was established in 1991 as a feasibility study for pit sludges buried at a DOE facility in Fernald, Ohio. The technology system utilizes several mixed waste streams requiring remediation as resources for vitrification to produce a stable and durable glass or slag final waste form for disposal. At Fernald, sludges, contaminated soils, and other various wastes are present that are amenable to vitrification. The benefit to this approach is that the volume of the final waste form is minimized since little or no additives are used, and vitrification results in additional volume reduction. This program uses an integrated technology approach that includes vitrification, soil washing, and waste water treatment systems and optimizes the overall system for cost and performance.

Keywords: Vitrification, Glass, Slag, Durability

278. Glass Compositional Envelope Study FY 1993
$1,400,000

DOE Field Office Contact: Steve Webster, (708) 252-2822
DOE HQ Program Manager: Grace Ordaz, (301) 903-7440
Catholic University Contact: Ian Pegg, (202) 319-6700

The purpose of this project is to provide information and develop waste glass forming systems to reduce costs and reduce cycle time from characterization to implementation. This will be accomplished by characterizing waste streams and glass crucible melts. Waste streams from sites will be analyzed and 50 kilogram samples will be sent to Catholic University to vitrify and characterize. The glass will be characterized for waste loading, viscosity, conductivity, redox state, crystallization and leachability. The compositional information will provide optimal formulations and determine applicability and potential benefits of Minimum Additive Waste Stabilization (MAWS) technology for any waste stream.

Keywords: Glass Characterization, MAWS, Catholic University

279. Extension of MAWS Concept to Glass Ceramic Waste Forms FY 1993 $175,000

DOE Field Office Contact: Steve Webster, (708) 252-2822
DOE HQ Program Manager: Grace Ordaz, (301) 903-7440
Argonne National Laboratory Contact: Xiangdong Feng, (708) 252-7362

The purpose of this work is to identify alternative final waste forms for waste streams not able to be disposed in glass such as scrap metals and sludges containing high amounts of Cr, Ni, Ti, Fe, Ca or Mg. Vitrification of these waste streams require low waste loading and large amounts of additives which is contrary to goals. Tailored slag has various crystalline and metal phases encapsulated into glass and shows promise as a waste form because of its durability, processing requirements and ability to incorporate large amounts of metal. The goal is to provide compositional ranges for the production of tailored slag and will complement the glass compositional envelope study being performed at Catholic University.

Keywords: Tailored Slag, MAWS

280. Plasma Centrifugal Furnace FY 1993 $175,000

DOE Field Office Contact: Steve Webster, (708) 252-2822
DOE HQ Program Manager: Grace Ordaz, (301) 903-7440
Argonne National Laboratory Contact: John Bates, (708) 252-4385

The objective of this project is to demonstrate Minimum Additive Waste Stabilization (MAWS) approach for use with the plasma centrifugal furnace. Soil and metal compositions will be modeled, using the Structural Bond Strength modeling approach developed by Argonne. Crucible studies on these modeled wastes and characterization of final waste forms will occur at Argonne for waste loading and durability. The goal is to recommend waste feed compositions to be used in the plasma centrifugal furnace. Characterization will be adapted from existing tests on high-level glass waste at Fernald/MAWS program. In addition, plasma centrifugal furnace glass form results will be compared to other glass melting methods because it may have advantages in processing high metal content waste streams.

Keywords: Plasma Centrifugal Furnace, MAWS

281. Plasma Arc FY 1993
$300,000

DOE Field Office Contact: Pamela Saxman, (505) 845-6101
DOE HQ Program Manager: Miles Dionisio, (301) 903-7639
Sandia National Laboratory Contact: Dale Blankenship, (505) 844-9694

The objective of this program is to develop plasma arc technology for characterization, treatment and disposal processes at Sandia National Laboratory for nuclear weapon components. The components contain radioactive, explosive and toxic materials such as foams and fillers that are not easily separated or characterized. The plasma arc process will destroy organic materials and allow metal recycling due to off-gas control, and ingot and glassified slag final products. Ingots contain copper which preferentially attracts precious metals such as gold, silver and palladium. Glassified slag collects undesirable metals like cadmium and arsenic. Volatile metals like mercury and lead will be captured in the off-gas for collection and recycling. The goal is to demonstrate plasma arc technologies on surrogate materials and actual weapons components to meet regulations and examine throughput capabilities for each system. This work may apply in the future to disposal faced by electronics manufacturers.

Keywords: Plasma Arc, Decontamination and Decommissioning

282. Fixed Hearth Plasma Arc for Mixed Waste Treatment (RETECH) FY 1993
$1,968,000

DOE Field Office Contact: G. Statts, (412) 892-5741
DOE HQ Program Manager: Paul Hart, (301) 903-7456
MSE Inc. Contact: R. Battleson, (406) 494-7287

The objective of this project is to test the Plasma Hearth Process (PHP) on low-level mixed waste surrogates, representative of wastes across the DOE complex. The goal is to demonstrate the viability of processing a wide range of wastes and determine if the enhanced waste form produced from the Plasma Hearth Process (PHP) will improve life-cycle costs over baseline technology. Primary and secondary waste stream composition from the plasma unit will be determined. This work will be discrete and shall not duplicate other plasma arc work funded by existing contracts or other research initiatives.

Keywords: Plasma Hearth Process, Low-Level Mixed Waste, RETECH

283. Plasma Hearth Process (ANL-W) Radioactive Waste Test FY 1993
$200,000

DOE Field Office Contact: Steve Webster, (708) 252-2822
DOE HQ Program Manager: Paul Hart, (301) 903-7456
Argonne National Laboratory-West Contact: Grant McClellan, (208) 533-7257

The purpose of this work is to test and evaluate a Plasma Hearth Process (PHP) unit to treat actual waste materials. Currently, a non-radioactive plasma unit exists in Ukiah, California. These tests will be performed on non-radioactive surrogate material, and surrogate waste materials containing radioactive tracers and actual radioactive waste. The goal of the work is to assess the performance of the plasma process on the actual wastes, and the fate of the radioactive contaminants upon treatment. This information will be used to develop bench scale design leading to full scale demonstration.

Keywords: Plasma Hearth Process, Non-Radioactive and Radioactive Surrogate Wastes

Materials Properties, Behavior, Characterization or Testing

284. Mixed Waste Program Support - Plasma Hearth Process FY 1993
$588,000

DOE Field Office Contact: Johnny Moore, (615) 576-3536
DOE HQ Program Manager: Paul Hart, (301) 903-7456
Martin Marietta Energy Systems Contact: I. Morris, (615) 574-0559

The objective of this project is to evaluate waste treatment performance of the plasma hearth process for treating waste materials directly to vitrified form with minimum characterization or pretreatment. The plasma process is commercially available technology with advantages in organics destruction, versatility, volume reduction and final waste form leachability. Simulated mixed waste will be evaluated on the existing lab scale plasma arc system to determine the range of mixed waste and off-gas systems design. These data will indicate process performance and lead to preconceptual design efforts for a prototype full scale plasma arc system including feed process, residuals handling and off-gas treatment. The project will conclude with the construction and demonstration of a prototype field scale plasma unit.

Keywords: Plasma Hearth Process

285. Waste Form Performance Criteria FY 1993 $100,000

DOE Field Office Contact: Deborah Trader, (509) 372-4035
DOE HQ Program Manager: Paul Hart, (301) 903-7456
Pacific Northwest Laboratory Contact: Richard Peters, (509) 376-4579

The objective of this project is to establish final waste form performance criteria to address environmental, technical, regulatory and economic issues. It will provide standards for performing waste form property characterization, and performance testing with views toward long term predictability of waste form behavior. The focus will be based on experience from high-level waste testing and will be in compliance with regulatory requirements. These activities will emphasize glass as the final waste form but other alternatives such as cement, polymers and ceramics, will be addressed.

Keywords: Waste Form Performance Criteria

286. Arc Melter Vitrification FY 1993 $650,000

DOE HQ Program Manager: Jaffer Mohiuddin, (301) 903-7965
EG&G Idaho Contact: Kevin Kostelnik, (208) 526-9642

The objective of this project is to demonstrate the applicability of Arc Melter Vitrification for the treatment of mixed wastes and contaminated soils and providing an extremely durable waste form for disposal. The field scale unit can process a nominal 1.5 tons per hour of buried waste type feeds and soils. The feed capabilities are limited by the screw feed system a full scale unit would handle objects larger than a 55 gallon drum. University, industry, in addition to other laboratory participants, are being solicited to accelerate the potential for technology transfer.

Keywords: Arc, Melter, Vitrification

287. Graphite DC Plasma Arc Melter FY 1993 $1,750,000

DOE HQ Program Manager: Jaffer Mohiuddin, (301) 903-7965
EG&G Idaho Contact: Kevin Kostelnik, (208) 526-9642

The objective of this project is to demonstrate the applicability of the Graphite DC Plasma Arc Melter for the treatment of mixed wastes and contaminated soils and providing an extremely durable waste form for disposal. This pilot-scale unit is expected to process a nominal .5 to 1.5 ton per hour of buried type feeds and soils. This furnace includes analytical instruments for making spatially resolved measurements of furnace and glass temperatures and on-line measurements of exhaust emissions, both in the furnace chamber and the off-gas.

Keywords: Graphite, DC, Plasma, Arc, Melter

OFFICE OF NUCLEAR ENERGY

	FY 1993
Office of Nuclear Energy - Grand Total	$123,047,000
Office of Uranium Programs	$ 14,770,000
Gaseous Diffusion	$ 6,770,000
Barrier Quality	2,960,000
Materials and Chemistry Support	3,810,000
Uranium-Atomic Vapor Laser Isotope Separation (U-AVLIS)	$ 8,000,000
Separator Materials	2,800,000
Uranium Processing	5,200,000
Office of Civilian Reactor Development	$ 31,347,000
Actinide Recycle Division	$ 31,347,000
High Temperature Gas-Cooled Reactors	$ 5,947,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 815,000
Fuel Process Development	815,000
Materials Properties, Behavior, Characterization or Testing	$ 5,132,000
Fuel Materials Development	1,015,000
Fuel Development and Testing	4,048,000
Graphite Development	25,000
Metals Technology Development	44,000

OFFICE OF NUCLEAR ENERGY (Continued)

	FY 1993
Office of Civilian Reactor Development (continued)	
Liquid Metal Reactors	$ 25,400,000
Materials Properties, Behavior, Characterization or Testing	$ 25,400,000
Fuel Performance Demonstration	5,000,000
Pyroprocess Development	5,500,000
Fuel Safety Experiments and Analysis	4,000,000
Core Design Studies	3,000,000
Fuel Cycle Demonstration	6,500,000
ALMR Technology R&D	1,000,000
Program Management	400,000
Office of Space and Defense Power Systems	$ 24,930,000
Radioisotope Power Systems Division	$ 2,630,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 2,105,000
Development of Improved Thermoelectric Materials for Space Nuclear Power Systems	375,000
Development of an Improved Process for the Manufacture of DOP-26 Iridium Alloy Blanks and Exploratory Alloy Improvement Studies	1,165,000
Carbon-Bonded Carbon Fiber Insulation Production Maintenance, Manufacturing Process Development and Product Characterization	565,000
Materials Properties, Behavior, Characterization or Testing	$ 525,000
Characterization of State-of-the-Art Thermoelectric Materials and Specialized Testing of Critical RTG Materials	150,000
Development of an Improved Carbon-Carbon Composite Graphite Impact Shell Replacement Material	375,000

OFFICE OF NUCLEAR ENERGY (Continued)

	FY 1993
Space Reactor Power Systems Division	$22,300,000
Thermoelectric Space Nuclear Power Systems Technology - SP-100	$15,700,000
Thermoelectric Cell Materials Development	5,700,000
Reactor Materials	2,100,000
Heat Transport Materials	5,400,000
Shield Materials	500,000
Reactor Control Drive Materials	2,000,000
Thermionic Space Nuclear Power System Technology	$ 6,600,000
Thermionic Fuel Element (TFE) Verification Program (DOE)	4,000,000
Thermionic Space Nuclear Reactor Design and Technology Demonstration Plan (DOD)	2,600,000
Office of Naval Reactors	$52,000,000*

*This excludes $63 million for the cost of irradiation testing in the Advanced Test Reactor (ATR).

OFFICE OF NUCLEAR ENERGY

The Office of Nuclear Energy conducts materials research and development through the Office of Uranium Enrichment, which became the Office of Uranium Programs on September 5, 1993, the Office of Civilian Reactor Development, the Office of Space and Defense Power Systems, and the Office of Naval Reactors. Summarized below are the areas of research in which the Department is currently engaged.

Office of Uranium Programs

The Department of Energy was authorized by the Atomic Energy Act of 1954, as amended, to provide toll uranium enrichment services. Customers delivered natural uranium containing about 0.7 percent uranium 235 to one of DOE's plants and, for a fee, DOE returned material enriched to 2-5 percent in the isotope uranium 235 for use in nuclear power reactors.

Revenues received by DOE for the enrichment of uranium were retained and used for the specific purposes of offsetting costs incurred by the Department in providing uranium enrichment service activities as authorized by Section 201 of Public Law 95-238, not withstanding the provisions of Section 3617 of the Revised Statutes (31 USC 484). The sum appropriated is reduced as uranium enrichment revenues are received during a fiscal year so as to result in no net fiscal year appropriations. Total obligations for all uranium enrichment activities in FY 1993 was approximately $1 billion.

At present in the United States, uranium is enriched in gaseous diffusion plants that force uranium hexafluoride (UF_6) gas through porous barriers. These plants are located at Portsmouth, Ohio, and Paducah, Kentucky. A diffusion plant at Oak Ridge, Tennessee, used since World War II, was placed in standby in 1985 and shut down in 1987. In 1985, the DOE determined that of all the new and competing processes under study the Uranium-Atomic Vapor Laser Isotope Separation (U-AVLIS) process had the best potential for providing the lowest cost uranium enrichment in the future.

As a precursor to potential privatization of uranium enrichment in the United States, a federal agency, the United States Enrichment Corporation (USEC) was created. In conformance to the USEC's mission, most of the gaseous diffusion activities that were the responsibility of DOE were transferred to the USEC on July 1, 1993. U-AVLIS activities were transferred to the USEC on October 1, 1993. The USEC has elected to fund U-AVLIS through July 1994, and has indicated it will decide at that time whether to proceed with commercializing the technology. The gaseous diffusion plants are now being operated by the USEC under a lease arrangement with DOE.

Materials R&D activities in FY 1993 within the Office of Uranium Programs were varied and, for the most part, classified Restricted Data. Approximately $15 million was used in these endeavors. Paragraph summaries of these activities are presented in the following text. The DOE contact is A. P. Litman, (301) 903-5777.

Gaseous Diffusion

Uranium as found in nature contains about 0.7 percent uranium 235 and the remainder is essentially non-fissionable uranium 238. The fissionable characteristics of uranium 235 are necessary and useful for power reactor fuel. To date, most nuclear reactors designed for producing electrical power require uranium 235 concentrations between 2 and 5 percent. Presently, uranium is enriched to the desired uranium 235 assay levels in gaseous diffusion plants. These plants operate on the principle that lighter weight gaseous isotopes have slightly higher average velocities and thus can be made to diffuse through a porous barrier more rapidly than heavier species. Two streams can be created, one enriched in the lighter isotope and one depleted. Because enrichment for a single cycle, or stage, is very small, a cascade of stages is required. For example, a plant constructed for producing 4 percent assay U-235 would contain about 1200 stages. Although many other methods for enrichment are still being investigated and another production technique is being used in parts of Europe, diffusion plants today still provide approximately 90 percent of the world's enrichment services.

288. Barrier Quality — FY 1993 $2,960,000

These studies include evaluation of the short- and long-term changes in the separative capability of the gaseous diffusion barrier and methods to recover and maintain barrier quality in the production plants. This activity is a long-term undertaking and will be maintained at appropriate levels of effort in the future.

Keywords: Nuclear Fuel Isotopic Separations, Gaseous Diffusion, Barrier, Uranium

289. Materials and Chemistry Support — FY 1993 $3,810,000

This activity involves the routine materials and chemistry support for the diffusion plants. It includes the characterization of contaminant-process gas cascade reactions, the physical and chemical properties of UF_6 substances. Also, the work incorporates studies of the corrosion of materials, failure analyses, improving trapping technology, and alternative materials replacement on a continuing basis.

Keywords: Nuclear Fuel Isotopic Separations, Uranium, Gaseous Diffusion

Uranium-Atomic Vapor Laser Isotope Separation (U-AVLIS)

The U-AVLIS process is based on utilizing the differences in the electronic spectra of uranium isotopes to induce the selective absorption required for isotopic separation. The process utilizes the controlled vaporization of uranium atoms from metal feed followed by selective excitation and ionization of uranium 235 using tunable lasers in the visible regions of the spectrum. The uranium 235 ions can then be removed from the vapor in a separator using electromagnetic methods. Collection of the product is as a liquid metal that is allowed to solidify upon withdrawal.

In June 1985, DOE selected U-AVLIS for further development and possible future deployment into the uranium enrichment enterprise. The primary emphasis for the U-AVLIS program in FY 1993 was to continue large-scale demonstrations of the entire U-AVLIS enrichment process in full size equipment. Available resources were focused on these demonstration goals which permitted the uranium demonstration system at Lawrence Livermore National Laboratory to operate continuously for 112 hours and process over one ton of uranium. As shown below, the U-AVLIS materials activities in FY 1993 were in support of the separator system and the uranium processing activities. The latter technologies would have strong economic leverage for a U-AVLIS production plant. The overall goal of uranium processing is to develop and demonstrate low-cost paths for integrating the U-AVLIS metal feed and product into the existing uranium oxide/fluoride nuclear fuel cycle. The uranium processing activities have been conducted at the Oak Ridge diffusion plant site by Martin Marietta Energy Systems.

290. Separator Materials | FY 1993 $2,800,000

This activity includes the selection and testing of alternative candidate structural and component materials and coatings for the U-AVLIS separator system. It also supports the fabrication of full size separator components and subsystems for verification tests, plus the off line operation of a full size separator.

Keywords: Enrichment, Uranium, Laser Isotope Separation, Uranium-Atomic Vapor Laser Isotope Separation (U-AVLIS)

291. Uranium Processing FY 1993
$5,200,000

This year experiments and design studies concentrated on alternatives for preparation of U-AVLIS feed from uranium ore. To support the back end of the fuel cycle, the design of a demonstration system for U-AVLIS metal product conversion to precursor oxide for light water power reactor fuel was continued. Interfacing continued with the private sector converters, metal makers, and fuel fabricators to lay the groundwork for efficient integration of U-AVLIS requirements into the nuclear fuel cycle, if U-AVLIS is selected to be commercialized.

Keywords: Enrichment, Uranium, Laser Isotope Separation, Uranium-Atomic Vapor Laser Isotope Separation (U-AVLIS)

Office of Civilian Reactor Development

Actinide Recycle Division

The mission of the Actinide Recycle program is to conduct the research, development, and testing activities required to demonstrate by 1998 the technical and economic feasibility of an innovative and highly diversion resistant nuclear fuel cycle technology which, if successful, has the potential to mitigate the long-term radioactive waste management problem.

The program is focused on development of a synergistic system comprised of two technology components: (1) an integral fast reactor/closed metal fuel cycle processing and fabrication system, and (2) light water reactor actinide recycle technology development. This synergistic system has the potential to extract actinides from Light Water Reactor (LWR) spent fuel and ultimately utilize this material as fuel in an Advanced Liquid Metal Reactor (ALMR) to produce electricity.

The scope of these activities include the following areas: fuel cycles; design and performance of high quality core components for fuels, blanket, and control systems; development of the structural materials used in these components and systems; development and demonstration of equipment, processes, and procedures for fabricating, processing, handling, and producing binary and ternary metal fuels, and components; sodium technology; standards and quality assurance; assuring a reliable high quality economical fuel supply for LMRs; destructive and nondestructive testing, examination, and evaluation of core components and the facilities and capabilities for conducting such examination; responsibility for engineering and supporting facilities; associated safety, safeguards, and nonproliferation; maintaining competent capabilities in several contractor organizations that conduct the R&D activities and program. These activities are responsive to the administration's policies and goals, the Energy Policy Act of 1992 and, the DOE programs that support them.

In-reactor and out-of-reactor property evaluations are being conducted on core materials, clad/ducts, fuels and absorber materials. Through irradiation testing in EBR-II, the Actinide Recycle Programs are developing, qualifying, and verifying the use of reference, improved and advanced metal fuels, and boron carbide absorbers, including full-size driver and blanket fuels, and absorber pins and assemblies. Fabrication development, evaluation, qualification, and verification are conducted on improved and advanced alloys including in-reactor qualification of pins, ducts, and assemblies. Improved insulation is being developed for advanced electromagnetic pumps. The testing for these programs is primarily conducted at government laboratories: Argonne National Laboratory at Chicago, Illinois and Idaho Falls, Idaho; and Oak Ridge National Laboratory at Oak Ridge, Tennessee.

High Temperature Gas-Cooled Reactors

The objective of this program is to develop the base technology, systems concepts, and reactor designs which will permit the Government, in cooperation with utilities and private industry, to commercialize the High Temperature Gas-Cooled Reactor (HTGR) and High Temperature Gas-Turbine Reactor (HTGTR). The materials interests include those required for the development of coated particle fuels, graphite moderator and reflector blocks, graphite core support blocks and posts and vessels. The DOE contact for these projects is P. Williams, (301) 903-2022.

Materials Preparation, Synthesis, Deposition, Growth or Forming

292. Fuel Process Development — FY 1993 $815,000

DOE Contact: P. Williams, (301) 903-2022
General Atomics Contact: R. F. Turner, (619) 455-2306

This work includes establishing, characterizing, and qualifying fabrication processes and equipment for the preparation of microsphere fuel particles of uranium-oxycarbide (UCO) coated with layers of pyrolytic carbon (2) and silicon carbide (1). Major processing operations include solution mixing, kernel forming, drying, calcining, and sintering. Coatings are applied in a fluidized-bed furnace at temperatures up to 1600°C. The objective is to develop kernel fabrication and coating specifications, which yield very low fractions of defective particles. This work also includes development of the process for fabricating the fuel compacts (short rods).

Keywords: Fuel, Ceramics, Sintering, Coatings, Chemical Vapor Deposition

Materials Properties, Behavior, Characterization or Testing

293. Fuel Materials Development

FY 1993
$1,015,000

DOE Contact: P. Williams, (301) 903-2022
General Atomics Contact: R. F. Turner, (619) 455-2306

This work includes development of the technology base required to design, qualify, and license the fuel systems for near-term steam cycle, gas turbine and advanced process heat HTGRs. These efforts are focused on the low enriched uranium-oxycarbide (UCO) fuel system. Major elements of the work include the preparation and evaluation of irradiation specimens, development and verification of fuel performance and fission product transport models, and preparation and updating of fuel specifications and a design data manual.

Keywords: Fuel, Ceramics, Coatings, Microstructure, Radiation Effects, Diffusion, High Temperature Service

294. Fuel Development and Testing

FY 1993
$4,048,000

DOE Contact: P. Williams, (301) 903-2022
ORNL Contact: M. J. Kania, (615) 576-4856

This work supports development of the technology base required to design, qualify, and license the fuels systems for steam cycle and gas turbine HTGRs. These efforts are focused on the low-enriched uranium-oxycarbide (UCO) fuel system. Major elements of the work include services associated with the design, assembly, and irradiation of fuel capsules, and post-irradiation examination work in support of qualification and licensing of the reference fuel system. This work also includes support of International Cooperatives with West Germany and Japan, and a fuel test program in the French CEA COMEDIE Test Facility.

Keywords: Fuel, Ceramics, Coatings, Microstructure, Radiation Effects, Diffusion, High Temperature Service

295. Graphite Development

FY 1993
$25,000

DOE Contact: P. Williams, (301) 903-2022
ORNL Contact: T. Burchell, (615) 576-8595

This work supports the evaluation and qualification of graphite materials for applications in HTGRs. Major goals of this work are to develop high strength graphites with sufficient stability under irradiation to be qualified for core components, and with sufficient oxidation resistance to be qualified for core support components. The major element of this work is the development of graphite materials test specifications and failure criteria required for reliable design analyses.

This work supports international cooperation on the evaluation and qualification of graphite materials for applications in HTGRs. Major goals of this work are to develop high strength graphites with sufficient stability under irradiation to be qualified for core components, and with sufficient oxidation resistance to be qualified for core support components.

Keywords: Graphite, Ceramics, Irradiation Effects, Strength, Corrosion, High Temperature Service

296. Metals Technology Development — FY 1993 $44,000

DOE Contact: P. Williams, (301) 903-2022
General Atomics Contact: A. A. Schwartz, (619) 455-2416

This work includes activities to characterize and qualify the metallic materials selected for applications in the HTGR system. Tasks involve work to establish the database required for design validations and code qualifications. Principal alloy is Alloy 800H.

Keywords: Alloys, Strength, Corrosion, Joining, Microstructure, High Temperature Service

Liquid Metal Reactors

Materials Properties, Behavior, Characterization or Testing

297. Fuel Performance Demonstration — FY 1993 $5,000,000

DOE Contact: Andrew Van Echo, (301) 903-3930
ANL Contact: Leon C. Walters, (208) 533-7384

Establish U-Pu-Zr fuel fabrication process, irradiation performance characteristics and high burn-up capability. Lead test achieved 19.3 and 16.0 a/o burn-up in tests in EBR-II and FFTF respectively, and were removed for PIE. Program plans to complete initial off-normal testing in EBR-II, including RBCB and fabrication variable tests and overpower transient tests.

Keywords: Breeder Reactor, Actinides, Fuel, Burn-up

298. Pyroprocess Development FY 1993 $5,500,000

DOE Contact: Eli I. Goodman, (301) 903-2966
ANL Contact: James J. Laidler, (708) 252-4479

Establish technical feasibility of the proposed pyroprocesses including electrorefining, waste treatment, and waste form production processes. Program will complete selection of optimum cathode configuration for electrorefining process, conduct engineering scale (10 kg) demonstration of electrorefining with uranium, and run laboratory-scale demonstration of waste treatment and waste form production processes. Process optimization and development of a commercially applicable flow sheet will be carried out.

Keywords: Waste Treatment, Electrorefining, Pyroprocesses

299. Fuel Safety Experiments and Analyses FY 1993 $4,000,000

DOE Contact: Harry Alter, (301) 903-3766
ANL Contact: Dean R. Pedersen, (708) 252-3335

Conduct analyses and experiments required for the demonstration of the safety performance of metallic fuel in fast reactor systems. Include transient fuel behavior, validated models and codes which describe fuel behavior, and safety mechanisms which contribute to inherent safety. Program will initiate analysis of high plutonium fuel to expand the database pertaining to safety margins, failure thresholds, and transient behavior.

Keywords: Reactor Safety, Actinides, Fuel, Inherent Safety, Transient Behavior

300. Core Design Studies FY 1993 $3,000,000

DOE Contact: Philip B. Hemmig, (301) 903-3579
ANL Contact: David C. Wade, (708) 252-4858

Provide direct support in developing optimized metallic core designs for ALMR and establish a validated design and safety analysis methodology suitable for initiation of detailed design and for licensing interactions. Conduct studies of fuel management strategies for the closed fuel cycle, including physics and economic impacts of self-sufficient uranium start-up versus maximized ratio start-up of sequential plant modules. Emphasize actinide self-consumption in the IFR metal fuel cycle to support the overall IFR waste management strategy. Develop materials control and accountancy system for testing in IFR Fuel Cycle Demonstration.

Keywords: Actinides, Reactor Design, Metal Fuel

301. Fuel Cycle Demonstration FY 1993
$6,500,000

DOE Contact: John Williams, (301) 903-9585
ANL Contact: M. J. Lineberry, (208) 533-7434

Provide for start-up of fuel cycle comprehensive remote operations demonstration including completion of equipment in FCF and start-up with irradiated fuel. Proceed to fabrication of first recycled U-Pu-Zr fuel assembly. Quantify the ultimate fuel cycle economics through development of commercial fuel cycle facility design and cost estimates.

Program will continue equipment development activities for remotized in-cell application, including reusable mold concept for injection-casting furnace, semi-automated pin processor, engineering-scale pyroprocessing equipment, etc. Refine and update commercial-scale fuel cycle facility design and cost estimates, including sensitivities to throughput requirements and develop initial set of prototype equipment systems.

Keywords: Fuels, Injection-Casting, Pyroprocessing, Metal Fuel Cycle, Remotized

302. ALMR Technology R&D FY 1993
$1,000,000

DOE Contacts: Philip B. Hemmig, (301) 903-3579
ANL Contact: Yoon I. Chang, (708) 252-4856

Comprehensive inherent safety testing with EBR-II, including incorporation of advanced reactor control technology and diagnostics systems, to demonstrate the passive safety aspects of the ALMR. Test and analysis support for ALMR mechanical components such as electromagnetic sodium pumps, auxiliary cooling systems, etc.

Keywords: Inherent Safety, Control Technology, Passive Safety, Sodium Pump

303. Program Management FY 1993
$400,000

DOE Contacts: Philip B. Hemmig, (301) 903-3579
ANL Contact: Yoon I. Chang, (708) 252-4856

Provide management for the ANL-LMR programs.

Keywords: Management

Office of Space and Defense Power Systems

Radioisotope Power Systems Division

The Radioisotope Power Systems Division responsibilities include the development, system safety and production of radioisotope powered thermoelectric generators (RTG) and dynamic power systems for NASA and DOD space and terrestrial applications and advancing base technologies for these power systems. Thus, applied materials research programs are supported in the areas of thermoelectric materials and devices, high temperature heat source materials, materials systems compatibility and safety related materials characterization and testing.

Materials Preparation, Synthesis, Deposition, Growth or Forming

304. Development of Improved Thermoelectric Materials for Space Nuclear Power Systems

FY 1993
$375,000

DOE Contact: W. Barnett, (301) 903-3097
Iowa State University, Ames Laboratory Contact: B. Cook, (515) 294-9673

The prime objective of this program is to apply and exploit the capabilities of the mechanical alloying process for the development of improved performance silicon-germanium (Si-Ge) type thermoelectric materials. The goal or target properties are average Figure of Merits, Z of 0.8 and 1.2 x 10^{-3}/°C over the temperature range 300 to 1000°C for "P" and "N" type materials, respectively. About 15 percent of the program was directed at exploring new potential thermoelectric materials.

During FY 1993, major emphasis continued to be placed on the optimization of mechanical alloying process and consolidation parameters for the production of low oxygen materials. Methods were developed to produce both "N" and "P" type Si-Ge type materials exhibiting improved thermoelectric properties, typically 15 to 30 percent above those of standard Si-Ge materials. Scale-up activities were initiated. Evaluation of hot isostatic pressing as an alternate process to vacuum hot pressing was initiated. Techniques for adding nano-size second phase particulates continued to be explored. Mechanical alloying continues to show excellent promise for the production of thermoelectric materials.

Keywords: Mechanical Alloying, Consolidation of Powder, Powder Synthesis, Semiconductors, Thermoelectrics

305. Development of an Improved Process for the Manufacture of DOP-26 Iridium Alloy Blanks and Exploratory Alloy Improvement Studies — FY 1993 — $1,165,000

DOE Contact: W. Barnett, (301) 903-3097
RNL Contact: E. P. George, (615) 574-5085

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. This process has proven effective in the FY 1993 production of DOP-26 alloy blanks and foil fabrication of the clad vent sets for the Cassini Mission. Production yields have exceeded our expected goals.

New computer-controlled electron beam melting and vacuum consumable arc melting facilities were qualified for use in the production process. Continued product characterization studies, particularly for simulated service conditions, have shown properties equivalent or superior to prior process product. Studies of alternate iridium alloy doping agents were continued with cerium plus low levels of thorium offering the most promise.

Keywords: Consumable Arc Melt, Extrusion, Noble Metal

306. Carbon-Bonded Carbon Fiber Insulation Production Maintenance, Manufacturing Process Development and Product Characterization — FY 1993 — $565,000

DOE Contact: W. Barnett, (301) 903-3097
ORNL Contact: C. E. Weaver, (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 1993 program encompassed (1) maintenance of production capability by both tube and plate billet production through the year, and (2) product characterizations with the focus on product uniformity and high temperature, ambient to 2000°C, thermal diffusivity and conductivity. Evaluation of the validity of current thermal diffusibility measurement methods and data reduction correction techniques for determination of high temperature (1000 to 2000°C) thermal conductivity of CBCF type materials was initiated. Preliminary exploratory studies of methods to lower very high temperature thermal conductivity of CBCF type structures was initiated.

Keywords: Insulators/Thermal, High Temperature Service, Fibers

Materials Properties, Behavior, Characterization or Testing

307. Characterization of State-of-the-Art Thermoelectric Materials and Specialized Testing of Critical RTG Materials — FY 1993 $150,000

DOE Contact: W. Barnett, (301) 903-3097
Iowa State University Contact: B. Cook, (515) 294-9673

This program is concerned with the evaluation and characterization of state-of-the-art Si-Ge/GaP and other "improved" silicon-germanium type thermoelectric materials. In FY 1993 a major effort was initiated for the development and validation of a steady state radial heat flow method for the measurement of the very high temperature thermal conductivity of CBCF insulation.

Keywords: Semiconductor, Thermoelectrics, Thermal Conductivity

308. Development of an Improved Carbon-Carbon Composite Graphite Impact Shell Replacement Material — FY 1993 $375,000

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 materials.

During 1993 the test matrix was expanded to include the standard FWPF material and six different reinforcement architectures. Procurement of test materials was completed and machining of test samples was initiated. A novel test method for measuring energy absorption during high velocity impact was developed and evaluation was initiated.

Keywords: Composites, Carbon-Carbon

Space Reactor Power Systems Division

The Space Reactor Power Systems Division (NE-52) has the responsibility to technically direct the unique federal functions in the United States of developing, demonstrating, and delivering nuclear reactor power systems for military and civilian space missions, and for special military terrestrial applications. Programs involve the design, testing, and validation of nuclear power systems for use in space and harsh environments. Activities include:

- space nuclear reactor power and propulsion system design,
- nuclear reactor fuels materials and components development and performance demonstration,
- heat transport, power conversion, and shielding technology, components, and system development and demonstration,
- computer analysis methods development and application,
- ground and flight system safety analysis.

Thermoelectric Space Nuclear Power System Technology

309. SP-100 Ground Engineering System Project — FY 1993 $15,700,000

DOE Contact: Lyle Rutger, (301) 903-6470
Martin Marietta Astro Space Contact: H. S. Bailey, (408) 365-6301

The objective of this program is to develop space reactor power system components for use in future civil, commercial, and defense applications. Included in this comprehensive program are numerous activities related to materials development, fabrication, and testing.

Principal materials activities are:

Thermoelectric Cell Materials Development ($5,700,000) - Fabrication of Si Ge multicell power converters incorporating Al_2O_3 insulators, niobium fiber compliant pads, tungsten-graphite electrodes using a variety of coatings, foils, brazes, and hot isostatic pressure bonds.

Reactor Materials ($2,100,000) - Development and testing of a high-temperature high-strength niobium-zirconium, 1 percent carbon alloy (NblZr), including techniques for processing the alloy and fabricating components from the alloy. Other materials work pursued included the testing of bonded Rhenium-NblZr fuel clad and other refractory special use materials.

Heat Transport Materials ($5,400,000) - Techniques were developed to fabricate a thermoelectric electromagnetic pump using explosive forming of niobium alloy ducts, and joining with thermoelectric cells, permanent magnets and Nb-clad copper busbars.

Shield Materials ($500,000) - Irradiation testing of lithium-hydride radiation shield material to characterize the behavior of lithium-hydride in prototypic radiation-temperature environments.

Reactor Control Drive Materials ($2,000,000) - Development of wear-resistant surfaces, bearings, and lubricants for operation in a high-temperature-radiation vacuum environment.

Keywords: Thermoelectric Cells, Refractory Metals, Tribology, Irradiation Testing, Space Reactors

Thermionic Space Nuclear Power System Technology

In June 1991, DOE, the Strategic Defense Initiative Organization, now the Ballistic Missile Defense Organization (BMDO), and the U.S. Air Force signed a Memorandum of Understanding establishing a Thermionic Space Nuclear Power System Technology Program, jointly funded by the three agencies, and managed by the DOE Headquarters Office of Nuclear Energy. The focus of the program is the Thermionic Space Nuclear Reactor Design and Technology Demonstration program, but also encompasses the Thermionic Fuel Element (TFE) Verification program which was initiated in 1986.

310. Thermionic Fuel Element (TFE) Verification Program

FY 1993
$4,000,000 - DOE
$0 - DOD

DOE Contact: C. Brown, (301) 903-6924
General Atomics Contact: R. Dahlberg, (619) 455-2997

The TFE Verification Program was initially established in 1986 to resolve the outstanding feasibility associated with the use of in-core TFEs in space reactor power systems. It is primarily aimed at demonstrating the long-term operational lifetimes of TFE materials, components, and fully-assembled TFEs through accelerated and real-time testing at high temperatures and under high radiation environments. General Atomics is the prime contractor. The main technical issues are TFE electrical characteristics, performance and swelling (constrained and unconstrained) of uranium dioxide fuel forms, ceramic insulator and seal integrity, and radiation resistance of graphite materials used for low-pressure cesium storage. High-temperature metallic materials involved are tungsten for the emitter (and fuel containment) and niobium for the collector. The outer diameter of the TFE is stainless steel which is cooled by flowing liquid sodium potassium (NaK). Alumina and yttria ceramics have been tested for insulators and seals. Graphite has been shown to maintain sufficient structural integrity to be used for cesium storage.

Keywords: Nuclear, Thermionic, Uranium Dioxide, Ceramics, Graphite, Tungsten, Niobium

311. Thermionic Space Nuclear Reactor Design and Technology Demonstration Plan

FY 1993
$0 - DOE
$2,600,000 - DOD

DOE Contact: C. Brown, (301) 903-6924
Rocketdyne Contact: J. Mills, (818) 586-9382
Space Power, Inc. Contact: J. Wetch, (408) 434-9500

The overall objective of this program is to design, develop, demonstrate, and advance the technology for a thermionic space nuclear reactor power system for military applications to a level consistent with performing a possible flight demonstration around the turn of the century. A 40 kWe end-of-life point design is the baseline using technology that is broadly applicable over the range of 5-40 kWe. Two separate contract teams began work in 1992, Rocketdyne Division of Rockwell International and Space Power, Inc. Both contractors have Russian subcontractors, and both are designing in-core TFE systems. A key difference is that Rocketdyne is designing a multicell TFE consisting of several individual thermionic cells connected in series, whereas Space Power, Inc., is designed a single-cell TFE where the TFE runs the entire length of the reactor core. In addition to testing of TFE materials and components, moderator and NaK cooling loop components will be tested.

Keywords: Nuclear, Thermionic, Uranium Dioxide, Ceramics, Graphite, Monocrystal, Molybdenum, Tungsten, Niobium, Yttrium Hydride, Zirconium Hydride, Hydrogen Getter

Office of Naval Reactors

The materials program supports the development and operation of improved and longer life reactors and pressurized water reactor plants for naval nuclear propulsion.

The objective of the materials program is to develop and apply, in operating service, materials capable of use under the high power density and long life conditions required of naval ship propulsion systems. This work includes irradiation testing of reactor fuel, poison, and cladding materials in the Advanced Test Reactor at the Idaho National Engineering Laboratory. This testing and associated examination and design analysis demonstrates the performance characteristics of existing materials as well as defining the operating limits for new materials.

Corrosion, mechanical property, and wear testing is also conducted on reactor plant structural materials under both primary reactor and secondary steam plant conditions to confirm the acceptability of these materials for the ship life. This testing is conducted primarily at two Government laboratories—Bettis Atomic Power Laboratory in Pittsburgh and Knolls Atomic Power Laboratory in Schenectady, New York.

One result of the work on reactor plant structural material is the issuance of specifications defining the processing and final product requirements for materials used in naval propulsion plants. These specifications also cover the areas of welding and nondestructive testing.

Funding for this materials program is incorporated in naval projects jointly funded by the Department of Defense and the Department of Energy. This funding amounts to approximately $115 million in FY 1993 including approximately $63 million as the cost for irradiation testing in the Advanced Test Reactor. The Naval Reactors contact is Robert H. Steele, (703) 603-5565

OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT

	FY 1993
Office of Civilian Radioactive Waste Management - Grand Total	$1,700,000
Materials Properties, Behavior, Characterization or Testing	$1,400,000
Waste Packages	$1,400,000
Device or Component Fabrication, Behavior or Testing	$300,000
Defense Waste Canisters	$300,000

OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT

Materials research is ongoing in the Office of Civilian Radioactive Waste Management in two areas: the development of canisters for containing the glass waste from the Defense Waste Processing Facility at the Savannah River Laboratory and the design of waste packages for eventual geologic disposal.

Materials Properties, Behavior, Characterization or Testing

312. Waste Packages — FY 1993 $1,400,000

DOE Contact: Dean Stucker, (702) 794-7275
Babcock and Wilcox Contact: Hugh Benton, (702) 794-1891

The modest materials effort for waste package design continued during the fiscal year. The scientific investigation plan was rewritten to include testing of corrosion-allowance materials. Equipment for testing these materials under humid and dry conditions was procured and set up. Preliminary work was conducted on thermal, criticality and structural analysis. The effort focused on new multi-purpose canister designs. Corrosion rates, cladding performance and design data were provided to the total system performance assessment effort.

Keywords: Waste Packages, Ferrous Metals, Geologic Repository

Device or Component Fabrication, Behavior or Testing

313. Defense Waste Canisters — FY 1993 $300,000

DOE Contact: Larry A. Hinson, (803) 557-1047
Westinghouse Contact: John Harbour, (803) 725-8725

Canisters for containing the glass waste from the Defense Waste Processing Facility at the Savannah River Technology Center (SRTC) are presently being produced by a conventional rolled and welded fabrication process for the cylindrical center section of the canister. The canister is completed by welding a top head and a bottom piece to the ends of the center section and a nozzle to the top head. Alternative fabrication processes are being investigated, including a deep-drawn canister and a spun (or flow-formed) canister.

Two deep-drawn prototype canisters fabricated by Norris Division of NI industries have been delivered to SRTC. The fabrication process begins with a forged cup of A314-88 304L stainless steel (0.75% max Si) that is deep-drawn to obtain canister dimensions of 118 inch length by 2 feet OD with a wall thickness of ⅜ inch (½ inch on the bottom). The initial prototype has one central girth weld at half-height. A nozzle section is also welded to the top. Testing of these canisters will involve filling with glass (at 500°C) followed by dimensional measurements, possible drop testing (bottom and angled top drops), metallographic examination and mechanical tests.

Two spun canisters have been ordered by SRTC from Spin Forge, Inc., with delivery expected in June 1994. The process begins with a forged and machined cup using A336 304L stainless steel, and has the capability of producing a spun cylinder to which a head can be electron beam welded. Tests similar to those described above are planned for these canisters.

Keywords: Waste Canisters, Glass Waste, Testing

OFFICE OF DEFENSE PROGRAMS

	FY 1993
Office of Defense Programs - Grand Total	$122,589,000
The Weapons Research, Development and Test Program	$122,589,000
Sandia National Laboratories	$ 65,443,000*
Engineered Materials and Processes Programs	$ 65,443,000*
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 6,304,000
Biomimetic Processing of Oriented Crystalline Ceramic Layers	300,000
Boron-Rich Solids	290,000
CVD Diamond/Diamond Powder Composites	90,000
CVD Diamond Growth Models	150,000
Development of LiF Coated Anodes for PBFA II	100,000
Diamond-Like Carbon Films	250,000
Improved Mechanical Properties of Ceramic Ferrites by Diffusion Induced Grain Boundary Migration (DIGM)	25,000
Ion Beam Modification of PLZT Thin Films	50,000
Nanoscale Engineering of Smart Membranes	50,000
Optical Properties of Potassium Titanyl Phosphate Derivatives	30,000
Sealing Glasses for Titanium and Titanium Alloys	397,000
Thermal Stability Studies of Diamond-Like Carbon Films	100,000
Chromate-Free Corrosion Resistant Coatings for Aluminum	400,000
Dynamic Wetting and Spreading of Solder	40,000
High-Temperature and Organic Superconductors	600,000
Intermetallic Compound Growth in Solder Joints	240,000
Nucleation in Chemical Vapor Deposition on Metal Films	80,000
Synthesis of Ti and TiO_2 Nanoparticles	40,000
Titanium Casting Face-Coat Development	291,000
Unalterable Magnetic Stripes	180,000
Bridged Poly-germsesquioxanes and Polysilsequioxanes	50,000

*Total funding includes unreported work (projects with proprietary, patentable or classified information).

OFFICE OF DEFENSE PROGRAMS (Continued)

	FY 1993
Sandia National Laboratories (continued)	
Engineered Materials and Processes Programs (continued)	
Materials Preparation, Synthesis, Deposition, Growth or Forming (continued)	
Carbon Film Nanoband Sensors	80,000
Development of a Scaleable, Flat-Flame Technology for the Synthesis of Diamond Films	150,000
Development of Solid Polymer Electrolytes for Lithium Rechargeable Batteries	100,000
Fuel Cell Applications for Novel Metalloporphyrin Catalysts	300,000
Fullerene-Xylene Copolymers	50,000
Low Dielectric and High Temperature Films for Multichip Modules	230,000
Microengineered Materials Development	150,000
Moisture Resistant Printed Wiring Board Materials	296,000
Porous Carbon Electrodes from a Microcellular Polymer	275,000
Supercritical Fluid Precipitated Polymer Membranes	200,000
A New Method for Promoting Photoresist Adhesion on Tungsten Films for Self-Aligned Refractory Gates on GaAs	50,000
Comparison of BOH and SiOH Reactivities in Boron-Doped SiO_2 Chemical Vapor Deposition Using Trimethyl Borate and Tetraethyl Orthosilicate	200,000
Magnetotransport in Strongly Coupled Double-Quantum-Well Structures	70,000
Particles in Rf Plasmas	150,000
The Growth of InSb Using Tri(dimethylamino)antimony and Trimethylindium	250,000
Materials Structure and Composition	$ 1,916,000
Structure of Microporous Glasses Derived from Borosilicates	401,000
Electronic Structure of Advanced Materials	150,000
Lubricant Films Deposited by Plasma Decomposition	72,000

OFFICE OF DEFENSE PROGRAMS (Continued)

	FY 1993
Sandia National Laboratories (continued)	
Engineered Materials and Processes Programs (continued)	
Materials Structure and Composition (continued)	
Phase Separation Kinetics in a Micelle System	190,000
Chemical Modification of Fullerenes	200,000
Electrorheological Fluids	150,000
Electrorheological Fluids in Shear Flow	100,000
Molecular Modeling of Polymer Liquids and Blends	363,000
Tailoring Interfaces with Block Copolymers	130,000
Thermal Decomposition Reaction Mechanisms of Bis(1-fluoro-1,1-dinitroethyl) formal (FEFO) and Bis(1-fluoro-1,1-dinitroethyl)difluoroformal (DFF)	100,000
Microstructures of InGaP Alloys: Ordering and Decomposition	60,000
Materials Properties, Behavior, Characterization or Testing	$19,315,000
Theoretical Calculation of the Direct to Indirect Transition in InAlGaP	35,000
Visible Light Emission from Porous Silicon Nanostructures	60,000
Advanced Energetic Materials	450,000
Ceramic and Glass Fracture	45,000
Characterization of Optical Fibers	63,000
Chemical Processing of Ceramic Thin Films	183,000
Crystallization of Solution-Derived Ferroelectric Thin Films	110,000
Diamond-Like Carbon Coatings	300,000
Diamond-Like Carbon Films for Protected Volumes	390,000
Dynamic Response of Concrete	100,000
Dynamic Testing of Armor Ceramics	150,000
Electronic Ceramic Granules for Lightning Arrestor Connectors (LAC)	160,000
Ferroelectric Thin Films for Nonvolatile Memories	500,000
Fluorination of Diamond and Diamond-Like Carbon Films	65,000

OFFICE OF DEFENSE PROGRAMS (Continued)

	FY 1993
Sandia National Laboratories (continued)	
Engineered Materials and Processes Programs (continued)	
Materials Properties, Behavior, Characterization or Testing (continued)	
Lightning Arrestor Connector (LAC) Granule Fracture Resistance Tests	80,000
Massively Parallel Simulation of Grain Boundary Evolution	151,000
Metal/Ceramic Brazing by Active Filler Metals	83,000
Silicon Nitride to Metal Joining	75,000
Structural Relaxations in Alkali Phosphate Glasses	111,000
Structure and Property Changes in Irradiated Glasses	20,000
Thixotropic Electrorheological Fluids	45,000
TiO_2-SiC Photocatalysts	40,000
Advanced Exclusion Barriers Study	750,000
Capillary Flow Solderability Study	120,000
Creep Properties of Silver-Copper and Silver-Copper-Titanium Braze Alloys	30,000
Diamond-Like Carbon Films for Stronglinks	478,000
Electrochemical Studies of Al-Based Intermetallic Precipitate Phases	65,000
Electrophoretic Deposition of Solid Lubricants	236,000
Fusion Welding of Advanced Borated Stainless Steels	300,000
High Energy Shock Physics	250,000
High Temperature Mechanical Properties of 82Au-18Ni and 62Cu-35Au-3N Braze Alloys	40,000
Intelligent Processing of Thin-Section Welded Assemblies	160,000
Lightweight Materials for Automotive Applications	692,000
Liquid Metal Surface Chemistry	50,000
Modeling the Vacuum Plasma Spray Process	34,000
Nanocluster Electronic Structure	150,000
QuikForm—Experimental Characterization Tool Development	90,000
Reaction Mechanisms of Solder Fluxes	120,000
Solid Film Lubricants for WR Applications (PRESS Support)	22,000
Solidification and Weldability of ThermoSpan Alloy	40,000
Solidification of Superalloys	200,000

OFFICE OF DEFENSE PROGRAMS (Continued)

	FY 1993
Sandia National Laboratories (continued)	
Engineered Materials and Processes Programs (continued)	
Materials Properties, Behavior, Characterization or Testing (continued)	
Specialty Metals Processing Consortium	4,197,000
Stimulated Chemistry of Amonia (NH_3) on Surfaces	70,000
Stockpile Support Capabilities	3,000,000
Surface Chemistry Soldering	200,000
Thermal Spray Technology for Cylinder Bore Coatings	780,000
Thermomechanical Fatigue Modeling	395,000
Weldability of an Advanced Titanium Alloy	20,000
Wetting and Mechanical Behavior of Interfacial Intermetallics in Solder Joints	80,000
Alkylene- and Arlyene-Bridged Polysiloxanes	75,000
Characterization of Moisture Adsorbed at Interfaces	100,000
Design and Fabrication of Inertial Confinement Fusion	245,000
Development of Improved Methods for Predicting and Validating Polymer Lifetimes in Weapon Environments	250,000
Electronic Properties of Fullerenes	38,000
Electronic Properties of Organic Materials	277,000
Fundamentals and Materials Studies on Fullerenes	200,000
Gas Permeation in Fullerenes	45,000
Low Melting "Weak Link" Dielectrics	60,000
One Container Sticky Foams for Safeguard	80,000
Optical Weak-Link Materials Development	80,000
Photo-Detoxification of Explosive Waste Streams	50,000
Resist Characterization for Soft-X-ray Projection Lithography	50,000
Role of Excited-State Singlet Oxygen in Polymer Degradation	200,000
Smart Materials and Structures	200,000
Techniques to Characterize Outgassing from Polymeric Microenvironments	800,000
Electrostatic Chuck Research	50,000
Hot Filament Carbon Chemical Vapor Deposition	75,000
Materials Science at High Pressure	435,000
Modeling Processing Effects for Porous Silicon Layers	20,000
Nonlinear Electrical Phenomenon in rf-Excited Plasmas	200,000

OFFICE OF DEFENSE PROGRAMS (Continued)

	FY 1993
Sandia National Laboratories (continued)	
Engineered Materials and Processes Programs (continued)	
Device or Component Fabrication, Behavior, or Testing	$10,822,000
Photosulfidation as Passivation Process for III-IV Compound Semiconductors	43,000
Polaronic Phenomena in Solids	100,000
Semiconductor Surface Defects	80,000
Technique Developed for Measurement of Electric Fields in High-Frequency Discharges	230,000
Variable-Temperature STM Measurements of Step Kinetics	80,000
Computer-Aided Advanced Ceramic Manufacturing	50,000
Ferroelectric Films for Optical Storage and Processing	700,000
Field Emission Flat Panel Displays	67,000
Ion Beam Modification of Glasses	50,000
Micro-Miniature Refrigerator Components	70,000
New Materials for SEMATECH Photolithography Stage	240,000
Thin-Film Decoupling Capacitors	500,000
Thin Film Solder Bonds for Sensor Assembly	208,000
Thin Film Transistors	50,000
Certification and Specification Exception Release Remediation Activities for MC4190M Thermal Battery	20,000
Copper on Teflon	75,000
FASTCAST Consortium	1,313,000
Laser Soldering of Sn Plated Brass Integrator Assembly Housings	20,000
Laser Welding Optimization Software	100,000
Lead-Free Solders for Electronics Assembly	278,000
New Common-Domain Specifications and Applications for Invar-Type Alloys	30,000
Printed Wiring Board and Interconnect Systems	200,000
SMARTWELD II—An Intelligent System for Concurrent Engineering	1,700,000
Substitute Cleaner for Lithium Thionyl Chloride Batteries	140,000
Supercritical Fluid View Cell	45,000

OFFICE OF DEFENSE PROGRAMS (Continued)

FY 1993

Sandia National Laboratories (continued)

Engineered Materials and Processes Programs (continued)

Device or Component Fabrication, Behavior, or Testing (continued)

Thin Film Solder Conductor as Thermal Weak Link	275,000
Cleaning Related Processes for Printed Wiring Boards	400,000
Development of Environmentally-Sound Removable Encapsulants	150,000
Endpoint Indicator for Printed Wiring Board	25,000
Environmental O-ring Seals—Properties, Aging and the Argon Method	250,000
Flexible Carbon Anodes for High Performance Batteries	100,000
Fully Integrated Optical Hydrogen Sensor	50,000
Lithography Employing Surface and Near Surface Imaging	250,000
MDA-Free Epoxy Encapsulant Formulations	268,000
Nonlinear Optical Materials and Devices Development	175,000
Organic Composite Materials	200,000
Toluene Diisocyanate-Free Rigid Polyurethane Encapsulation Foams	200,000
Commercial Development of Porous Silicon Humidity Sensors	20,000
Engineered Photocatalysts for the Detoxification of Waste Water	300,000
Folded Cavity Second Harmonic Generation of a Nd:YAG Laser	30,000
Gate-Controlled "Artificial Impurities" Fabricated with Nanostructure Airbridges	100,000
High Sensitivity Moisture Sensors	1,200,00
Hybrid Shubnikov-deHaas-Photoluminescence Analysis of 2-D Electron Density in PHEMT Structures with Heavily-Doped Contact Layers	50,000
Matrixed Field Emitter Arrays	40,000
Midwave (4 m) Infrared Emitters with Biaxially Compressed InAsSb Active Regions	200,000
Phosphorus-Containing Precursors for III-V Semiconductors	50,000
Rapid Methods for Calculating Reflectance Spectra of Growing Semiconductor Films for Applications in Process Control	100,000

OFFICE OF DEFENSE PROGRAMS (Continued)

	FY 1993
Sandia National Laboratories (continued)	
Engineered Materials and Processes Programs (continued)	
Instrumentation and Facilities	$12,086,000
Real Time Control of MBE by Optical Based Flux Monitoring (OFM)	200,000
Semiconductor Wafer Cleaning	810,000
Sensors for Process Control	30,000
Shallow Zn Ion Implantation for GaAs Junction Field Effect Transistors	200,000
Surface Science of Compound Semiconductor Epitaxy	300,000
Theory and Computer Simulation of Low-Temperature, rf-Driven Plasmas Relevant to Plasma Processing	150,000
Analytical Capabilities	4,500,000
Analysis of Crystalline Silicotitanate (CST) for Cs-Extraction from Radwaste	112,000
Beam Characterization of a Materials Processing CO_2 Laser	12,000
Booster for Tandem	1,200,000
Characterization of Quartz Resonators	40,000
Chemometrics Methods Developments	220,000
Diagnostics for Supercritical Water Oxidation of Hazardous Wastes	70,000
Helium Leak Testing of Integrated Circuit Packages	12,000
Ion Induced Roughening and Smoothing of SiO_2 Films	80,000
Massively Parallel Quantum Chemistry Code Development	100,000
Mechanism of Lithium Ion Production from the PBFA II Anode	100,000
Noninvasive Alcohol Monitor	35,000
Optical Diagnostics for Process Control in Steelmaking	315,000
Parallel Numerical Libraries for Materials Modeling Programs	201,000
Phase Identification in the Scanning Electron Microscopy by Backscattered Electron Kikuchi Patterns	60,000
Porous Silicon Photoluminescence and K-Map X-ray Diffraction	100,000
Quantitative Materials Characterization by Nuclear Microprobe Analysis	770,000

OFFICE OF DEFENSE PROGRAMS (Continued)

	FY 1993
Sandia National Laboratories (continued)	
Engineered Materials and Processes Programs (continued)	
Instrumentation and Facilities (continued)	
Resonant Ionization Detection of Atomic H from Surfaces	70,000
Scanning Tunneling Microscope for CVD Processes	80,000
Sorting of Waste Plastics Using Near Infrared Spectroscopy and Neural Networks	254,000
Studies on Triboluminescent Materials	25,000
Techniques for Measuring Outgassing Characteristics of Polycarbonate Polymers	140,000
Tritium Monitor	50,000
Weapon Component Characterization for Disposition	400,000
X-ray Reflectivity Characterization of Thin Film Structures	100,000
Microstrain in Diamond Films	20,000
Scattering Center Development	150,000
Beam Quality Measurements and the Proposed ISO Standard	100,000
High Energy, High Flux Pulsed Ion Beams for Surface Modification	300,000
Medical Applications of Ion Beam Induced Radiation	250,000
Photoluminescence Analysis of Tetragonal Mercuric Iodide	30,000
Radiation Microscopy	200,000
Time-of-Flight Heavy Ion Backscattering Spectroscopy	300,000
Lawrence Livermore National Laboratory	$30,119,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 4,473,000
Inorganic Aerogels	100,000
Organic Aerogels	325,000
Engineered Nanostructure Laminates	330,000
Sol Gel Coatings	325,000
KDP Growth Development	600,000
Advanced Finishing Development	850,000

OFFICE OF DEFENSE PROGRAMS (Continued)

	FY 1993
Lawrence Livermore National Laboratory (continued)	
Materials Preparation, Synthesis, Deposition, Growth or Forming (continued)	
Synthesis and Scale-up	250,000
Doped Polymers for ICF	200,000
Plasma Polymer Coating Development	900,000
Polymer Films by RF Sputtering	125,000
Excimer Laser Micromachining	468,000
Materials Properties, Behavior, Characterization or Testing	$ 4,313,000
Advanced Synchrotron Radiation Study of Materials	365,000
Structural Transformation and Precursor Phenomena	200,000
PALX Low Vulnerability High Explosives for 155mm Artillery Shells	200,000
Very High Energy Density Materials	1,350,000
Interfaces, Adhesion and Bonding	300,000
Laser Damage: Modeling and Characterization	400,000
KDP Characterization	300,000
Damage Testing	730,000
Energy Transfer Dynamics in Energetic Materials	308,000
Processing-Structure-Property Correlation in Laminated Metal Composites	160,000
Instrumentation and Facilities	$21,333,000
Scanning Tunneling Microscopy (STM) and Atomic Force Microscopy (AFM)	546,000
Pyrochemical Technology Development	5,000,000
Thermoelectric Materials with Exceptional Figures of Merit	325,000
Capacitive Deionization as an Alternative to Ion Exchange	795,000
Trilayer Josephson Junctions (Technology Transfer Initiative)	250,000

OFFICE OF DEFENSE PROGRAMS (Continued)

	FY 1993
Lawrence Livermore National Laboratory (continued)	
Instrumentation and Facilities (continued)	
Critical Parameters of Superconducting Materials LDRD (Departmental)	427,000
Lithium Cell Development	500,000
High Explosives Lead Laboratory Program	1,000,000
Environmentally Safe Disposal of Explosive Wastes: SERDP Project	1,800,000
Laminated Metal Composites for Aerospace Applications	700,000
Fatigue of Metal Matrix Composites	300,000
Molecular Dynamics Simulation Studies of Radiation Effects in Solids	60,000
Fundamental Studies of Particle-Solid Interactions	180,000
Radiation Effects in Materials for Inertial Confinement Fusion	50,000
Novel Materials for Optoelectronics and Photonics	500,000
Uranium Manufacturing Lead Lab Program	3,900,000
Plutonium Manufacturing Lead Lab Program	5,000,000
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
Plasma-Flame Spraying Technology	300,000

OFFICE OF DEFENSE PROGRAMS (Continued)

	FY 1993
Los Alamos National Laboratory (continued)	
Materials Preparation, Synthesis, Deposition, Growth or Forming (continued)	
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

OFFICE OF DEFENSE PROGRAMS (Continued)

	FY 1993
Los Alamos National Laboratory (continued)	
Laboratory Directed Research and Development	$10,982,000
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
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

OFFICE OF DEFENSE PROGRAMS (Continued)

	FY 1993
Los Alamos National Laboratory (continued)	
Laboratory Directed Research and Development (continued)	
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

OFFICE OF DEFENSE PROGRAMS (Continued)

	FY 1993
Los Alamos National Laboratory (continued)	
Laboratory Directed Research and Development (continued)	
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 FY93 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

Engineered Materials and Processes Programs

This report includes summaries selected to present the diversity of materials research, development and application projects conducted for the Office of Defense Programs. Funds for the work include the RD&T program, the Technology Transfer Initiative program, the Stockpile Surveillance program, and the Laboratory Directed Research and Development program. Some projects with proprietary, patentable, or classified information are not reported.

Sandia's materials program is coordinated through the Materials Science and Technology Council. This council develops the strategies and business plans to assure the ability of the Laboratories to fulfill its missions for the Department of Energy.

The mission of the Engineered Materials and Processes program is to deliver reliable, comprehensive, integrated solutions to meet the materials and process needs of our customers. Teaming within Sandia and partnering with industry, other labs, and academia, we perform research, development and applications engineering for DOE, other government agencies, and U.S. industry.

Materials Preparation, Synthesis, Deposition, Growth or Forming

314. Biomimetic Processing of Oriented Crystalline Ceramic Layers — FY 1993 $300,000

DOE Contact: Maurice Katz, (202) 586-5799
SNL Contact: Joe Cesarano, (505) 272-7624

This project serves to combine the concepts and methodology of biochemistry and materials science to develop a biomimetic processing technique for oriented crystalline ceramic thin films. Langmuir-Blodgett (LB) films are used to form two-dimensional crystalline arrays of organic molecules and synthetic biochemical analogs on silicon substrates. The order of chemical functional groups extending from the LB film serves as a template atomically to control the nucleation and growth of a crystalline inorganic film from solution. The project focuses on validation of this theory by coupling experimentation with state of the art characterization techniques and very powerful computational molecular modeling. Ultimately we are trying to fabricate oriented crystalline thin films of electroceramics and develop a technology utilizing LB technology for medical, semiconductor, optoelectronic, and "smart" material applications.

Keywords: Ceramics, Biomimetic, Film

315. Boron-Rich Solids — FY 1993 $290,000

DOE Contact: G.J. D'Alessio, (301) 903-6688
SNL Contact: Terry L. Aselage, (505) 845-8027

Boron-rich solids are refractory materials with unusual structures and bonding. Among boron-rich solids one finds wide-bandgap electronic insulators, small-bipolaronic semiconductors, materials with high conductivities and even superconductors. Our program aims to develop a fundamental understanding of the unusual properties of these solids in relation to their distinctive structures. We also attempt to utilize these properties in novel applications. Many boron-rich solids are reported to resist structural damage normally induced in conventional materials by bombardment with ions, neutrons, and high-energy electrons. We have initiated a program to understand this radiation tolerance. Additionally, we have developed several device concepts that utilize this potential radiation tolerance. A solid-state neutron detector based on the difference in neutron absorption between the ^{10}B and ^{11}B isotopes has been developed. A prototype device has been fabricated and will be tested. Concepts for the potential solid-state conversion of the energy of high-energy ions to electrical energy have been explored with a local company.

Keywords: Ceramics, Boride

316. CVD Diamond/Diamond Powder Composites FY 1993
$90,000

DOE Contact: Maurice Katz, (202) 586-5799
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Diamond exhibits a unique combination of extraordinary properties including (1) above 300K, the highest thermal conductivity, (2) optical transparency from the far ultraviolet to the far infrared, (3) superlative hardness and (4) exceptional X-ray transmittance. Certain potential applications for diamond, e.g.: (1) thermal conductors for cooling dense electronic packages, (2) optical windows and (3) strong refractory, inert, low density material for load bearing structures require relatively thick, shaped coatings of free-standing pieces of diamond with tailored surface finishes. At the present time, there are a number of problems associated with forming predominantly chemical vapor deposited (CVD) diamond with the above properties. Frequently, as a result of flaws, intrinsic stress. fractal growth patterns, etc., the properties of CVD diamond only approach the properties of the best natural diamond. Depositing predominantly CVD diamond is an energy intensive, and because of the concentrations of hydrogen required, potentially dangerous process. We are developing processes for forming thick, shaped, CVD diamond/diamond powder composites with tailored surface topographies and controllable densities that may be superior to predominantly CVD diamond for many applications.

Keywords: Ceramics, Composite, Diamond, Microporous, Preparation

317. CVD Diamond Growth Models FY 1993
$150,000

DOE Contact: G.J. D'Alessio, (301) 903-6688
SNL Contact: Michael E. Coltrin, (505) 844-7843

Low-pressure and low-temperature growth via chemical vapor deposition opens up many potential markets for diamond films. Diamond's unique properties include high thermal conductivity for thermal management applications, extreme hardness and low friction for protective coating applications. CVD diamond is usually grown from hydrocarbon sources like methane. However, halogenated sources offer the possibility of reduced growth temperatures, thereby increasing the range of material types that can be coated. We are developing quantitative computer models of diamond CVD to aid in process optimization. These complex models require as input information about the fundamental mechanisms of diamond growth. We have obtained the Molecular Mechanics program MM3 and are using it to calculate thermochemical properties of diamond surface structures.

Keywords: Ceramics, CVD, Diamond

318. Development of LiF Coated Anodes for PBFA II FY 1993
$100,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: John E. Maenchen, (505) 845-8963

A LiF thin film is currently used as an ion source in the PBFA II project. The LiF coating is deposited on the inside surface of a stainless steel, cylindrical anode. The surface of the coated anode must be as smooth as possible to minimize the divergence of the Li ions' trajectories after they are liberated from the coating. It is also desirable to preheat the anode to desorb contaminants from the surface of the LiF coating before Li ion liberation. The factor of two difference in the thermal expansion coefficient of LiF and stainless steel can lead to significant stress generation at the interface between the two materials during this thermal treatment. The thermally generated stress can, in-turn, cause the coating to delaminate from the anode. This project is focused on (1) modifying the anode surface preparation and LiF coating processes to minimize surface roughness and (2) identifying and testing thin film materials with thermal expansion coefficients intermediate between stainless steel and LiF as adhesion promotion layers.

Keywords: Ceramics, Coating

319. Diamond-Like Carbon Films FY 1993
$250,000

DOE Contact: Maurice Katz, (202) 586-5799
SNL Contact: Michael P. Siegal, (505) 845-9453

A major impediment for the use of diamond films in semiconductor device applications has been the lack of a process for the growth of smooth diamond films without the need to polish a substrate surface with diamond grit for the creation of nucleation sites. The nucleation of diamond grains on a given substrate surface is generally the rate-limiting step for growth as well as the advent for rough morphologies (10-15 mm) and poor surface coverage for films < 10-20 mm thick. In addition, diamond films are generally grown at high temperatures (900°C) that are incompatible with most device processing technologies. Diamond-like carbon (DLC), on the other hand, can grow on most surfaces at room temperature without any substrate pretreatment. DLC can be thought of as an amorphous mixture of sp^2- and sp^3-bonded carbon atoms with physical and electronic properties intermediate between diamond and graphite. A new pulsed-laser deposition (PLD) system has been assembled for the growth of DLC thin films. An excimer laser (l = 248 nm) is used to ablate a pyrolytic graphite target under high-vacuum. The energetic carbon species (12 - 50 eV) generated in the PLD process condense on the cold substrate with a high fraction of sp^3-bonded carbon atoms.

Keywords: Ceramics, Diamond

320. Improved Mechanical Properties of Ceramic Ferrites by Diffusion Induced Grain Boundary Migration (DIGM)

FY 1993
$25,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: S. Jill Glass, (505) 845-8050

Ceramic ferrites are used in components such as safing wheels, and in numerous commercial applications such as transformer cores, antenna cores, deflection magnetics for particle accelerators, etc. Although the primary properties of interest are the magnetic and electrical properties, the inherent brittleness of ceramic ferrites is a problem in many applications. Because the magnetic properties are often optimized at larger grain sizes, traditional ceramic toughening approaches such as adding reinforcement whiskers or fibers, or zirconia particles, are not viable approaches because they tend to limit grain growth. The toughening approach that we are exploring is to change the grain boundary morphology from smooth to wavy. This change can occur under conditions that lead to diffusion-induced grain boundary migration. In ceramic ferrites, which typically have extremely weak grain boundaries, the production of wavy grain boundaries is expected to enhance the fracture resistance by mechanical interlocking of adjoining grains.

Keywords: Ceramics, Fracture, Ferrite

321. Ion Beam Modification of PLZT Thin Films

FY 1993
$50,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: J. Charles Barbour, (505) 844-5517

Ferroelectric materials such as lead lanthanum zirconate titanate (PLZT) in thin-film form are important for optical storage devices, but in order to make these materials competitive with current device schemes, a method is needed to improve their photosensitivity. Ion implantation has been used in the past to increase the near-UV and visible-light photosensitivity in bulk PLZT (277 micron thick) by ion implantation with noble gas ions, and Al or Cr ion. The cause of this increase in photosensitivity is not fully understood, although it is thought to be related to a change in the near surface dielectric constant. This work has used the effects of ion-beam modification on PLZT thin films (630 nm thick) in order to alter the dielectric constant (e) uniformly throughout the film thickness and obtain a measure of the change in e as a function of damage. This modification is expected to increase the near-UV photosensitivity of these films; and in fact, preliminary results show that implantation to a fluence of $2x10^{14}$ Ar/cm^2 at 80 keV does also increase the sensitivity to longer wavelength light. Further, the recovery of the original dielectric constant with post-implant annealing was examined.

Keywords: Ceramics, Dielectric, Ferroelectric, Film, Optical

322. Nanoscale Engineering of Smart Membranes

FY 1993
$50,000

DOE Contact: Maurice Katz, (202) 586-5799
SNL Contact: Douglas A. Loy, (505) 844-4445

Project summary withheld because information is patent sensitive.

Keywords: Ceramics, Microporous

323. Optical Properties of Potassium Titanyl Phosphate Derivatives

FY 1993
$30,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Mark L. F. Phillips, (505) 844-8969

This project synthesizes and characterizes a family of nonlinear optical ceramic oxides isostructural with $KTiOPO_4$ (KTP) in which lanthanide and transition metal ions partially replace Ti, causing optical absorptions at visible and near IR wavelengths. These absorptions introduce anomalous dispersion, which may shift the noncritical phase matching wavelength of KTP to allow efficient doubling at diode laser wavelengths (ca. 750-900 nm). Before target phases for crystal growth can be selected, compositions with both appropriately located absorption bands and significant optical nonlinearity must be identified. These compositions can easily be synthesized as powders using solid state and/or low-temperature hydrothermal methods.

Keywords: Ceramics, Optical

324. Sealing Glasses for Titanium and Titanium Alloys

FY 1993
$397,000

DOE Contact: Maurice Katz, (202) 586-5799
SNL Contact: Richard K. Brow, (505) 845-8047

Project summary withheld because information is patent sensitive.

Keywords: Ceramics, Glass, Seals

325. Thermal Stability Studies of Diamond-Like Carbon Films FY 1993
$100,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: John E. Parmeter, (505) 844-8898

There is currently much interest in films of amorphous carbon/hydrogen, also known as diamond-like carbon or simply DLC. The DLC films, prepared from plasma CVD of hydrocarbons, can be prepared such that they have similar physical properties (i.e. hardness, optical band gap) to diamond, and can be grown at much higher rates. It is thus envisioned that DLC can serve as a more economical substitute for diamond coatings in some applications. However, the thermal stability of DLC is a key factor in determining its usefulness that has not previously been investigated thoroughly. We have therefore undertaken a study of the thermal stability of DLC grown on tungsten and aluminum substrates using Raman spectroscopy, Auger spectroscopy, and thermal desorption measurements.

Keywords: Ceramics, Diamond, Failure

326. Chromate-Free Corrosion Resistant Coatings for Aluminum FY 1993
$400,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Rudy G. Buchheit, (505) 844-6904

Project summary withheld because information is patent sensitive.

Keywords: Metals, Coating, Corrosion, Environment, Surface, Treatments

327. Dynamic Wetting and Spreading of Solder FY 1993
$40,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Elizabeth A. Holm, (505) 844-7669

The as-solidified shape of a solder bump is determined by the equilibrium shape of the liquid droplet, which is controlled by surface tension. In this project, we are developing computer simulations for the evolution of solder droplet shapes under various processing conditions. These processing parameters include substrate wettability, spatial and temporal variations in solder surface tension, and pad and lead geometry and arrangements. The goal of the project is to identify processing conditions which result in the formation of desirable and undesirable droplet shapes. In the first stage of this project, we are studying the effects of varying substrate wettability on sessile drop shape. In particular, we have examined the "solder donut" problem, in which a solder droplet is deposited on a patch of poorly-wet substrate surrounded by wettable substrate. We developed a computer code, utilizing the Surface Evolver software package, which models this problem.

Keywords: Metals, Joint, Modeling, Solder

328. High-Temperature and Organic Superconductors FY 1993
$600,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Eugene L. Venturini, (505) 844-7055

Materials exhibiting high-temperature superconductivity offer unique potential applications in energy, technology and defense areas. Our broad research efforts have concentrated on improved synthesis, materials understanding and property determination as well as prototype demonstrations in three synergistic areas: (1) fundamental structure and physics on selected single crystal systems, (2) thin films of Tl-containing cuprates and yttrium barium cuprate (Y-123), and (3) bulk materials complementing our thin film studies. This effort to date has allowed Sandia to maintain a leadership role in the field with the only sustained effort in crystal growth and characterization, the first successfully fabricated thin films based on the Tl-materials and the only laboratory to develop some understanding of the complex phase chemistry and stability in the Tl-materials. This has led to a wide range of microelectronic device developments, such as the flux flow transistor and confocal resonator.

Keywords: Metals, Superconductors

329. Intermetallic Compound Growth in Solder Joints FY 1993
$240,000

DOE Contact: Maurice Katz, (202) 586-5799
SNL Contact: Kenneth L. Erickson, (505) 844-4133

Intermetallic compound growth occurs at the solder/substrate interface of solder joints through solid state diffusion processes. Long term aging data describing the growth of intermetallic compound layers are valuable for long term reliability predictions of electronic assemblies. An accurate computer model of solder/substrate reactions permits the prediction of substrate solderability and joint functionality beyond the time periods of traditional laboratory tests. The objective of this study was to acquire experimental intermetallic growth data on the 63Sn-37Pb/copper and 100Sn/copper systems. The intermetallic layer thickness values as a function of time provided the appropriate input to computer models developed with the objective to predict longer term intermetallic compound growth. Electron microprobe analysis was performed on the intermetallic layers to verify their concentration profile(s); these data were also required as input for the model operation.

Keywords: Metals, Joining, Modeling

330. Nucleation in Chemical Vapor Deposition on Metal Films FY 1993
$80,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Thomas M. Mayer, (505) 844-0770

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 are investigating 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 apply a complementary set of measurements, including macroscopic probes of composition and structure (XPS and X-ray reflectivity) and microscopic imaging of nuclei (high temperature STM). This program gives us the unique ability to study nucleation of thin films in CVD processes, *in situ,* and to follow the structural evolution of thin films. We intend to use this ability to understand the relationship of various dynamic processes (e.g. diffusion, ligand dissociation, site specificity, etc.) to the structural evolution of the material. We hope to develop methods of controlling nucleation through surface chemical and structural modification. This would be useful in controlling growth mode and microstructure of films, selective film deposition, and nanostructure fabrication.

Keywords: Metals, Interfaces

331. Synthesis of Ti and TiO_2 Nanoparticles FY 1993
$40,000

DOE Contact: Maurice Katz, (202) 586-5799
SNL Contact: Jess P. Wilcoxon, (505) 844-3939

Metal and semiconductor nanoparticles have unique properties that make them very attractive as catalysts. For example, because of their extremely small size, very large surface areas are generated leading to significant improvement in the catalytic efficiency of a given material. Also, because the band gap shifts as a function of particle size, it becomes possible to tailor the light absorption properties of semiconductor nanoparticles and, hence, adjust the energy required to generate trapped surface electrons for use in solution chemical reactions. The first step in investigating the properties of such materials is to establish reliable methods of synthesizing them. Titanium nanoparticles were produced in a glove box by adding TiI_4 or $TiCl_4$ to an inverse micelle solution consisting of 10 percent C12E5 surfactant in dry octane. Reduction of the titanium salt was accomplished through the addition of a stoichiometric amount of $LiBH_4$ (2M in THF). Chemical reaction was denoted by the evolution of gas bubbles. Stable, transparent, colorless solutions were produced. Subsequent analysis using light scattering and electron microscopy confirmed the formation of relatively monodisperse,

~5 nm diameter particles. Electron diffraction confirmed a titanium structure for these particles.

Keywords: Metals, Cluster

332. Titanium Casting Face-Coat Development FY 1993 $291,000

DOE Contact: Maurice Katz, (202) 586-5799
SNL Contact: Michael C. Maguire, (505) 845-3105

Project summary withheld because information is patent sensitive.

Keywords: Metals, Melting, Net Shape, Solidification

333. Unalterable Magnetic Stripes FY 1993 $180,000

DOE Contact: Maurice Katz, (202) 586-5799
SNL Contact: Terry J. Garino, (505) 845-8762

Project summary withheld because information is patent sensitive.

Keywords: Metals, Magnetic

334. Bridged Poly-germsesquioxanes and Polysilsequioxanes FY 1993 $50,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Douglas A. Loy, (505) 844-4445

Project summary withheld because information is patent sensitive.

Keywords: Organic, Synthesis

335. Carbon Film Nanoband Sensors FY 1993 $80,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Clifford L. Renschler, (505) 844-0324

Project summary withheld because information is patent sensitive.

Keywords: Organic, Coating, Electrode, Film, Foam, Microporous, Polymer, Sensors

336. Development of a Scaleable, Flat-Flame Technology for the Synthesis of Diamond Films

FY 1993
$150,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Kevin F. McCarty, (510) 294-2067

We are developing a combustion technology that can be scaled to manufacture diamond films of arbitrary size. Presently, commercialization of synthetic diamond films is hindered by the lack of an economical way to rapidly deposit large area films. We have conceived two burner designs, the "coflow" and "trumpet bell." Both result in radially uniform fluxes to surfaces and they optimize the use of reagents. Furthermore, both the coflow and trumpet-bell burners are inherently scaleable designs. Using a trumpet-bell burner, we have grown uniform films of diamond from a substrate-stabilized flat flame of $C_2H_2/H_2/O_2$. Computational modeling is being used to understand and optimize the chemical vapor deposition (CVD) process. The modeling is also evaluating whether untried but potentially advantageous processes (such as oscillating/pulsating flames, preheated feed gases, and lower cost feed gases) warrant experimental investigation.

Keywords: Organic, Diamond, Films, Combustion, CVD, Materials Synthesis

337. Development of Solid Polymer Electrolytes for Lithium Rechargeable Batteries

FY 1993
$100,000

DOE Contact: Maurice Katz, (202) 586-5799
SNL Contact: Charles Arnold, Jr., (505) 844-8728

The purpose of this work was to develop new solid ion-doped gels that have ionic conductivities that are at least comparable to those reported in the literature but which are compositionally stable and are safe to use in lithium rechargeable batteries. To accomplish this goal, we needed to set up a glove box facility and develop suitable fixtures for evaluation of the electrical properties of our films. Our approach was different from that of previous workers in that we focused on aprotic solvents that had lower vapor pressures than propylene carbonate and used lithium salts that could be used safely in battery applications.

Keywords: Organic, Electrolyte, Polymer

338. <u>Fuel Cell Applications for Novel Metalloporphyrin Catalysts</u> FY 1993
$300,000

DOE Contact: Maurice Katz, (202) 586-5799
SNL Contact: Tom Klitsner, (505) 844-1901

The efficiency and reliability of fuel cells is largely determined by the performance of catalysts at both the fuel and air electrodes. Our objective is to develop catalysts from a new class of metalloporphyrin materials that overcome the limitations of current catalytic materials (primarily platinum). Problems being encountered with current catalysts include: susceptibility to poisoning, poor stability, lower catalytic activity than desired, and poor matching of redox potentials. By the appropriate addition of molecular sidegroups, metalloporphyrin materials can be tailored to overcome these problems and provide more optimal catalytic performance under real fuel cell conditions. Computer-aided molecular design is used to guide this work in an iterative process which includes synthesis, characterization, and testing in actual fuel cells.

Keywords: Organic, Catalyst

339. <u>Fullerene-Xylene Copolymers</u> FY 1993
$50,000

DOE Contact: Maurice Katz, (202) 586-5799
SNL Contact: Douglas A. Loy, (505) 844-4445

Project summary withheld because information is patent sensitive.

Keywords: Organic, Polymer

340. <u>Low Dielectric and High Temperature Films for Multichip Modules</u>
FY 1993
$230,000

DOE Contact: Maurice Katz, (202) 586-5799
SNL Contact: Randall S. Saunders, (505) 844-1760

Project summary withheld because information is patent sensitive.

Keywords: Organic, Coating, Dielectric, Film, Microporous, Polymer

341. Microengineered Materials Development FY 1993
$150,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Tamara A. Ulibarri, (505) 844-5279

The goal of this project is to synthesize inorganic/organic nanocomposite materials which combine the strength of ceramics with the toughness of polymers. Sol-gel methods allow the production of homogeneously reinforced materials without the costly mixing or lay-up steps required in conventional systems. By controlling the reaction conditions, we should be able to reliably carry out the designed synthesis of new composite materials with superior properties. However, before this can be achieved a fundamental understanding of the relationship between the synthetic protocol, structure and mechanical properties must be gained. To this end, sol-gel techniques have been used to synthesize inorganic/organic composite materials under controlled reaction conditions.

Keywords: Organic, Composite, Polymer, Ceramics

342. Moisture Resistant Printed Wiring Board Materials FY 1993
$296,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Linda A. Domeier, (510) 294-2350

One goal of the Materials Team within the NCMS PWB Consortium is the development of laminate materials which can be thermally processed, including solder exposures, without the need for pre-baking cycles to eliminate absorbed moisture. Such moisture is widely recognized within the industry as a source of defects such as measles and blisters. Project planning included a broad survey of the previous work in this area. The results of that survey indicate that the nature of the interphase materials, present at the resin-fiber interface, is a key parameter in determining the moisture sensitivity of PWB and other composites. The composition and morphology of this complex region are in turn determined by the coupling agents applied to the glass and also by the glass surface itself and the bulk matrix resin. Recent studies have confirmed that the level of moisture at this interface region is indeed significantly higher than found in the bulk matrix material.

Keywords: Organic, Composite, Fiber, Polymer

343. Porous Carbon Electrodes from a Microcelluar Polymer FY 1993 $275,000

DOE Contact: Maurice Katz, (202) 586-5799
SNL Contact: Robert R. Lagasse, (505) 845-8333

Project summary withheld because information is patent sensitive.

Keywords: Organic, Battery, Carbon, Foam, Membrane

344. Supercritical Fluid Precipitated Polymer Membranes FY 1993 $200,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: James H. Aubert, (505) 844-4481

Project summary withheld because information is patent sensitive.

Keywords: Organic, Foam, Membrane, Microporous, Supercritical

345. A New Method for Promoting Photoresist Adhesion on Tungsten Films for Self-Aligned Refractory Gates on GaAs FY 1993 $50,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Michael E. Bartram, (505) 844-1619

The use of self-aligned tungsten (W) gates on GaAs to fabricate refractory gates in field effect transistors (FET) has not been widespread, due in part to the early preference of the WSi/GaAs Schottky contact properties. However, W gates offer the advantage of less fabrication complexity, lower cost, and lower sheet resistances than WSi. This latter attribute allows a better high frequency response for larger gate widths and the possibility of local routing with W to provide a more compact layout in integrated circuits. In order to incorporate these advantages, for the first time, a procedure has been developed for promoting adhesion of 0.8 micron gate length patterns between W films on GaAs and a photoresist. This method has facilitated the fabrication of self-aligned refractory gates in FETs.

Keywords: Semiconductor, Metallization

346. Comparison of BOH and SiOH Reactivities in Boron-Doped SiO_2 Chemical Vapor Deposition Using Trimethyl Borate and Tetraethyl Orthosilicate

FY 1993
$200,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Michael E. Bartram, (505) 844-1619

The addition of dopants for the modification of materials properties is often accompanied by changes in the deposition kinetics. This altered chemistry suggests that the dopant precursors increase the complexity of the chemical vapor deposition (CVD) process. For example, the addition of trimethyl borate (TMB) to a thermal tetraethyl orthosilicate (TEOS) CVD process produces boron-doped SiO_2 with a lower reflow temperature for surface planarization in VLSI devices but also increases the overall deposition rate of SiO_2. As such, the study of the TMB TEOS system is a unique opportunity to advance the important technology of boron-doped SiO_2 CVD as well as expand the rich science behind the effect of dopants on growth. For these reasons, the relative rates of boranols and silanols reacting with TEOS were studied with FTIR under conditions similar to those used industrially. This comparison has direct bearing on understanding the growth of boron-doped SiO_2 films from TEOS and TMB sources since previous work suggests strongly that surface boranols and silanols are present during the thermal CVD process. In addition, the reactions of TEOS on SiO_2 without boranols were studied at 300 and 1000K.

Keywords: Semiconductor, CVD, Oxides

347. Magnetotransport in Strongly Coupled Double-Quantum-Well Structures

FY 1993
$70,000

DOE Contact: Maurice Katz, (202) 586-5799
SNL Contact: S. Ken Lyo, (505) 844-3718

Recently semiconductor double-quantum-well structures (DQWS) have been receiving increasing attention, because they offer many novel physical phenomena and new concepts of device applications. The basic physics of the structure is tunneling between the two wells. Depending on whether the tunneling is strong or weak, the tunneling is coherent or incoherent. The subject of this report is on the coherent tunneling when the two QW's are strongly coupled. It is desirable to investigate what other new phenomena are expected for DQWS from coherent tunneling not only from the academic point of view but also to maximize their full potential application. We find that applying external magnetic fields in the quantum-well plane (studied very rarely in the past) alters the electronic and magnetotransport properties in a significant way.

Keywords: Semiconductor, Electronic, Ceramics

348. Particles in Rf Plasmas FY 1993
$150,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Richard J. Buss, (505) 844-3504

Project summary withheld because information is CRADA Sensitive.

Keywords: Semiconductor, Cleaning, Deposition, Etching, Plasma

349. The Growth of InSb Using Tri(dimethylamino)antimony and Trimethylindium FY 1993
$250,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Kevin C. Baucom, (505) 844-1191

There is considerable interest in the growth of InSb for use in long wavelength devices, high-speed circuitry and magnetic Hall devices. Trimethylantimony (TMSb) is currently the primary antimony source for the growth of InSb-based devices by metal organic vapor deposition (MOCVD). TMSb has a decomposition temperature ~450°C. An alternative antimony source allowing reduced pyrolysis temperature is needed because of a possible intrinsic p-type defect which exists in epitaxial layers grown at temperatures >400°C. There is also interest in the reduction of background carrier concentration by the development of higher purity sources and reduced carbon impurities by the elimination of methyl groups. For these reasons, we have examined the growth of InSb using TDMASb ($[(CH_3)_2N]_3Sb$) which has no methyl groups bound directly to the antimony atom.

Keywords: Semiconductor, Compound, CVD

Materials Structure and Composition

350. Structure of Microporous Glasses Derived from Borosilicates FY 1993
$401,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Dale W. Schaefer, (505) 844-7937

The leaching of a sacrificial phase is one of the oldest methods of achieving microporosity in glasses. The mechanism of pore formation has long been attributed to phase separation in the precursor unleached glass. Our work calls this model into question and suggests a new perspective to understand and control porosity in borosilicates. A comparison of the small-angle X-ray scattering profile of leached and unleached Vycor borosilicate glass (supplied by Corning Glass) demonstrated negligible scattering in the precursor unleached glass. Calculation of the expected intensity based on a fully phase separated silica/boria precursor shows that the precursor is not phase separated. The result led us to postulate that the interconnected pore structure of leached glasses is imposed during the dissolution of the boria and is not the result of a spinodal pattern in the precursor.

Keywords: Ceramics, Microporous

351. Electronic Structure of Advanced Materials — FY 1993 $150,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Alfred C. Switendick, (505) 844-2013

The purpose of these investigations is to calculate the electronic structure of a variety of advanced materials: hydrides, borides, carbides, nitrides, oxides, aluminides and silicides. From these calculations various physical properties are calculated to include equilibrium structures, cohesive energies, heats of formation, electronic charge density distributions for comparison with experimental X-ray measurements, optical and phonon spectra, mechanical moduli and Fermi surface properties. From the understanding derived from these calculations, one can guide the synthesists in preparing new materials with desired properties.

Keywords: Metals, Electronic

352. Lubricant Films Deposited by Plasma Decomposition — FY 1993 $72,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Michael T. Dugger, (505) 844-1091

Many solid lubricants currently in use employ high VOC (volatile organic constituent), toxic, flammable, or ozone-depleting solvents in their formulation or as carriers during deposition. The increasing emphasis on environmental safety and health requires the development of alternative lubricants to those presently in use in weapons-related miniature mechanisms, and it is unclear whether new formulations expected from commercial lubricant vendors will fulfill these requirements. In this work, plasma decomposition of gaseous precursors is explored as a mechanism for forming lubricative thin films. Plasma decomposition of fluorocarbon gases is commonly used in semiconductor manufacturing to deposit thin dielectrics, and in dry etching. This process produces films with the necessary low reactivity, thickness control and ability to coat complex shapes to be considered as solid lubricants. The objective of this project is to examine the tribological performance of films deposited on ferrous substrates by plasma decomposition from a variety of gaseous precursors, and relate friction and wear performance to film structure and composition.

Keywords: Metals, Coating, Tribology, Analysis, Organic, Plasma

353. Phase Separation Kinetics in a Micelle System

FY 1993
$190,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Jess P. Wilcoxon, (505) 844-3939

Spinodal decomposition is the process by which a multicomponent material separates into inhomogeneous microdomains. Spinodal decomposition is generally deleterious, since material properties degrade when microphase separation occurs. For example, microphase separation so severely degrades nuclear reactor confinement vessels that sixteen reactors have had to be prematurely shut down. An understanding of the kinetics of spinodal decomposition is thus essential to the prediction of operating lifetimes of materials. We are now discussing, with Boston University, a collaboration wherein we would perform long time small angle X-ray scattering studies, at the Brookhaven National Light Source, of domain growth in metal alloys used in reactors.

Keywords: Metals, Materials Properties

354. Chemical Modification of Fullerenes

FY 1993
$200,000

DOE Contact: Maurice Katz, (202) 586-5799
SNL Contact: Paul A. Cahill, (505) 844-5754

Fullerenes are new molecular allotropes of carbon first discovered in 1985 in the ablation of graphite, and which are now available in quantity for $90/gram ($C_{60}$). The race to find applications for these unique materials is extremely competitive and may hinge on chemical modification of the basic cage structure. Such chemical modifications target optimization of structural, solubility, electronic, or optical properties. Methods for attaching addends are needed and the reactivity patterns must be determined. Efficient chemical synthesis of complex derivatives also requires the capability to model reactivity of unfunctionalized and functionalized fullerenes. Through experimental and computational studies of several fullerene hydrides, including $C_{60}H_2$, $C_{70}H_2$, and $C_{60}H_4$, we have learned much about the kinetics and thermodynamics of addition to the soluble fullerenes. The level of theory required to model these compounds is now known, as is the pattern of electrophilic addition to singly modified fullerenes.

Keywords: Organic, Fullerene, Modeling, Synthesis

355. Electrorheological Fluids FY 1993
$150,000

DOE Contact: Maurice Katz, (202) 586-5799
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An Electrorheological (ER) fluid is normally a low-viscosity colloidal suspension, but when an electric field is applied, the fluid undergoes a reversible transition to a solid, being able to support considerable stress without yield. The commercial possibilities for such fluids are enormous, including clutches, brakes, valves, shock absorbers, and stepper motors. However, performance of current fluids is inadequate for many proposed applications. Our goal is *to engineer improved fluids* by investigating the key technical issues underlying the solid-phase yield stress and the liquid to solid switching time. Our studies focused on the field-induced interactions between colloidal particles that lead to solidification, the relationship between fluid structure and performance (viscosity, yield stress), and the time evolution of structure in the fluid as the field is switched on or off.

Keywords: Organic, Dielectric, Electrorheological, Modeling

356. Electrorheological Fluids in Shear Flow FY 1993
$100,000

DOE Contact: Maurice Katz, (202) 586-5799
SNL Contact: James E. Martin, (505) 844-9125

Electrorheological (ER) fluids are particle suspensions that quickly and reversibly solidify when a strong electric field is applied, due to a mismatch in the dielectric constant or conductivity of the particles and the suspending liquid. This mismatch results in induced particle dipoles that cause particle chaining along the electric field lines. When a large shear stress is applied to a soft ER solid, a viscous flow is induced that is strongly shear thinning. Because the viscosity can be moderated by the electric field, ER fluids have potential for applications in electromechanical actuators such as fiber spinning clutches, shock absorbers, etc. In collaboration with T.C. Halsey, Univ. of Chicago, we have developed an "independent droplet model" to describe the complex rheology of ER fluids. However, rheology is only an indirect test of the structural changes predicted by this model, so we have sought direct structural evidence, such as that provided by light scattering, to evaluate the model.

Keywords: Organic, Electrorheological

357. Molecular Modeling of Polymer Liquids and Blends

FY 1993
$363,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
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Polymer alloys (including polymer blends and copolymers) consisting of mixtures of existing polymers are versatile materials which could satisfy many future needs for advanced materials. This is particularly important in view of the stringent OSHA restrictions on chemicals which makes the synthesis of new polymers difficult. Unfortunately, even empirical rules governing the relationship between structure and properties are not available for polymer alloy systems. Because of the chainlike nature of polymers, the mixing behavior of polymer systems is much more complex than that of metallic alloys. The objective of this program is to develop the capability to calculate the structure, thermodynamic properties and phase diagrams of polymer alloys for engineering applications. For this purpose we have developed the polymer reference interaction site model or PRISM theory.

Keywords: Organic, Modeling

358. Tailoring Interfaces with Block Copolymers

FY 1993
$130,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Michael S. Kent, (505) 845-8178

Block copolymers are active interfacial modifiers, and are used to enhance adhesion between a polymeric matrix and a solid surface, to control the domain size in incompatible polymer blends, and to stabilize colloidal dispersions. Our objective is to tailor interfacial properties through the use of molecularly designed block copolymers. To this end we are working to understand the relationships between chain architecture, the interactions between copolymer segments and the bulk materials, the conformations of copolymers at interfaces, and interfacial properties. Controlled synthesis of block copolymers is a key element in this program. The detailed structure of block copolymers at polymer-polymer, solid-polymer, and liquid-air interfaces is being investigated with neutron and X-ray reflectivity. This work is funded through two related projects.

Keywords: Organic, Adhesive, Film, Surface, Analysis, Scattering, Reflection

359. Thermal Decomposition Reaction Mechanisms of Bis(1-fluoro-1,1-dinitroethyl) formal (FEFO) and Bis(1-fluoro-1,1-dinitroethyl)difluoroformal (DFF) FY 1993
$100,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Richard Behrens, (510) 294-2170

Bis(1-fluoro-1,1-dinitroethyl)formal (FEFO, I) is the energetic liquid ingredient used in the explosive formulations for the Transferable Insensitive Explosive (TIE) program and the Paste Extrudable Explosive (PEX) based booster systems. The difluoro-derivative of FEFO, bis(1-fluoro-1,1-dinitroethyl)difluoroformal (DFF, II), also has potential applications in such systems. Simultaneous thermogravimetric modulated beam mass spectrometry (STMBMS) technique has been applied to measure the vapor pressures and evaluate the thermal decomposition chemistry of FEFO and DFF.

The resulting DH_{vap} and vapor pressure at 25°C are 20.3 ± 0.2 kcal/mol and 0.4 ± 0.1 millitorr for FEFO, and 17.3 ± 0.2 kcal/mol and 5.1 ± 1.1 millitorr for DFF. The thermal decomposition of FEFO indicates there are five major pyrolysis pathways. The results suggest that FEFO initially decomposes at 150°C by rearrangement of the nitro group ($-NO_2$) to the nitrite group (-O-NO), followed by loss of NO. Between 200°-230°C, further pyrolysis yields a large-molecular weight product, $C_3H_5NO_5F_2$, and the backbone structure breaks apart through three primary pathways; one yielding CO_2 (possibly N_2O), one yielding CH_2O and CO, and one yielding a ring, C_3H_2NOF.

Keywords: Organic, Energetic, Analysis, Chemical

360. Microstructures of InGaP Alloys: Ordering and Decomposition FY 1993
$60,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: David M. Follstaedt, (505) 844-2102

Alloys of InGaP are of considerable interest for their electro-optical properties since they have the highest energy direct bandgap of the III-V compound semiconductor alloys. $In_{0.48}Ga_{0.52}P$ alloys can be grown lattice-matched to GaAs by Metal Organic Chemical Vapor Deposition (MOCVD), and are being used to make practical devices such as Vertical Cavity Surface Emitting Lasers (VCSELS) and light emitting diodes. Higher bandgaps (shorter wavelength light) are desirable, but have been found to be reduced (from 2.0 eV to 1.9 eV) for growth at intermediate temperatures due to atomic ordering of In and Ga. We are using Transmission Electron Microscopy (TEM) to examine key alloys from a previous study of bandgaps and growth conditions, and find: (1) Strong ordering (Cu-Pt) at 675°C where the bandgap is lowest, and (2) Spinodal-like decomposition in all alloys. We are investigating further to learn how the structures form and to control their effect on electronic properties.

Keywords: Semiconductor, Compound

Materials Properties, Behavior, Characterization or Testing

361. Theoretical Calculation of the Direct to Indirect Transition in InAlGaP

FY 1993
$35,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Jeff S. Nelson, (505) 844-4395

The InAlGaP alloy system is one of the most promising materials for visible light emission from red to yellow-green. As the emission wavelength is shortened further into the green by increasing the Al concentration, the material suffers a drastic decrease in emission intensity; at high Al concentrations InAlGaP becomes an indirect gap semiconductor. An accurate estimate of the direct-indirect (G-X) crossing with increasing Al concentration is needed to place an upper bound on the short wavelength characteristics of InAlGaP, as well as provide physical insight into alternate band gap engineering schemes to achieve strong green light emission.

Keywords: Semiconductor, Electronic

362. Visible Light Emission from Porous Silicon Nanostructures

FY 1993
$60,000

DOE Contact: Maurice Katz, (202) 586-5799
SNL Contact: Michael J. Kelly, (505) 844-4031

Although the property of visible luminescence from porous silicon was discovered more than 30 years ago, a renewed interest due to the recent discovery of fairly high quantum efficiency photoluminescence has resulted in numerous publications examining the composition and morphology of porous silicon and their relation to the mechanism of porous silicon photoluminescence. Porous silicon is typically formed by anodization in an aqueous hydrofluoric acid electrolyte. As yet, no mechanistic model for photoluminescence from porous silicon has been universally accepted. Proposed mechanisms include: (1) quantum size effects in the porous silicon nanostructures affecting the electronic band structure of silicon; (2) photoluminescence from Si-O-H polymeric compounds such as siloxene; (3) photoluminescence due to the presence of silicon hydride species, and (4) light emission from hydrogen-terminated amorphous silicon structures. Our goal here is to obtain experimental evidence that supports or refutes the proposed photoluminescence mechanisms.

Keywords: Semiconductor, Optoelectronics

363. Advanced Energetic Materials — FY 1993 $450,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Robert A. Graham, (505) 844-1931

The dynamic compaction processes resulting from high pressure shock loading are involved in weapons surety efforts involving high explosives, energetic responses of ballotechnic energetic materials, and materials synthesis and processing of ceramic powders. The ability to predict and model these behaviors is critical to successful applications yet there is little data on the deformation processes. The project has developed an experimental capability to study the details of the compaction process with controlled impact loading and the use of piezoelectric polymer gauges to detect the deformation. In a cooperative effort with LANL the project is studying the compaction and initiation of reaction of the high explosive HMX. Both modeling and experimental efforts are in progress. It has been observed that the pressure required to compress 65 percent dense powder is found to be about 250 MPa, an exceptionally low value. Below that pressure the compression waves are highly dispersive.

Keywords: Ceramics, Powders

364. Ceramic and Glass Fracture — FY 1993 $45,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Edwin K. Beauchamp, (505) 845-8495

The objective of this project is to provide a sound basis for failure analysis and predictions of mechanical performance of components containing glasses and ceramics. In our past work, we have had to assume that tabular values were appropriate for these calculations. We routinely use indentation fracture to measure fracture toughness of glasses and to determine local stresses on surfaces of these materials.

Keywords: Ceramics, Electronic, Failure, Fracture, Analysis, Fractography

365. Characterization of Optical Fibers | FY 1993 $63,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Saundra L. Monroe, (505) 845-8227

Optical fibers, used to transmit Nd/YAG laser energy in the DOI (Direct Optical Initiation) system, have extremely high energy transmission requirements. Our objective was to identify fiber face and bulk fiber defects and localized inhomogeneity that could interfere with the required high energy transmissions. Work performed for this project included mechanical and chemical characterization of multimode fused silica core/fluorine doped silica clad 400 micrometer diameter optical fibers.

Keywords: Ceramics, Fiber, Glass, Optical

366. Chemical Processing of Ceramic Thin Films | FY 1993 $183,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Robert W. Schwartz, (505) 272-7629

Ceramic thin films prepared by solution deposition are of interest for a variety of applications ranging from membranes to ferroelectric films for optical memories. Understanding the effects of precursor structure, film processing conditions, and heat-treatment schedules on film densification and crystallization is necessary to prepare ceramic thin films with optimized properties for these different applications. We are studying the processing-property relationships in ceramic film fabrication by synthesizing precursors with different structures and converting these precursors to the ceramic phase using different heat-treatment schedules.

Keywords: Ceramics, Dielectric, Ferroelectric, Film

367. Crystallization of Solution-Derived Ferroelectric Thin Films | FY 1993 $110,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: James A Voigt, (505) 845-9044

It is well recognized that the electrical properties of ferroelectric thin films can be strongly influenced by film microstructure. As Sandia's device work expands into optoelectronic applications of ferroelectric thin films, the ability to control film microstructure becomes even more important, since film surface roughness, residual porosity, grain size and orientation all impact film optical quality. Our research is directed at determining the fundamental processes involved in the transformation of solution-derived thin films from the as-prepared amorphous state to the crystalline ferroelectric state. The information gained from this project will be used to determine conditions for processing films with improved properties for optoelectronic applications.

Keywords: Ceramics, Ferroelectric, Film, Modeling, Solution

368. Diamond-Like Carbon Coatings FY 1993 $300,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Michael P. Siegal, (505) 845-9453

Project summary withheld because information is CRADA sensitive.

Keywords: Ceramics, Diamond

369. Diamond-Like Carbon Films for Protected Volumes FY 1993 $390,000

DOE Contact: Maurice Katz, (202) 586-5799
SNL Contact: Edward McKelvey, (510) 294-2396

Diamond-like carbon (DLC) thin films resemble diamond in their extreme hardness, lubricity, and chemical inertness. These properties make the films of interest for protective and barrier coating applications. Second year LDRD research has focused on testing and improving the chemical resistance of DLC coatings. The major problem in achieving this goal has been to reduce defects in the coating. Defects have been reduced by understanding how defects occur and improvements in the deposition process.

Keywords: Ceramics, Diamond, Film

370. Dynamic Response of Concrete FY 1993 $100,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Dennis E. Grady, (505) 844-2799

Concrete is widely used as a fortifying material in military structures, and its resistance to impact or explosive loading varies significantly with preparation technique, chemistry, and character of the aggregate. In the present program we are investigating the dynamic strength and related material properties critical to the needs of computational models use for structural response analysis. In this research, aggregate concretes are subjected to controlled impact loading to determine dynamic constitutive properties of the materials. High-resolution velocity interferometry is the principal experimental diagnostic used to provide the necessary material property data. From such data dynamic compression and strength relations are determined for specific concretes and used to develop appropriate computational models.

Keywords: Ceramics, Failure, Fracture, Modeling, Concrete

371. Dynamic Testing of Armor Ceramics

FY 1993
$150,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Dennis E. Grady, (505) 844-2799

High-strength ceramics offer significant advantages over steel in both heavy armor and light armor applications in armored military vehicles. Unique properties of low density and ultra-high strength combine to provide attractively-low weight-to-strength ratios. Critical properties include mechanical strength and dynamic equation-of-state issues. To understand and optimize these properties through improved chemistry and microstructure, we are performing dynamic testing through controlled impact methods. Ceramics which are currently under study in this program include silicon carbide, boron carbide, aluminum nitride, silicon nitride, aluminum oxide and titanium diboride. Equation-of-state and dynamic strength properties are investigated by examining the evolution of impact-generated large amplitude shock waves with high-resolution velocity interferometry diagnostics.

Keywords: Ceramics, Carbide, Failure, Fracture, Modeling, Nitride

372. Electronic Ceramic Granules for Lightning Arrestor Connectors (LAC)

FY 1993
$160,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Bruce A. Tuttle, (505) 845-8026

The reliability of radars depends, in part, on surge protection devices known as lightning arrestor connectors (LACs). Ceramic granules provide the active medium which is responsible for controlled breakdown in LACs. Within the B61 radar, the granules must meet a series of electrical and temperature requirements. Here we report the results of three ongoing studies. Of concern is the reliability of varistor granules subjected to specified temperature and electrical conditions that might be experienced during operation of the radar. In addition, the requisite properties of lead titanate-lead magnesium niobate (PT-PMN) granules as an active medium for the development of a hermetic "super" LAC must be determined and compared with that of the varistor granules. Finally, the use of polyimide carbon composites for use as an organic washer that will provide a high conductivity electrical path in the LAC chamber at elevated temperatures is a subject for investigation.

Keywords: Ceramics, Electronic, Ferroelectric, Fracture

373. Ferroelectric Thin Films for Nonvolatile Memories FY 1993
$500,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Bruce A. Tuttle, (505) 845-8026

Project summary withheld because information is CRADA sensitive.

Keywords: Ceramics, Electronic, Ferroelectric, Film

374. Fluorination of Diamond and Diamond-Like Carbon Films FY 1993
$65,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Diane E. Peebles, (505) 845-8087

Diamond and diamond-like carbon (DLC) films are currently being widely evaluated for wear resistant coatings for mechanical applications. The potential benefit of such films is based on their properties - high thermal conductivity, resistance to high temperatures and corrosive environments, high hardness, extreme wear resistance and low friction coefficient. However, some studies suggest that diamond and DLC films may be susceptible to degradation in high humidity environments. Fluorination of the diamond and DLC films may reduce susceptibility to moisture degradation and could improve the corrosion resistance while lowering the friction coefficient, similar to the benefits of fluorocarbon polymers over hydrocarbon polymers. If this is the case, fluorinated diamond and DLC films would provide exceptional performance as wear resistant and protective coatings. This program will evaluate several methods of fluorinating commercially-obtained diamond and DLC films. The goal of the program is to understand and evaluate the surface chemistry and environmental stability of the fluorinated diamond and DLC films relative to non-fluorinated films.

Keywords: Ceramics, Coating, Diamond, Analysis, Surface, Organic, Plasma

375. Lightning Arrestor Connector (LAC) Granule Fracture Resistance Tests FY 1993
$80,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: S. Jill Glass, (505) 845-8050

Ceramic granules are used to provide controlled breakdown in components known as lightning arrestor connectors. The electrical properties that define granule performance are the fast-rise breakdown voltage and insulation resistance. There is evidence to suggest that unacceptable increases in fast rise breakdown voltage may be related to granule fracture during extended random vibration testing. Granule fracture could also compromise component performance if granule fragments are lost through gaps between the pins and the web. The objectives of our program were to identify a test to measure the fracture resistance of ceramic granules and to determine the relative fracture strengths of the various granule materials. The pressure-compaction test appears to be the best method for determining granule fracture resistance and the test is now being implemented as part of the granule product specification at Martin Marietta Specialty Components (MMSC) in Pinellas, FL. Calculations have been made to estimate stresses that granules are subjected to during extended random vibration tests to determine a cut-off strength. We have also begun work on microstructural modifications to improve the fracture resistances of PT-PMN granules.

Keywords: Ceramics, Dielectric, Electronic, Fracture, Varistor

376. Massively Parallel Simulation of Grain Boundary Evolution — FY 1993 $151,000

DOE Contact: Maurice Katz, (202) 586-5799
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Microstructural evolution in polycrystalline materials is exceedingly complex. Grain boundary motion depends on the local boundary environment (i.e. pores, particles, dissolved impurities, temperature gradients, strain gradients, surface effects, and crystallographic misorientation) and the dynamic evolution of these features. Current tools for understanding microstructural evolution include analytical models, continuum and discrete computer simulations, and a large experimental database. We will combine these approaches to characterize microstructural evolution and service reliability for ceramic and metallic films. The goal of this project is to develop a computer simulation which predicts the microstructural evolution and stability of ceramic and metallic films subjected to diffusional fluxes.

Keywords: Ceramics, Coating, Modeling, Metals, Microstructure

377. Metal/Ceramic Brazing by Active Filler Metals — FY 1993 $83,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Paul T. Vianco, (505) 844-3429

Brazing with active filler metals is the preferred method of joining metal and ceramic components used in heat engine applications. Solid state reactions at the filler metal/substrate interface can take place under elevated temperature service conditions. Such changes can significantly affect the performance of the braze joints. Several braze alloy/metal and ceramic substrate diffusion couples were assembled. The couples were then aged for suitable temperatures and time to promote the formation of reaction products at the interface. The interfacial microstructure would then be analyzed for layer thickness and composition so a to characterize the effects of elevated temperatures on the braze joint interface.

Keywords: Ceramics, Joining, Modeling

378. Silicon Nitride to Metal Joining

FY 1993
$75,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: S. Jill Glass, (505) 845-8050

Ceramic to metal joining has numerous applications both in defense programs and in the commercial sector. Although joining of aluminum oxide (Al_2O_3) to metals such as Kovar has been done for many components (switch tubes, neutron tubes, plasmatrons), and is generally well understood, our knowledge of joining to high performance ceramics such as Si_3N_4 is limited. Our objective in this program was to develop the technology for producing both intermediate (400-500°C) and high temperature (>700°C) Si_3N_4 to metal joints. To produce joints for both temperature ranges we have examined the use of active metal (Ti) brazes in the Ag-Cu and Au-Ni families. We have studied the effects of braze temperature, time, and atmosphere, and ceramic surface preparation, including surface finish and heat treatment, on joining in both systems.

Keywords: Ceramics, Composite, Joining, Nitride

379. Structural Relaxations in Alkali Phosphate Glasses

FY 1993
$111,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Richard K. Brow, (505) 845-8047

When a glass is rapidly cooled to a lower temperature, the system retains some degree of "memory" of its original state. The time dependence of the structural relaxation process responsible for returning the system to equilibrium is highly non-linear and non-exponential. These relaxation processes are typically evaluated by characterizing macroscopic thermodynamic properties like enthalpy or volume. One important consequence of this behavior is that the glass stress state will exhibit similar time dependencies. The current lack of understanding about the causes and magnitude of these nonlinear relaxation mechanisms translates into unpredictable dimensional analyses for glass processing for glass metal sealing and high temperature flat panel display manufacturing.

Keywords: Ceramics, Glass

380. Structure and Property Changes in Irradiated Glasses FY 1993
$20,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Richard K. Brown, (505) 845-8047

The property changes associated with gamma irradiation of glass are well-known, but poorly understood. Most glasses, for example, will densify when irradiated and borosilicate glasses will compact more than fused-silica. when glasses are first soaked in hydrogen, some compositions actually expand instead of compact when irradiated. There has been much speculation in the literature about different atomic modifications to the glass structure which might account for such property changes, but little spectroscopic evidence to support such claims. We have examined a variety of glasses by solid state nuclear magnetic resonance spectroscopy and by electron spin resonance (ESR) spectroscopy in order to develop a molecular level understanding of the property changes in irradiated glasses.

Keywords: Ceramics, Glass

381. Thixotropic Electrorheological Fluids FY 1993
$45,000

DOE Contact: Maurice Katz, (202) 586-5799
SNL Contact: Terry J. Garino, (505) 845-8762

Electrorheological fluids, colloidal suspensions that develop an apparent yield stress in an electric field, have a variety of applications in robotics and in automobiles. Desirable properties of electrorheological fluids include a low off-field viscosity, a high yield stress, wide temperature range of operation and stability against particle settling. We have been studying the behavior of electrorheological fluids consisting of ceramic particles, such as barium titanate, in hydrocarbon liquids, such as dodecane, which function due to the mismatch in dielectric constant between the two phases. However, due to the huge density mismatch between these two materials (5.9 and 0.75 g/cm^3, for barium titanate and dodecane respectively) particle settling could potentially keep these fluids from practical use.

Keywords: Ceramics, Ferroelectric, Electrorheological Fluid, Organic

382. TiO_2-SiC Photocatalysts FY 1993
$40,000

DOE Contact: Maurice Katz, (202) 586-5799
SNL Contact: Terry J. Garino, (505) 845-8762

Titanium oxide powders have been shown to be effective photocatalysts for removing low levels of organics and metals from water. Because of the relative position of its band gap with respect to that of titania, silicon carbide should have photocatalytic properties complementary to those of titania. Therefore, the goal of this project is to develop a mixed titania-silicon carbide photocatalyst capable of removing a wide range of contaminants from water. We are initially studying the photocatalytic properties of bulk SiC before attempting to study the more complex case of powders.

Keywords: Ceramics, Inorganic Powders

383. Advanced Exclusion Barriers Study — FY 1993 $750,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Richard J. Salzbrenner, (505) 844-9408

Nuclear weapon safety depends on the "exclusion barrier" which surrounds vital portions of the weapon, separating them from outside stimuli. To assure nuclear safety, all communication with the external world must be limited to controlled channels which are protected by strong link and weak link components. Nuclear safety is assured only if the exclusion barrier remains intact (i.e., continuous) through all normal operating conditions as well as during all accident environments (including fire, crush, impact, high voltage, lighting, etc.). The response to accidental mechanical loading has historically been difficult to quantify. We have developed and applied new capability in finite element modeling to accurately characterize large scale deformation behavior. Design-of-experiment strategies allow the efficient determination of the effects of geometry, material selection, and their interactions on barrier behavior. Results from parametric studies are being distilled into guidance for designers and nuclear safety analysts. The capabilities being developed in this project are "dual use," and can be applied in critical manufacturing technologies such as sheet forming, and forging.

Keywords: Metals, Environment, Failure, Fracture

384. Capillary Flow Solderability Study — FY 1993 $120,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: F. Michael Hosking, (505) 845-8401

Project summary withheld because information is patent sensitive.

Keywords: Metals, Electronic, Modeling, Solder, Surface

385. Creep Properties of Silver-Copper and Silver-Copper-Titanium Braze Alloys

FY 1993
$30,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: John J. Stephens, (505) 845-9209

Project summary withheld because information is patent sensitive.

Keywords: Metals, Braze, Creep, Manufacturing, Modeling

386. Diamond-Like Carbon Films for Stronglinks

FY 1993
$478,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Michael T. Dugger, (505) 844-1091

Solid film lubricants currently used for electromechanical components in weapons employ hazardous solvents, are line-of-sight processes, or do not possess reproducible friction and wear characteristics. The application requires materials with reproducible and low friction and wear properties, long-term chemical stability when exposed to oxygen, water vapor and a cyclic thermal environment, and quantifiable, inspectable fabrication processes. Diamond-like carbon (DLC) films possess many of these qualities, and deposition from RF plasma decomposition of carbonaceous gases allows substrates to be immersed in a plasma, thus coating all surfaces of non-planar shapes simultaneously. A potential difficulty associated with depositing DLC on ferrous surfaces is the solubility of carbon in the substrate, which may lead to poor adhesion. The goal of this project is to develop a DLC coating process for lubrication of ferrous electromechanical component parts.

Keywords: Metals, Coating, CVD, Dry Lubricant, Tribology

387. Electrochemical Studies of Al-Based Intermetallic Precipitate Phases

FY 1993
$65,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Rudy G. Buchheit, (505) 844-6904

A variety of Al-based intermetallic compounds have been synthesized in bulk form for study by conventional electrochemical and surface analytical techniques. Results obtained have been used to understand the role of finely dispersed precipitate particles in localized corrosion. The solid solubility of most metals in aluminum is usually less than 1 wt%. As a result, Al-alloys usually contain a variety of submicrometer intermetallic particles. These particles can serve as initiation sites for corrosion during aqueous processing and cleaning procedures, or during exposure to service environments. Although it is widely known that these particles induce local attack, the exact role of these particles is not well understood. Thorough understanding of the electrochemical behavior of intermetallic compounds has enabled the development of methods for mitigating localized corrosion. In this project, we have defined the electrochemical behavior of several intermetallic compounds and applied this information to aid in the understanding of localized corrosion mechanisms.

Keywords: Metals, Alloy, Corrosion

388. <u>Electrophoretic Deposition of Solid Lubricants</u> <u>FY 1993</u> $236,000

DOE Contact: Maurice Katz, (202) 586-5799
SNL Contact: Michael T. Dugger, (505) 844-1091

Project summary withheld because information is patent sensitive.

Keywords: Metals, Coating, Dry Lubricant, Surface, Tribology

389. <u>Fusion Welding of Advanced Borated Stainless Steels</u> <u>FY 1993</u> $300,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Charles V. Robino, (505) 844-6557

Project summary withheld because information is CRADA sensitive.

Keywords: Metals, Joining, Weld

390. <u>High Energy Shock Physics</u> <u>FY 1993</u> $250,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Lalit C. Chhabildas, (505) 844-4147

This is an experimental program on hypervelocity impact of metals at pressures and temperatures that have never before been accessible in the laboratory. Pressures approximating 10 Mbar and temperatures approaching 10 eV states (1 eV$\sim 10^4$K) can be achieved using the Sandia Hypervelocity Launcher. These measurements will provide the first laboratory data on the behavior of materials under shock loading to produce melt and vaporization at impact velocities of 10 km/s.

Keywords: Metals, Analysis, X-ray, Shock, Melting, Vaporization

391. High Temperature Mechanical Properties of 82Au-18Ni and 62Cu-35Au-3N Braze Alloys

FY 1993
$40,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: John J. Stephens, (505) 845-9209

Recent work on high temperature mechanical properties of braze alloys at our laboratory has included a number of investigations on Ag-base braze alloys. While Ag-base braze alloys are widely used in industry, there are a number of applications where Ag-base alloys cannot be used. Often this is due to vapor pressure requirements at a certain temperature, but it can also be caused by the need for mechanical strength at elevated temperatures. For both of these reasons, Cu- or Au-base braze alloys can offer better performance than Ag-base braze alloys. We have recently characterized the elevated temperature mechanical properties of two such alloys, namely the 82Au-18Ni (Nioro) and 62Cu-35Au-3Ni (Nicoro) alloys. Both alloys were studied in tension, using miniature samples machined from 1/8 inch diameter rod.

Keywords: Metals, Alloy, Creep, Joint, Manufacturing

392. Intelligent Processing of Thin-Section Welded Assemblies

FY 1993
$160,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
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The overall goal of this project is to develop engineering tools to predict and measure distortion in thin-section welded assemblies. Our approach integrates validated 3-D numerical techniques (tailored to welding), improved materials' response model for Ti-6-4, application and development of advanced diagnostics and sensors, as well as development of experimental strategies for validation of the numerical predictions. The project has been divided into three primary phases with specific goals. Phase I, which was completed in August of 1993, generated a valid thermal-mechanical model for predicting distortion (thin-plate buckling) in unrestrained, autogenous (no filler metal) gas tungsten arc welds on 1 mm thick Ti-6-4. Phase II is aimed at extending that model to fixtured butt-welded plates of Ti-6-4. All of the experimental data required for validation of the thermal-mechanical model has been generated at Sandia and is being statistically evaluated at P&W. Completion of the numerical analyses is expected in early December. Phase III of the project will require the simulation of filler metal additions to the model. Generation of the experimental test matrix is underway.

Keywords: Metals, Intelligent Processing, Joining, Manufacturing, Modeling

393. Lightweight Materials for Automotive Applications | FY 1993 $692,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Michael C. Maguire, (505) 845-3105

Project summary withheld because information is patent and CRADA sensitive.

Keywords: Metals, Melting, Microstructure, Solidification

394. Liquid Metal Surface Chemistry | FY 1993 $50,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Robert R. Rye, (505) 844-9194

Spreading of liquid metals on solid surfaces is central to a number of practical technologies. Despite its wide spread use, in some cases for millennia, the surface chemistry of this apparently simple process is only poorly understood, if at all. We are probing the physical effects in spreading by video recording the spreading of Pb-Sn alloys on specially prepared Cu samples. By creating accurately known groves in polished Cu we have created conditions where motion of the liquid alloy is driven by capillary forces down the groves at rates as high as ~3 cm/sec while spreading of liquid metal on the flat surface is negligible. That this rapid spreading along the grove is dominated by capillary forces is supported by several observations. With strong evidence in hand indicating that motion of the liquid Sn-Pb alloys is driven by capillary forces, it should now be possible to develop a theoretical description of this motion, and work is in progress at Case-Western Reserve and Sandia to develop such a theoretical description.

Keywords: Metals, Solder

395. Modeling the Vacuum Plasma Spray Process | FY 1993 $34,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Richard A. Neiser, (505) 845-3016

A computer-based model of the vacuum plasma spray process is being used to investigate the velocity and energy states of sprayed particles under a wide variety of operating conditions. The goals of this computer modeling are to reduce the amount of experimentation required to identify acceptable spraying conditions and to improve our understanding of the process. The work performed in this project employs both an analytical/numerical model of the vacuum plasma spray process and statistical modeling.

Keywords: Metals, Coating, Modeling, Ceramics

396. Nanocluster Electronic Structure FY 1993
$150,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Dwight R. Jennison, (505) 845-7737

Recent breakthroughs in the manufacture of nanoclusters using inverse-micelles and the possibility of revolutionary catalytic properties have stimulated our theoretical effort to understand both clean and adsorbate covered clusters. We have chosen the local density functional (LDF) method for our research program. This method has proved successful for understanding adsorbates on extended surfaces, and allows us to compare extended surfaces with nanoclusters. We have successfully studied 13-atom icosahedral clusters of Ag and Cu. We have found a substantial compression (~8 percent) of the internal atom in the clean clusters; this compression is largely relieved upon hydrogen chemisorption. We have also calculated 13-atom Cu clusters with two hydrogen atoms chemisorbed. By comparing total energies as a function of H-H distance, we find weak interactions beyond nearest neighbor three-fold-hollow sites. The solution of convergence problems on transition metal clusters was a major milestone. We have now demonstrated the capability to study adsorbates on clusters of interesting size. There are very few multi-dimensional PESs for adsorbed molecules. We find considerable sensitivity in the electron stimulated desorption dynamics to details of the PES.

Keywords: Metals, Cluster

397. QuikForm—Experimental Characterization Tool Development FY 1993
$90,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
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In support of Sandia's emerging responsibility to develop advanced manufacturing technologies, the Materials and Process Sciences Center and the Engineering Sciences Center have initiated a program titled QuikForm. The goal of this program is to develop a suite of computer-based design tools to facilitate and accelerate the design of dies for sheet metal forming. We feel that such tools could easily be adapted to other processing technologies, such as forging, extrusion, rolling, and drawing. Such a capability could prove of great utility in the rapidly evolving DOE weapons complex, allowing agile manufacturing of formed metal components to be a reality. For QuikForm to realize its potential, a number of technologies must be developed to a state of application readiness. One of these is our ability to perform experimental characterization of sheet materials to provide the necessary parameters in the new, computationally-efficient constitutive models which will be developed. Decades of research on sheet formability have demonstrated the extreme sensitivity of forming predictions to subtle variations in assumed material constitutive behavior. As part of this project, we are pursuing the development of a suite of experimental capabilities to support the QuikForm initiative.

Keywords: Metals, Fracture, Intelligent Processing, Manufacturing, Modeling

398. Reaction Mechanisms of Solder Fluxes

FY 1993
$120,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Henry C. Peebles, (505) 845-8921

Project summary withheld because information is patent and CRADA sensitive.

Keywords: Metals, Interfaces, Joining, Solder, Surface

399. Solid Film Lubricants for WR Applications (PRESS Support)

FY 1993
$22,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Michael T. Dugger, (505) 844-1091

The use of solid lubricants in weapons-related electromechanical mechanisms is widespread. Desired properties are reproducible friction and wear, long-term chemical stability and good adhesion upon exposure to weapon environments. Poor performance and more stringent environmental safety and health regulations require the use of alternative lubricants. It is unclear whether new formulations expected from commercial vendors will fulfill these requirements. Alternatives are sought for bearing lubrication as well as for sliding and impact within electromechanical mechanisms. Close communication between the design and production agencies is required to insure that materials compatibility and manufacturing issues are addressed. The goal of this work is to facilitate communication and technology transfer on solid lubrication between the production agencies and weapons system designers, component designers, and materials scientists at Sandia. This is accomplished through regular meetings of a Solid Film Lubrication Working Group, consisting of staff from Allied Signal/Kansas City Division and Sandia. Sandia participants include systems engineers, component designers, and materials scientists who provide guidance to production agency internal programs aimed at replacing the hazardous lubricants that are currently in use.

Keywords: Metals, Coating, Dry Lubricant, Treatments, Tribology

400. Solidification and Weldability of ThermoSpan Alloy FY 1993 $40,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Charles V. Robino, (505) 844-6557

ThermoSpan alloy is a low coefficient of thermal expansion precipitation hardenable superalloy with high tensile and rupture strengths. The alloy is based on the Fe-Co-Ni system and utilizes chromium additions for improved environmental resistance. This material has potential applications in a variety of Sandia designed components such as electrical feedthroughs, headers, and other glass/metal sealing applications. In order to realize these applications an understanding of the solidification behavior and a weldability database must be established. The experimental study includes differential thermal analysis (DTA) of solidification behavior, weldability evaluation by Varestraint testing, hot ductility testing by Gleeble thermo-mechanical simulations, and service weldability testing. Optical and electron microscopy is being used to characterize solidification microstructures and for identification of solidification phases. For comparison of the hot cracking tendency of ThermoSpan with other alloys used in similar applications, Varestraint samples of ThermoSpan, Pyromet Alloy CTX 909, and Pyromet Alloy 718 have been evaluated in parallel.

Keywords: Metals, Joining, Solidification, Weld

401. Solidification of Superalloys FY 1993 $200,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Brian K. Damkroger, (505) 845-3105

The processing response and performance of nickel-base superalloys are strongly affected by their solidification structure, as characterized by microstructural scale, relative amounts of microconstituents, overall homogeneity, extent of micro and macrosegregation, and the presence of solidification defects. Efforts currently being conducted under the Specialty Metals Processing Consortium are directed toward understanding and controlling the macroscopic conditions bounding the solidification process. The goal of this study is to characterize the response of two Ni-based superalloys to these solidification conditions and their stability. The variables in this study include thermal gradient, solidification rate, and niobium content. This program examines the solidification response of Alloys 625 and 718, with respect to these variables, under conditions representative of industrial scale remelting processes.

Keywords: Metals, Melting, Microstructure, Solidification

402. Specialty Metals Processing Consortium FY 1993
$4,197,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Brian K. Damkroger, (505) 845-3105

The Specialty Metals Processing Consortium (SMPC) is a group of ten specialty metals producers and users who contract with the DOE and Sandia to perform research in the areas of specialty metals melting and processing. The SMPC research program has just completed the third year of a five year contract and has active efforts in the areas of Vacuum Arc Remelting (VAR), Electroslag Remelting (ESR), and Product Characterization and Quality. The SMPC was formed to conduct basic research in the area of specialty metals processing, and to enhance the technology base of the domestic industry. The ultimate goals of the SMPC are to increase the competitiveness of the U.S. industry and to ensure a consistent supply of premium quality material for DOE applications.

Keywords: Metals, Manufacturing, Melting, Solidification

403. Stimulated Chemistry of Amonia (NH_3) on Surfaces FY 1993
$70,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Alan R. Burns, (505) 844-9642

Nitridation of substrate surfaces (e.g., GaN) is critical in the development of barriers in electronic and optoelectric devices. Thus we are motivated to study the fundamental processes, dissociation and desorption, which occur as a result of electronic excitation of adsorbed NH_3. We have succeeded in characterizing in detail the electronically-excited processes which give rise to both dissociation and desorption of adsorbed NH_3 on Pt(111). We were able to unambiguously show that desorption and dissociation arise from two distinct excited states: (1) desorption occurs via ~6 eV excitation of the lone-pair electrons at the N atom, (2) dissociation occurs via the ~12-15 eV excitation of the N-H bonding electrons. Our results directly impact the understanding of how the many degrees of freedom of a polyatomic molecule can determine the fate of electron- or photon-driven surface processes. These experimental results guide our theoretical efforts to model both the ground and excited-state potential energy surfaces. A separate report addresses our efforts to model the potential energy surfaces for this molecular adsorbate system.

Keywords: Metals, Chemisorption, Electronic, Surface, Analysis, Spectroscopy

404. Stockpile Support Capabilities

FY 1993
$3,000,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Robert J. Eagan, (505) 845-8943

Stockpile Surveillance programs require tests, analysis, materials and process certification activities. This project supports those critical capabilities. To fulfill Sandia's mission in stockpile surveillance, the materials organizations provide expert support in materials and process analysis, test interpretation, and production support. This project assures that critical capabilities, staff, and equipment meet the needs of this program.

Keywords: Metals, Capabilities

405. Surface Chemistry Soldering

FY 1993
$200,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Diane E. Peebles, (505) 845-8087

Soldering wetting is a complicated process involving many interrelated steps, including spreading, oxide removal and intermetallic formation. Very little is known about the basic mechanisms, kinetics or thermodynamics of these processes, in spite of the length of time that soldering has been a common joining technique. For instance, it is "known" that surface oxides inhibit solder wetting and that a solder flux is used to "clean" the surface and remove the surface "oxides." However, no detailed studies of wetting versus surface composition have been completed. It is not known how much oxygen must be present on a surface in order to inhibit wetting. It is also not known whether other surface contaminants, like carbon, chlorine or sulfur have similar effects on wetting. This program is designed to study the basic surface chemistry and physics of solder wetting in the absence of any fluxing agents, including the mechanisms and dynamics of each of the component steps discussed above. Studies will be conducted with tin and tin/lead solder on substrates of copper and other materials of commercial or DOE interest.

Keywords: Metals, Cleaning, Interfaces, Solder, Surface

406. Thermal Spray Technology for Cylinder Bore Coatings

FY 1993
$780,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Mark F. Smith, (505) 845-3105

Project summary withheld because information is CRADA sensitive.

Keywords: Metals, Coating, Modeling, Surface

407. Thermomechanical Fatigue Modeling

FY 1993
$395,000

DOE Contact: Maurice Katz, (202) 586-5799
SNL Contact: Darrel R. Frear, (505) 845-90237

Solder joints in electronic systems join materials with different coefficients of thermal expansion. When the systems encounter temperature fluctuations strain is imparted to the solder joints. This cyclical strain causes the solder joints to fail resulting in a reliability issue for the electronic system. Current methodologies used to predict the lifetime of solder joints are based on empirical curve fitting routines that do not take into account the solder alloy and its microstructure nor the fact that real electronic systems undergo conditions of thermomechanical fatigue. A new approach is being developed that integrates experimental results and computational finite element techniques to predict fatigue life.

Keywords: Metals, Joining, Microstructure, Packaging, Solder

408. Weldability of an Advanced Titanium Alloy

FY 1993
$20,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Brian K. Damkroger, (505) 845-3105

One class of advanced titanium alloys, "burn-resistant" alloys, offer the potential to replace Ni-based superalloys in several jet engine applications, thereby significantly improving the overall engine performance. Other applications include mineral and chemical processing, and power generation equipment. At present however, the widespread application of these alloys is limited by material production and fabrication difficulties, arising from limited hot ductility and a tendency toward grain boundary failure. Two ways this problem manifests itself are weld cracking and edge cracking during hot rolling. This program is set up to characterize the microstructural response and mechanical behavior of one burn-resistant alloy, (Alloy C, Ti-35V-15Cr), to a wide range of welding cycles. The goal is to develop a level of understanding sufficient to support the production and welding of Alloy C and similar alloys.

Keywords: Metals, Joining, Manufacturing, Solidification

409. Wetting and Mechanical Behavior of Interfacial Intermetallics in Solder Joints

FY 1993
$80,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Darrel R. Frear, (505) 845-9023

Intermetallic compounds form at the interface between the solder and substrate surface. The presence of an intermetallic is often an indicator for good wetting but, after aging, the increased thickness of intermetallics has also been cited as a possible cause for poor joint reliability. A great deal of information exists for the common near eutectic Sn-Pb alloy, but new solder alloys are being developed for special applications (such as lower and higher melting temperatures) and solders that contain no lead. There is a lack of fundamental understanding of the properties of the intermetallics that form with these new solders (due to concerns over lead as a heavy metal toxin). The areas that need to be quantified are which intermetallics form, their growth kinetics, and the mechanical properties of the intermetallics in a solder joint. This work is a cohesive study of a variety of solder systems to develop a fundamental understanding of the role of intermetallics on solder joint properties and behavior.

Keywords: Metals, Joining, Microstructure, Packaging, Solder

410. Alkylene- and Arylene-Bridged Polysiloxanes — FY 1993 $75,000

DOE Contact: Maurice Katz, (202) 586-5799
SNL Contact: Douglas A. Loy, (505) 844-4445

The purpose of this research is to determine the effect of lower crosslink density on the porosity of gels prepared by sol-gel processing hydrocarbon-bridged ethoxysilane monomers. Sol-gel processing of tetraalkoxysilanes affords porous silica. If one of the ethoxy groups is replaced with an organic group (alkyl or aryl) a siloxane network material is formed. If the organic group acts as a bridge between two triethoxysilyl groups a bridged polysilsesquioxane results in which there are a maximum of three siloxane bonds to each silicon atom in the monomer repeat unit. This high degree of sterically unhindered functionality or crosslinking allows gels to form at relatively low monomer concentrations while simple (un-bridged) triethoxysilanes forms gels only under extreme conditions. The bridging groups can be used to control porosity in the materials. Surface areas range from non-porous to 1880 m^2/g. Potential applications of bridged siloxane gels include hydrogen getters, catalyst supports, chromatographic and membrane separation systems.

Keywords: Organic, Polymer

411. Characterization of Moisture Adsorbed at Interfaces — FY 1993 $100,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Michael S. Kent, (505) 845-8178

Adsorbed moisture is believed to be a key element in debonding failures of a variety of interfaces important to weapon systems and commercial applications. This project is a study of the concentration profile of adsorbed moisture at interfaces by X-ray and neutron reflection. The objective is to characterize the profile of adsorbed moisture as a function of surface treatments in order to establish conditions which lead to hydrophobic interfaces.

Keywords: Organic, Adhesive, Polymer, Surface, Analysis, Scattering, Reflection

412. Design and Fabrication of Inertial Confinement Fusion — FY 1993 $245,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: James H. Aubert, (505) 844-4481

Target experiments, designed to study the stopping power of ion beams and the resulting radiation fields, are being conducted in the Pulsed Power Sciences Center on the Saturn and PBFA II accelerators. Target designs are developed in order to test a specific physical process and corresponding code prediction. The designs are for specific ion beams (composition and energy) and often utilize materials that are both challenging to prepare and to manipulate into the designed geometric arrangement. These materials include thin metal foils, thin polymer films, and low-density foams.

Keywords: Organic, Coating, CVD, Film, Foam

413. Development of Improved Methods for Predicting and Validating Polymer Lifetimes in Weapon Environments — FY 1993 $250,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Kenneth T. Gillen, (505) 844-7494

The Arrhenius methodology, which assumes a linear relationship between the log of the time to a certain amount of degradation and the inverse absolute temperature, has been used for many years as a means of predicting thermal lifetimes of weapon materials and components. The goals of our program are to rigorously assess the applicability of this approach. In particular, we are trying to determine (1) when and why Arrhenius behavior is followed under accelerated conditions, and (2) whether methods can be developed to better assure that the linearity assumed in extrapolated predictions can be experimentally confirmed. The materials being studied include several elastomers, including two which are frequently used as weapon environmental seals (butyl B612-70 and EPDM SR793B-80).

Keywords: Organic, Aging, Modeling, O-ring, Polymer, Seals

414. Electronic Properties of Fullerenes FY 1993
$38,000

DOE Contact: Maurice Katz, (202) 586-5799
SNL Contact: R. Glen Kepler, (505) 844-7520

The recently discovered fullerenes are an exciting new class of materials with many potential applications. During the last period we began our studies by studying the changes in photoconductivity of films of poly(methylphenylsilane) (PMPS), a s-conjugated polymer which is an excellent photoconductor, induced by doping with C_{60} molecules. The results of that study led us to now look at heterojunctions between polysilanes and C_{60}. During this period we prepared heterojunctions of poly(methylphenylsilane), PMPS, and C_{60} by spin casting a 100 nm thick film of PMPS on an indium-tin oxide (ITO) coated glass plate and then evaporating a 100 nm thick layer of C_{60} on top of the PMPS film. The ITO served as one electrode and the second electrode was a 100 nm film of aluminum evaporated on top of the C_{60} layer. When light from a monochromator with a wavelength at the peak of the C_{60} absorption band was incident on the junction through the ITO, an open circuit voltage of 1.6 V was developed and a short circuit current quantum efficiency of 0.6 percent electrons/photon absorbed. These numbers are considerably higher than those reported for a C_{60}/PPV heterojunction.

Keywords: Organic, Electronic, Fullerene

415. Electronic Properties of Organic Materials FY 1993
$277,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: R. Glen Kepler, (505) 844-7520

The electronic properties of organic materials pertinent to a variety of applications are being determined with the present emphasis on conjugated polymers and on those properties relevant to polymeric light emitting diodes. Recent emphasis has been on the electronic states of s-conjugated polymers, which exhibit high fluorescence quantum efficiencies and are thus potential light emitting diode materials. We have used absorption, fluorescence, electro-absorption, two-photon and photoconductivity spectroscopies to locate and characterize the various states pertinent to possible applications in nonlinear optics and light emitting diodes and the s-conjugated polymers have served as model compounds to test and develop appropriate theoretical models.

Keywords: Organic, Electronic, Polymer

416. Fundamentals and Materials Studies on Fullerenes — FY 1993, $200,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Bruno Morosin, (505) 844-9125

The fullerenes are the new form of carbon which has recently commanded enormous interest. Further, these materials represent individual entities which are nanostructured clusters, known to be tailorable, but currently the separation of the metal-containing entities (having potential use as low-grüniesen materials) into pure compounds still remains to be solved. In order to investigate fundamental properties as well as the potential of these materials for such applications as catalyst substrates, gas filters and optical shutters, solvent free, high purity materials are necessary. Single crystals are needed to determine intrinsic properties. Fundamental studies to date have involved collaborations with individuals from other laboratories (Argonne, U of Penn, BTL, LANL) on the pressure dependence of the superconducting transitions for alkali-metal intercalated materials. We have also performed pressure studies on (1) the dynamic behavior of fullerene molecules in their normal lattices, (2) the intercalation of gas molecules in intersticies, (3) and the reaction of C_{60} with H_2 gas. An LDRD also independently supports the practical aspects for realizing the potential of separating technologically important gases using fullerenes as "lattice sieves."

Keywords: Organic, Synthesis, Properties

417. Gas Permeation in Fullerenes — FY 1993, $45,000

DOE Contact: Maurice Katz, (202) 586-5799
SNL Contact: Roger A. Assink, (505) 844-6372

Fullerene C_{60} forms a face-centered-cubic crystal at room temperature. We found that simple gases such as hydrogen, nitrogen and oxygen readily diffuse into and out of the octahedral sites of the lattice. Most membrane separation processes are based on amorphous polymeric films. These disordered materials contain a distribution of pore sizes through which the molecules to be separated diffuse at different rates. Because the pore size distribution is very broad, the permselectivity of polymeric membranes is usually quite low, resulting in poor separation factors and/or multiple stage separation. Pore size in C_{60} is not determined by the random packing of polymeric chains, but by the lattice parameters of the crystal. In principle, the pore size of this material, which corresponds to the channels between interstitial sites, is unimodal. Thus these materials have the potential to exhibit enormous separation factors for suitable gas pairs.

Keywords: Organic, Fullerene, Membrane, Analysis, Resonance, Spectroscopy

418. Low Melting "Weak Link" Dielectrics FY 1993
$60,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Charles Arnold, Jr., (505) 844-8728

Project summary withheld because information is patent sensitive.

Keywords: Organic, Capacitor, Dielectric, Polymer

419. One Container Sticky Foams for Safeguard FY 1993
$80,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Peter B. Rand, (505) 845-8695

Our Sandia-developed one container sticky foams are used in many Safeguard applications as dispensable deterrents. These foams are packaged in pressure vessels and foam when the solutions are released to atmospheric pressure. The current solvent/blowing agent is a chlorofluorocarbon (CFC). This must be replaced to allow us to continue to use sticky foams. The replacement must be an adequate solvent for the sticky resins and also diffuse slowly enough to form stable foams. Only low boiling solvents are useful. Another requirement which severely limited our choices was non flammability. The sticky resins are blends of styrene butadiene elastomers, high melting point thermoplastic resins, plasticizing oils, chlorinated paraffin fire retardants, and silicone surfactants. The reformulated foam must be a drop-in replacement for the current formulation to avoid redesign of the dispensing systems.

Keywords: Organic, Foam

420. Optical Weak-Link Materials Development FY 1993
$80,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Paul A. Cahill, (505) 844-5754

An optical, thermal weak link built into a TSSG (trajectory sensor signal generator) would provide a significant enhancement in a device currently designed only to measure acceleration. Furthermore, an optical system would provide signal isolation from electrical noise that could lead to false signal generation. An ideal system would contain an optically readable code written in a thermally erasable medium. This code would be indefinitely stable at 74°C, but would rapidly and irreversibly be erased at temperatures as close as possible to 74°C. Our approach is to use a polymer which undergoes a phase transition (glass transition) slightly above 74°C (because the viscosity of a polymer typically may vary by several orders of magnitude across such a transition). Such a polymer would also have both an opaque and transparent state such that a code could be recorded. We have identified, obtained and continue to test a polymer which meets these requirements.

Keywords: Organic, Optical, Polymer

421. Photo-Detoxification of Explosive Waste Streams FY 1993 $50,000

DOE Contact: Maurice Katz, (202) 586-5799
SNL Contact: Clifford L. Renschler, (505) 844-0324

Environmental regulations of explosive waste streams are expected to soon become much more stringent. Current techniques for explosive disposal rely heavily on filtration, evaporation, and burning. The generators of these waste streams, including Pantex, will be forced to adopt other methods of disposal. We have now finished an experimental program which showed that it is possible to photodegrade the most common explosive waste streams generated at Pantex via laser-induced remediation. Our objective was to determine if laser-induced photo-degradation could be made more efficient or cost-effective than photo-remediation with conventional light sources. Analysis of the photo-destruction rate data for TNT, RDX, and pink water have now been completed. Exponential losses were observed, indicating pseudo-first order kinetics. Since our data were taken under conditions of total light absorption, scale-up to higher power lasers and high (multi-gallon per hour) explosive throughput should be feasible.

Keywords: Organic, Catalyst, Energetic, Explosive

422. Resist Characterization for Soft X-ray Projection Lithography FY 1993 $50,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Glenn D. Kubiak, (510) 294-3375

We are characterizing resist materials for use in soft X-ray projection lithography (SXPL). SXPL uses 14 nm radiation and reflective imaging systems to project high-resolution, sub-tenth micron demagnified images onto a photoresist. SXPL using a laser plasma source illumination is being developed at Sandia with AT&T for the lithographic definition of 0.15 micron features required for 1 Gbit DRAM. Due to the extremely high photoabsorption cross sections of all elements at 14 nm, traditional photoresists do not yield adequate resolution in SXPL. Additionally, precise experimental values of absorptance at 14 nm, required for predictive modeling of resist performance, have not been available for any resist. We are investigating the sensitivity, lithographic performance, absorptance, and photodesorption of new resists in an effort to develop a sensitive, high resolution resist which does not liberate highly absorbing contaminants onto the reflective imaging optics.

Keywords: Organic, Lithography, Polymer, Modeling

423. Role of Excited-State Singlet Oxygen in Polymer Degradation FY 1993 $200,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Roger L. Clough, (505) 844-3492

Aging and degradation is an almost universal problem for polymeric materials under a wide range of environments. In most cases, oxidation is the major degradation pathway. Oxidative degradation is highly complex: many aspects of the underlying mechanisms are not understood. The most extensively studied material oxidation mechanism involves free-radical-mediated chemistry. A second oxidation mechanism, involving the participation of the first electronically excited state of the oxygen molecule (singlet oxygen) has been the subject of much speculation during the past two decades. Studies of this mechanism have proven difficult, and the literature contains a number of conflicting reports on the subject. We have been able to apply a time-resolved spectroscopic technique, in which we observe the near-infra-red phosphorescence signal of singlet oxygen formed from oxygen molecules dissolved inside solid polymer materials. This allows us, for the first time, to directly observe singlet oxygen in polymers and to monitor parameters, such as formation yield and lifetime, in polymer systems of interest. This technique is now providing information on singlet oxygen interactions in polymers, and should lead to enhanced capability in material design for improved stabilization, and in material lifetime prediction.

Keywords: Organic, Aging

424. Smart Materials and Structures FY 1993 $200,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Jay Spingarn, (510) 294-3307

Smart materials and structures are highly integrated assemblies incorporating sensors, actuators, local intelligence, and communication. These materials offer adaptability in uncertain or inhospitable environments. Critical to the successful implementation of these materials is the use of composite manufacturing technology, as well as understanding the interrelationships between the host materials and the sensors and actuators. Work is continuing for characterizing and implementing fiber optic-based interferometric strain sensors, which will have the greatest impact on state of health monitoring systems. A simple peak counting program has been written to track our existing extrinsic Fabry-Perot sensors whose output is sinusoidal. The measured strain values compare well with traditional strain gages for surface mounting. An absolute strain measuring system based on a resonant cavity (extrinsic Fabry-Perot) is now available. This will allow us to track strains through the entire fabrication process.

Keywords: Organic, Composite, Fiber, Polymer

425. Techniques to Characterize Outgassing from Polymeric Microenvironments

FY 1993
$800,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Dale C. McIntyre, (505) 272-7621

Further reduction in particulate contamination in semiconductor device manufacturing environments will be required to meet the future challenges of producing devices with decreased dimensions. Using microenvironments to provide very clean environments on a local (wafer level) scale is an alternative that can reduce the technological demands and cost (capital and operating) of providing comparable contamination levels in an entire clean-room manufacturing facility. However, there have been indications that outgassed constituents from polymeric microenvironment materials can condense on Si wafers during storage. These condensed contaminants may impact device processing and thus device performance. This project is focused on: (1) developing standard high sensitivity outgassing testing techniques for evaluating polymeric microenvironment materials of construction and (2) evaluating the use of prototype commercial surface acoustic wave (SAW) sensors as high sensitivity, real time monitors for condensable, outgassed, organic contaminants found in microenvironments, minienvironments, and cleanrooms.

Keywords: Organic, Polymer

426. Electrostatic Chuck Research

FY 1993
$50,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Carleton H. Seager, (505) 844-9168

Project summary withheld because information is patent and CRADA sensitive.

Keywords: Semiconductor, Oxides

427. Hot Filament Carbon Chemical Vapor Deposition FY 1993
$75,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Robert R. Rye, (505) 844-9194

The most widely used method for low temperature diamond formation involves a hot tungsten filament in the presence of dilute mixture of hydrocarbon in hydrogen with growth occurring on a near-by substrate. Despite the widespread interest in low temperature diamond formation, efforts to refine the processing conditions have been limited by the lack of understanding of this process. This is especially true for reactions that occur at the tungsten filament. We have shown that the only reactions that occur at the tungsten filament, other than hydrogen dissociation, are decomposition of the hydrocarbon to carburize the tungsten filament. Thus, it is clear that a main function of the hot tungsten filament is to serve as a source of carbon, with the species leaving the surface being equivalent to those from sublimation of graphite. This explains why diamond growth occurs with such an extremely wide range of hydrocarbon species.

Keywords: Semiconductor, Carbon

428. Materials Science at High Pressure FY 1993
$435,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: George A. Samara, (505) 844-6653

By decreasing the interatomic separation, one of the most fundamental variables in the study of the properties of matter, high pressure plays a crucial role in materials science. The variation of properties with pressure provides insight into the physics and allows testing of proposed models. Pressure also induces phase transitions, allows access to regions of the phase diagram of materials difficult or impossible to achieve in any other way, and makes possible novel materials synthesis. Additionally, static high pressure results are necessary for the understanding of shock-wave phenomena. This program capitalizes on all of these attributes of high pressure research. Materials and phenomena of current interest are: defects and deep levels in semiconductors, organic and inorganic superconductors, electronic transport in boron-rich solids, piezoelectric polymers, fullerenes and phase transitions.

Keywords: Semiconductor, Compound

429. Modeling Processing Effects for Porous Silicon Layers FY 1993
$20,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Joel O. Stevenson, (505) 845-8652

Porous silicon has myriad applications in the microelectronics industry and can be selectively processed to form a variety of insulators, conductors, and micromachined structures. While preparing thick sacrificial porous silicon layers to form thin single crystal silicon membranes for the determination of interstitial oxygen in silicon, we observed unexpected processing effects and evidence of high stress areas. Since an understanding of material morphology is a prerequisite to tailoring specific structures, we have begun a modeling study to estimate the magnitude of the interfacial stress generated during the porous silicon formation process and to evaluate the effects of such stress on the quality of the underlying single crystal silicon.

Keywords: Semiconductor, Silicon

430. Nonlinear Electrical Phenomenon in rf-Excited Plasmas FY 1993
$200,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Paul A. Miller, (505) 844-8879

Electrically excited plasmas are widely used in the manufacture of microelectronic circuits. Previous workers have largely ignored the electrical nonlinearity of the voltage-vs.-current characteristics of plasmas. Recent industrial results have demonstrated the importance of nonlinear interactions between the plasmas and their rf power supplies. However, little is presently understood in detail of the use, control, or mitigation of most such phenomena. One important nonlinear phenomenon is "period doubling" (PD) and the accompanying generation of subharmonics of the excitation frequency. This consists of an alternation between two states of the plasma on successive cycles of the excitation waveform. This behavior is a fundamental mathematical property of essentially all dynamical systems with two or more degrees of freedom, and it is generally a precursor to chaos. We now are in a position to exploit in two different ways the understanding gained from the model and the laboratory experiments. First, we know how to suppress PD in systems in which its presence is undesirable. Second, we can induce PD (and also higher levels of period multiplication) to achieve different processing conditions that may yield superior process performance.

Keywords: Semiconductor, Plasma

Device or Component Fabrication, Behavior or Testing

431. Photosulfidation as Passivation Process for III-IV Compound Semiconductors

FY 1993
$43,000

DOE Contact: Maurice Katz, (202) 586-5799
SNL Contact: Carol I. H. Ashby, (505) 844-2303

Project summary withheld because information is patent sensitive.

Keywords: Semiconductor, Compound, Passivation, Analysis, Spectroscopy

432. Polaronic Phenomena in Solids

FY 1993
$100,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: David Emin, (505) 844-3431

Polarons are charge carriers that are bound within potential wells produced by displacements of the atoms of condensed matter. Polarons form in ionic solids, polymers, molecular crystals and amorphous semiconductors. Small polarons are confined to a single site and move by phonon-assisted hopping. Large polarons extend over multiple sites and move as heavy massed quasi-free carriers. We study how polaron formation dramatically affects electronic and optical properties of solids.

Keywords: Semiconductor, Oxides

433. Semiconductor Surface Defects

FY 1993
$80,000

DOE Contact: Maurice Katz, (202) 586-5799
SNL Contact: Brian S. Swartzentruber, (505) 844-6393

Although it is known that defects control the growth of epitaxial structures and, ultimately, their electronic properties, very little is known about their formation and stability on an atomic scale. Using variable-temperature STM we have explored the nature of surface vacancies on the Si(001) surface. The number of vacancies that we observe on the surface is largely sample and treatment-history dependent. Highly doped samples generally have many more defects than lower doped samples. As sample surfaces are repeatedly prepared *in situ*, the defect level tends to increase due to exposure to the residual gas and/or contaminants leaching off of the sample mount. It is clear that the surface defect density is largely process dependent. As the size of fabricated structures decreases, surface defects will become the limiting factor that determines the quality of the final device. By understanding the origin and kinetic behavior of these defects we can better control the processing conditions that lead to their generation.

Keywords: Semiconductor, Silicon

434. Technique Developed for Measurement of Electric Fields in High-Frequency Discharges

FY 1993
$230,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Kenneth E. Greenberg, (505) 844-1243

High-frequency plasma systems are used to etch and deposit materials during the fabrication of integrated circuits. These plasma systems have proven to suffer from reliability and reproducibility problems. Furthermore, due to the highly complex nature of the plasmas, development of new etching and deposition processes is typically arduous. Knowledge of the fundamental mechanisms occurring in plasma systems and accurate plasma models would greatly increase the ability to control and optimize presently used plasma processes, and to efficiently develop new processes. We have developed a technique that can be used to measure electric-field strengths in high-frequency (13.56 MHz) helium discharges. The technique is based on observation of the Stark structure of helium Rydberg levels. This technique allows the measurement of electric fields in high-frequency helium discharges with a high degree of spatial resolution.

Keywords: Semiconductor, Plasma, Microelectronics, Electric Field, Parallel-Plate Discharge, Plasma Etching

435. Variable-Temperature STM Measurements of Step Kinetics

FY 1993
$80,000

DOE Contact: Maurice Katz, (202) 586-5799
SNL Contact: Brian S. Swartzentruber, (505) 844-6393

A number of surface properties are affected by defects. It is generally believed that steps serve as an important class of active sites on the surface. Steps can control the nucleation and subsequent growth of epitaxial and 3-D overlayers. The chemical reactivity of the surface, as well as the sticking and surface diffusion of adsorbed species can be altered by the presence of steps. Using the variable-temperature STM we have acquired movies of the time evolution of the atomic-scale arrangement of steps on Si(001) at temperatures up to 450°C. At temperatures between 225 and 350°C we have performed quantitative measurements of the details of the individual step rearrangement events by recording the differences of the step positions in sequential frames of the movies. In the context of this simple model we can extract the activation energy for step rearrangement events. We measure an activation energy of 1.3 ± 0.3 eV for atom attachment to and detachment from the step, and a difference in activation energies of 0.180±0.060 eV for events occurring at straight sections of the step versus kink sites. The understanding gained through the study of the Si(001) model provides a general insight into the kinetic properties of steps.

Keywords: Semiconductor, Silicon

436. Computer-Aided Advanced Ceramic Manufacturing FY 1993 $50,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Kevin G. Ewsuk, (505) 272-7620

Ceramic component fabrication involves multiple processes ranging from raw materials beneficiation to post-sintering machining. Member companies of the Association of American Ceramic Component Manufacturers (AACCM) have identified forming, binder burnout, and sintering as three critical areas where improved understanding and control would contribute to improved product quality and yield, and reduced manufacturing costs. Seven member companies of the AACCM have signed letters of intent to work with Sandia National Laboratories (SNL) and Los Alamos National Laboratory (LANL) to apply process science and computer methodologies being developed and employed at DOE national laboratories for advanced materials processing to develop improved processes and process controls to form ceramics. Modeling and experiments will be conducted to develop a personal-computer based, software package that can be used to design new ceramic forming processes, and troubleshoot problematic processes. This package will also serve as a demonstrative and prototypic model to develop comparable packages for binder burnout and sintering.

Keywords: Ceramics, Modeling, Manufacturing

437. Ferroelectric Films for Optical Storage and Processing FY 1993 $700,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Duane B. Dimos, (505) 844-6385

Lead zirconate titanate based films, exhibit a combination of electrooptic and photo-induced properties that make them attractive materials for optical storage and processing applications. Optically-generated information can be stored by using light to induce changes in the hysteresis behavior of the film. Since the value of an individual bit is defined by the remanent polarization, the information is stored in a nonvolatile manner. The stored information can be readout photometrically due to the polarization-dependent change in birefringence. We are currently evaluating the optical storage and readout responses of sol-gel derived films in an effort to make a nonvolatile, read/write optical memory and related devices, such as spatial light modulators. To optimize the materials properties, we are also studying the fundamental aspects of the electrooptic and photo-induced properties, especially the storage photosensitivity.

Keywords: Ceramics, Electrooptic, Ferroelectric, Optical, Sol Gel

438. Field Emission Flat Panel Displays

FY 1993
$67,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Carol S. Ashley, (505) 845-8931

The technical aim of this program is to develop a manufacturable technology for field-emission, flat-panel displays which will feature relaxed cleanliness constraints, higher efficiency low-voltage phosphors, and reduced lithographic requirements. The expected reduced capital investment and enhanced yields compared to current Active-Matrix Liquid Crystal Display (AMLCD) technology will allow competition with the now-dominant AMLCD technology used by Japanese firms to control 95 percent of the world market for flat panel displays. We are continuing to work toward the development of inexpensive, manufacturable routes to stable, high efficiency, low-voltage phosphors for the fabrication of phosphor screens. We are also preparing prototype screens using sol-gel films to bind conventional phosphor powders to a glass substrate. Films for potential non-photolithographically defined masks are being prepared by loading sol-gel films with a sacrificial phase which is subsequently removed to leave a distinct pattern of holes.

Keywords: Ceramics, Electrooptic

439. Ion Beam Modification of Glasses

FY 1993
$50,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: George W. Arnold, (505) 844-3848

There are increasing applications of ion-implanted SiO_2 in future semiconductor heterostructures and as components in optical computers. For example, in patterning wave guides into glass substrates and the high-fluence implantation of metals into such waveguides to form colloids for enhancing the intensity-dependent refractive index. Past work in the Ion Solid Interactions and Defect Physics Department at Sandia and in collaboration with Padova University (Italy) has shown that the implantation damage depth can increase to twice the TRIM predicted ranges at high collisional energy deposition values (10^{22}-10^{23} keV/cm^3) as indicated by changes in many important properties such as etching rates and depths, alkali depletion depth, and the distribution depth of the implanted ions. This phenomenon is not well understood and provides the motivation for the present investigation.

Keywords: Ceramics, Glass, Optical, Preparation, Waveguide

440. Micro-Miniature Refrigerator Components FY 1993 $70,000

DOE Contact: Maurice Katz, (202) 586-5799
SNL Contact: Terry J. Garino, (505) 845-8762

Micro-miniature refrigerators have numerous military, space and commercial applications. We are developing two components that will improve the performance of micro-miniature refrigerators. The first is an adaptive orifice to control gas expansion in a Joule-Thomson refrigerator to optimize performance and to conserve gas, as these devices are commonly powered by a compressed gas bottle. The second component is a miniature compressor that would replace the gas bottle supply. We have designed a mini-compressor based on bismuth oxide oxygen conductor. At moderate temperatures, ~500°C, bismuth oxide is capable of readily conducting oxygen when an electric field is applied across it so that oxygen can be made to go from a low pressure side in contact with air, to a high pressure side. Our design consists of a patterned layer of doped bismuth oxide 50 mm thick between two substrates.

Keywords: Ceramics, Ferroelectric, Piezoelectric

441. New Materials for SEMATECH Photolithography Stage FY 1993 $240,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Darrel R. Frear, (505) 845-9023

Project summary withheld because information is CRADA sensitive.

Keywords: Ceramics, Modeling, Nitride

442. Thin-Film Decoupling Capacitors FY 1993 $500,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Duane B. Dimos, (505) 844-6385

High-performance decoupling capacitors are a critical part of multi-chip module systems. Thin-film decoupling capacitors are being developed to replace multi-layer ceramic capacitors for next-generation packaging architectures. Thin-film capacitors, that can be embedded into multi-chip modules, should lead to decreased package volume and improved high-speed performance. Ferroelectric lead zirconate titanate films are being investigated for this application since these films satisfy the material requirements of high dielectric constant (e~1000), low loss, and good insulating properties. These films are fabricated using sol-gel techniques and fired at low-temperatures (< 650°C), which makes their processing compatible with a goal of full integration. Discrete thin-film decoupling capacitors are being fabricated on silicon wafers for use in a prototype digital signal processing multi-chip modules.

Keywords: Ceramics, Dielectric, Ferroelectric, Film, Packaging, Sol Gel

443. Thin Film Solder Bonds for Sensor Assembly FY 1993 $208,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Paul T. Vianco, (505) 844-3429

Microsensors are being developed which incorporate single crystal quartz resonators for frequency control and silicon micromachining for packaging technology. A joining technique was required to assemble the quartz resonator and silicon lids that would accommodate tight dimensional control, provide adequate strength, and have the capacity to absorb thermal mis-match strains. It was determined that solder films based upon indium would be most appropriate since the material is inherently very ductile and the precious metal content would be adequate to effect a fluxless soldering processes. The indium-containing solders could be deposited by physical vapor deposition which allowed for precise control of the bond thickness as permit batch processing of the devices. A mechanical tension test was used to quantify the strength of the thin film bond as a function of processing and bond thickness.

Keywords: Ceramics, Joining, Piezoelectric

444. Thin Film Transistors FY 1993 $50,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Carleton H. Seager, (505) 844-9168

Project summary withheld because information is CRADA sensitive.

Keywords: Ceramics, Ferroelectric

445. Certification and Specification Exception Release Remediation Activities for MC4190M Thermal Battery FY 1993 $20,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Gerald A. Knorovsky, (505) 844-1129

The MC4190M Thermal Battery is a MAST component produced at Eagle-Picher Industries (EPI), Joplin, MO. In order to proceed with production activities, the closure weld schedule had to be certified by a SNL Welding Metallurgist according to requirements of

SS324637F. The welds are made in 304 stainless steel using the pulsed Gas Tungsten Arc process in a standing edge geometry. Certification samples provided by EPI were found to be nonconforming based upon metallographic examination. The areas of nonconformance included an excessive number of passes being used (three) when only two are allowed, insufficient penetration of the weld fusion zone, and excessive size porosity. Nevertheless, it was judged that the welds were functional and a Specification Exception Release (SXR) was written allowing their acceptance. As part of remediation activities mandated by the SXR, the weld schedule was re-examined.

Keywords: Metals, Batteries, Joining, Steel, Weld

446. <u>Copper on Teflon</u> — <u>FY 1993</u> $75,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Robert R. Rye, (505) 844-9194

Project summary withheld because information is patent sensitive.

Keywords: Metals, Electronic, Organic, Dielectric

447. <u>FASTCAST Consortium</u> — <u>FY 1993</u> $1,313,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Frank J. Zanner, (505) 845-3085

An effort is currently underway to assist the domestic Investment Casting Industry to form a Consortium called FASTCAST which will oversee funding and provide technical guidance in the building of a investment casting tool kit at Sandia. This effort will complement our already functioning program that is internally funded by DOE/DP. Major technical work will center around developing a rule-based system to design and evaluate the performance of the gating system. FASTCAST demonstrations of the system at current status were presented to the Investment Casting Institute (ICI) Board of Directors in Dallas, TX, at the ICI annual technical meeting in Chicago, IL, and to the Sandia Defense Programs sponsoring organization. Three industry members have agreed to Incorporate FASTCAST in Delaware and then to solicit members in a CDB announcement. Industry lawyers are currently drafting up the legal documents for incorporation.

Keywords: Metals, FASTCAST, Manufacturing, Melting

448. Laser Soldering of Sn Plated Brass Integrator Assembly Housings FY 1993
$20,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: David M. Keicher, (505) 845-8365

Laser soldering was proposed as an alternative process for producing closure joints on Sn plated brass integrator assembly housings after joints produced using hand soldering methods and electrically conductive epoxies failed to provide desirable results. The localized heating properties provided by lasers can be used to overcome the high thermal diffusivity of the brass and produce good solder joints while minimizing the heat input to the structure. Joints produced using hand soldering methods (i.e. a soldering iron) exhibited good electrical shielding properties; however, the excessive heating required to produce these joints caused thermal damage to the electronic components contained within the housings. Conversely, using an electrically conductive epoxy did not provide satisfactory electrical properties.

Keywords: Metals, Electronic, Joining, Joint, Solder

449. Laser Welding Optimization Software FY 1993
$100,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Phillip W. Fuerschbach, (505) 845-8877

The SMARTWELD computer system is an SNL developed technology for rapid response manufacturing of welded assemblies. The demonstration computer system illustrates the feasibility of integrating Sandia's unique expertise in design, analysis, and fabrication software application tools. For the tasks in SMARTWELD where software is not already developed, new software must be written. A primary goal of SMARTWELD is to incorporate into the computer system, mature welding technology that has been developed for past defense programs. An important requirement for a rapid response expert welding system is the determination of a practical set of weld parameters (weld schedule) that will produce the weld as required by the design process. Sandia has been for several years developing an empirical model of the laser welding process that is ideally suited for the task of weld schedule prediction.

Keywords: Metals, Intelligent Processing, Manufacturing, Modeling

450. Lead-Free Solders for Electronics Assembly

FY 1993
$278,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Paul T. Vianco, (505) 844-3429

Reducing the amount of lead introduced into the environment by manufacturing processes has included the examination of lead-bearing solders used in electronic assemblies. A collaborative effort is being conducted with AT&T/Bell Laboratories, Engineering Research Center to fabricate circuit board prototypes using commercially available and Sandia proprietary lead-free solders. Test vehicles were used to determine the feasibility of alternative solders for electronic assembly by assessing the number and kinds of defects observed on the circuit boards. Several of the test vehicles were then subjected to preliminary reliability testing by thermal cycling the units at SNL. The surface mount technology developed with AT&T is being extended to the assembly of components at Martin Marietta Specialty Components (MMSC). In addition, hand soldering techniques using lead-free solders were developed at Allied Signal/Kansas City Division (AS/KCD) through assembly of the inverter board for the Simple Firing Set (Focal Point). Solder joint defects were assessed for each of the solders in order to assess the feasibility of substituting these lead-free solders on this assembly. Initial reliability data is being collected by observing solder joint integrity following thermal shock and thermal cycling exposure. Functional units are also being built to determine compatibility of the solder process with the electrical operation of the assembly.

Keywords: Metals, Joining, Solder

451. New Common-Domain Specifications and Applications for Invar-Type Alloys

FY 1993
$30,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: John J. Stephens, (505) 845-9209

The low thermal expansion alloys Fe-36Ni (Invar) and Fe-32Ni-5Co (Super Invar) are used for a number of precision instrument and component applications where minimal thermal expansion near room temperature is required. Two separate activities have been initiated involving these alloys: (1) a new ASTM specification is being developed to cover a wide range of product forms for standard Invar, free-machining Invar and Super Invar; (2) an assessment has been made of the feasibility of using Super Invar as a braze interlayer for metal/Si_3N_4 braze joints. The specification activity has been motivated by a lack of comprehensive common-domain specifications for Invar-type alloys. The latter activity is driven by the need to identify interlayer materials that can match the thermal expansion of Si_3N_4 over significant ranges of temperatures in order to minimize residual stresses in brazed Si_3N_4 parts.

Keywords: Metals, Alloy, Braze, Joining, Steel

452. Printed Wiring Board and Interconnect Systems

FY 1993
$200,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: N. Robert Sorensen, (505) 844-5558

This project addresses critical areas of generic, pre-competitive technologies needed to enable the utilization of next generation electrical components on printed wiring boards. Maintaining a solderable surface during processing and storage can be extremely important. Defects in the surface can results in dewetting or product rework or rejection. The ultimate objective of this program is to develop a reliable soldering technology which is compatible with the environment through improved understanding of soldering processes. Objectives include characterization of aging & stressing of printed wiring boards, development of non-destructive surface inspection technique, and an understanding of copper inhibitor interactions and their effect on soldering. Improved solderability has been demonstrated after environmental exposure by using organic inhibitors. Both imidazole and benzotriazole (BTA) improved solderability, but the BTA provided the best conditions for solderability. Both BTA and imidazole have been evaluated for atmospheric corrosion resistance, with BTA providing the highest degree of protection. With both BTA and imidazole, solderability is maintained, even after accelerated environmental testing.

Keywords: Metals, Batteries, Joining, Steel, Weld

453. SMARTWELD II—An Intelligent System for Concurrent Engineering

FY 1993
$1,700,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Kim W. Mahin, (505) 844-2222/(510) 294-3582

SMARTWELD is a new initiative at Sandia National Laboratories, which integrates computer-aided design, information networking, computer simulation, process optimization and machine controls into a unique system for concurrently designing both the process and the product for optimum manufacturability and performance. Over the past seven months, the SMARTWELD project has succeeded in physically linking diverse people, applications, and information in an integrated, collaborative workstation environment. The physical models being integrated into SMARTWELD tailor its current application specifically to welding. However, the networking framework designed for SMARTWELD is generic and provides the framework for developing a whole suite of SMARTPROCESSING initiatives. The objective of SMARTPROCESSING, as well as SMARTWELD, is to use this integrating framework to capture our materials and processing expertise, to maintain our capabilities in design and manufacturing, and to provide a continual path for process improvement.

Keywords: Metals, Intelligent Processing, Joining, Manufacturing, Modeling

454. Substitute Cleaner for Lithium Thionyl Chloride Batteries

FY 1993
$140,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Carol L. J. Adkins, (505) 845-9119

There are currently several fabricators of the lithium thionyl chloride cells being used for aging, safety, and reliability tests conducted by Sandia. Each is using different cleaning techniques. The batteries fabricated at Sandia, specifically, use chlorofluorocarbons as a primary parts cleaning technique. These solvents will soon be unavailable and there was a need to learn more about possible alternative cleaning solvents. At Sandia, the primary battery piece part contaminants are fingerprints, Apiezon L grease, and high vacuum silicon grease. The chosen cleaner must be able to remove both organics and the salts found in fingerprints. Currently, the parts are vapor cleaned at Sandia in Freon TMS. The alternate solvents tested were d-limonene, ethyl lactate, Actrel 4493L, supercritical carbon dioxide, and Oakite Citridet. D-limonene is being implemented as a Freon and TCE replacement solvent at AlliedSignal/Kansas City and there is a large body of knowledge that has been gathered on this product. Citridet is a d-limonene/surfactant mixture that is used at dilute concentrations in water and can be rinsed with water. This solvent is being investigated as an alternative by the thermal battery engineers. The other solvents are under consideration as alternatives both at Sandia and at Allied Signal-Kansas City.

Keywords: Metals, Cleaning

455. Supercritical Fluid View Cell

FY 1993
$45,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Carol L. J. Adkins, (505) 845-9119

There is currently much work being done to determine if there is a niche that supercritical carbon dioxide (SC-CO_2) can fill in the area of alternative solvents. An important aspect of this research is determination of the solubility of relevant contaminants in SC-CO_2. We assembled a high pressure view cell in order to perform these solubility and phase separation studies. An alternate technique, known as the "dynamic" method, can also be used measure solubilities. This method involves passing SC-CO_2 through a packed bed of the material being tested at slow enough flowrates that equilibrium is achieved, and then capturing and quantifying the material carried through by the carbon dioxide. However, this technique is difficult to use with liquids—entrainment is an issue. The high pressure view cell is ideal for measuring the solubility of liquids and allows us to visually determine the cloud and dew points for a material in high pressure carbon dioxide. These equilibrium properties are critical in understanding how a practical SC-CO_2 cleaning system would operate.

Keywords: Metals, Cleaning

456. Thin Film Solder Conductor as Thermal Weak Link FY 1993 $275,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Larry D. Miller, (505) 844-2568

The safety of nuclear weapons under adverse environmental conditions depends upon sensors in the arming, fuzing, and firing electronics to detect such circumstances and enact the proper system response. The implementation of a thin film "thermal weak link" is being evaluated as a means to disable system functions upon exposure of the weapon to elevated temperatures. The first-principle weak link concept being evaluated uses electrical conductor paths of binary metal thin films which melt upon exposure to elevated temperatures, thereby irreversibly opening the signal path of the electronic circuit. The alloy films are deposited as separate layers of each of the constituents by evaporation techniques. Various metal thicknesses, conductor path configurations, and substrate materials are being evaluated for optimum performance of the weak link.

Keywords: Metals, Electronic, Solder

457. Cleaning Related Processes for Printed Wiring Boards FY 1993 $400,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Edwin P. Lopez, (505) 845-9181

Project summary withheld because information is CRADA sensitive.

Keywords: Organic, Adhesive, Cleaning, Compatibility

458. Development of Environmentally-Sound Removable Encapsulants FY 1993 $150,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Charles A. Arnold, (505) 844-8726

Project summary withheld because information is patent sensitive.

Keywords: Organic, Encapsulant, Foam, Polymer

459. Endpoint Indicator for Printed Wiring Board FY 1993
$25,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Pamela P. Ward, (505) 844-2038

The production of multilayered printed wiring boards consists of laminating several conductive layers (typically copper) isolated by nonconductive polymer. The resulting assembly is then drilled through to allow the mounting of connectors and components. During the drill-through process, a "smear" may develop. A smear results when the insulating layer is heated to the point where the polymer flows through the hole to form an insulator over copper contact where none is desired. One method of removing the smear is via a plasma desmear process. The difficulty in performing a desmear operation is determining when the process is complete. An endpoint indicator is required to determine when the polymer has been removed to the degree desired. Optical emission spectroscopy is one method of monitoring a plasma etch process. With this method, the plasma environment can be explored without perturbing the process. The method consists of a spectrophotometer measuring the plasma light via a monochromator. By observing the spectra of the plasma discharge, the components of the etchant gasses and plasma products can be determined.

Keywords: Organic, Cleaning, Composite, Electronic, Plasma

460. Environmental O-ring Seals—Properties, Aging and the Argon Method FY 1993
$250,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Kenneth T. Gillen, (505) 844-7494

Environmental O-ring seals are used in most weapons to protect the interior from the ingress of potentially harmful quantities of such substances as water vapor and oxygen. Two components contribute to the ingress, permeation through the O-rings and leakage between the O-ring and its metal-mating surface. It is difficult to estimate the latter since it will depend on the long-term aging characteristics of the seal and on other factors hard to predict (e.g., leaks may occur during low temperature exposures). Our O-ring program is attempting to address such issues by studying the aging (from surveillance units and from accelerated aging studies) of important O-ring materials used in weapons and the quality of O-ring parts when received. In addition, we have suggested and are pursuing an easy, inexpensive method for estimating the lifetime ingress of oxygen and water vapor into a weapon based on the analysis of the argon gas content in the weapon's interior.

Keywords: Organic, Aging, Modeling, O-ring, Polymer, Seals

461. Flexible Carbon Anodes for High Performance Batteries FY 1993
$100,000

DOE Contact: Maurice Katz, (202) 586-5799
SNL Contact: Robert R. Lagasse, (505) 845-8333

Flexible carbon electrodes may allow development of high capacity rechargeable batteries useful for applications ranging from electric vehicles to small portable electronic devices such as cellular phones. Previous work at Sandia has shown that rigid, porous carbons produced by pyrolyzing poly(acrylonitrile) perform extremely well as anodes for rechargeable lithium batteries. The goal of the present work is to determine if the same performance can be achieved in a flexible carbon anode. Flexibility would allow the anode to be wound in a layered structure with the cathode and separator to produce a high capacity, low cost battery. The approach has been to develop a process for converting commercially available poly(acrylonitrile) yarn into a flexible carbon and then to evaluate its electrochemical performance.

Keywords: Organic, Battery, Carbon, Electrode

462. Fully Integrated Optical Hydrogen Sensor FY 1993
$50,000

DOE Contact: Maurice Katz (202) 586-5799
SNL Contact: Michael B. Sinclair, (505) 844-5506

Compact sensing devices are required for a number of applications including safeguard and security monitoring, manufacturing process control, health monitoring, environmental protection and restoration. The goal of this project is to develop a technology demonstrator for a new class of sensors that are compatible with microelectronic packaging. The prototype sensor consists of an organic optical waveguide which is integrated with sources and detectors on a single GaAs chip. The sensing function is accomplished via interaction of the optical energy propagating along the waveguide with external perturbations which may be mechanical, chemical, or thermal in origin.

Keywords: Organic, Polymer, Sensors, Waveguide

463. Lithography Employing Surface and Near Surface Imaging FY 1993
$250,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: David R. Wheeler, (505) 844-6631

Project summary withheld because information is patent and CRADA sensitive.

Keywords: Organic, Lithography, Polymer, Semiconductor

464. MDA-Free Epoxy Encapsulant Formulations

FY 1993
$268,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Linda A. Domeier, (510) 294-2350

Neutron generators and other DOE components currently use epoxy encapsulants cured with MDA (methylene dianiline), a regulated carcinogen. Alternative epoxy formulations using less hazardous curing agents while still meeting or improving on other requirements are needed and have been the target of an on-going multi-site program. The particular formulations developed at Sandia/CA have utilized combinations of aliphatic amine curing agents to obtain the desired balance of toughness, Tg and other processing and performance characteristics. The preferred formulation based on this approach, designated Formula 456, has been endorsed as a replacement material for MDA cured epoxies. Formula 456 contains 25 parts of Dow's XU-71790 acrylic rubber modified epoxy, 50 parts of Epon 826, and 25 parts of a 1:1 blend of Jeffamine D-230 and Ancamine 2049. The Dow epoxy contains 40 percent of a phase separated acrylic rubber which helps provide an exceptional combination of low viscosity and processability. An extensive database on Formula 456 is now available and further qualification testing in specific applications is underway. A companion formulation, Formula 459, is also under evaluation for applications where very low viscosities and low CTE values are critical. Formula 459 does not contain the rubber modifier present in Formula 456.

Keywords: Organic, Adhesive, Encapsulant, Polymer

465. Nonlinear Optical Materials and Devices Development

FY 1993
$175,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Paul A. Cahill, (505) 844-5754

Project summary withheld because information is CRADA sensitive.

Keywords: Organic, Electrooptic, Nonlinear, Optical, Polymer

466. Organic Composite Materials

FY 1993
$200,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Jay R. Spingarn, (510) 294-3307

Composite materials offer designers and engineers extraordinary flexibility in tailoring directional properties and combining mechanical, electrical, thermal, chemical, and optical behavior to optimize system performance. Effective utilization of this added flexibility requires an understanding of the strong interactions between design, manufacturing, test, and materials characterization. The goal of this program is to develop the tools to effectively support a diverse set of customers, both internal and external. Experimental work was completed on the toroidal pressure vessels developed for Surety applications. Work continues on developing a compressive failure model for filament wound cylinders with Stanford University. Composite hardware has been provided for on-going SNL projects. A material evaluation study was conducted and two large test panels were provided for possible retrofitting of the Aft Cover for the B83.

Keywords: Organic, Composite, Fiber, Polymer

467. Toluene Diisocyanate-Free Rigid Polyurethane Encapsulation Foams — FY 1993 — $200,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Peter B. Rand, (505) 845-8695

Many Sandia-designed electronic assemblies, such as firesets, are encapsulated with rigid polyurethane foam. This is done to improve the mechanical ruggedness of the assembly and provide environmental protection. Polyurethane has been a very popular encapsulant over the last ten years, because it reduces thermally induced stresses, when compared with other encapsulants. The current foam is formulated with toluene diisocyanate (TDI), which is a suspected human carcinogen. The foam developed at Sandia/New Mexico has been selected by a DOE multi-agency group to replace the currently used TDI based encapsulation foam. Our foams utilize the same polyester polyol used in the TDI based foams. This was done to maintain the toughness of the current encapsulation foams. The foam is formulated with polymeric isocyanates (polymethylenepolyphenylisocyanate - PMDI) rather than TDI.

Keywords: Organic, Encapsulant, Foam

468. Commercial Development of Porous Silicon Humidity Sensors — FY 1993 — $20,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Terry R. Guilinger, (505) 845-9043

Project summary withheld because information is CRADA sensitive.

Keywords: Semiconductor, Etching, Silicon

469. Engineered Photocatalysts for the Detoxification of Waste Water FY 1993
$300,000

DOE Contact: Maurice Katz, (202) 586-5799
SNL Contact: Michael R. Prairie, (505) 844-7823

Solar photocatalytic detoxification provides an attractive new approach for the treatment of polluted water. The best available technology uses a TiO_2 photocatalyst because it is active, robust, and non-toxic. Unfortunately, TiO_2 only absorbs UV light. This limits the efficiency of solar applications to the fraction of the solar spectrum which is UV, about 5 percent. Also, the choice of TiO_2 limits the application of photocatalysis to only a few toxic metals. This project includes development of a new generation of photocatalysts designed to enhance solar detoxification by using (1) adsorbed porphyrin dyes to effectively capture a larger portion of the solar spectrum, (2) molecular modeling techniques to design biomimetic catalysts for isolation and detoxification of dilute toxic waste components and (3) a novel SiC/TiO_2 photocatalytic diode for extending the applicability of photocatalysis to a much wider range of toxic metals. The key technical challenges are binding the porphyrins to various substrates to form active and stable waste treatment catalysts, optimizing the catalysts for broad applicability, optimally deploying the photocatalysts, and fabricating a powder form of a dual semiconductor photocatalyst for reductive treatment of polluted water.

Keywords: Semiconductor, Compound, Oxides, Electrochemistry, Organic, Catalyst, Modeling

470. Folded Cavity Second Harmonic Generation of a Nd:YAG Laser FY 1993
$30,000

DOE Contact: Maurice Katz, (202) 586-5799
SNL Contact: David M. Keicher, (505) 845-8365

In development of a 3-D packaging process for silicon multichip modules, laser drilling was determined to be the process of choice for producing vias through the bulk silicon material. However, silicon, and most ceramic insulators, are essentially transparent to the fundamental wavelength of the preferred high power, Nd:YAG laser. Thus, the second harmonic is critical for laser machining these materials. Also, it is generally found that the second harmonic wavelength provides improved processing performance over the fundamental wavelength from the Nd:YAG laser due to the significantly higher volumetric absorption of many materials at the shorter wavelength. However, the two-mirror resonator geometry possessed by typical second harmonic lasers limited the frequency doubled output power to no greater than one half the maximum power available at the fundamental wavelength. This limitation reduced the overall efficiency of the laser system and limited the second harmonic performance. By using a folded cavity configuration, the second harmonic light generated in the forward direction in the cavity is reflected back through the second harmonic crystal to be combined with the second harmonic light generated in the backwards direction. Extraction of the beam at this point allows essentially all of the second harmonic light produced within the cavity to utilized.

Keywords: Semiconductor, Laser, Packaging, Silicon

471. Gate-Controlled "Artificial Impurities" Fabricated with Nanostructure Airbridges

FY 1993
$100,000

DOE Contact: Maurice Katz, (202) 586-5799
SNL Contact: Jerry A. Simmons, (505) 844-8402

As present day electronic devices are scaled down to increasingly smaller sizes, understanding of the quantum effects which dominate in the small limit is becoming increasingly crucial. In the small size limit the electron wavefunction remains coherent across the entire device, and the presence of a single impurity can determine the device's behavior. Devices based on tunneling through lower-dimensional states also hold great promise for high speed applications. Our objective is to fabricate single impurity-like potentials and study resonant tunneling through the individual electron states associated with them, as well as how those states evolve with the enhanced electron-electron interactions occurring at high magnetic fields.

Keywords: Semiconductor, Compound, Electronic, Lithography

472. High Sensitivity Moisture Sensors

FY 1993
$1,200,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Raymond P. Goehner, (505) 844-9200

Project summary withheld because information is patent and CRADA sensitive.

Keywords: Semiconductor, Sensors, Organic

473. Hybrid Shubnikov-deHaas-Photoluminescence Analysis of 2-D Electron Density in PHEMT Structures with Heavily-Doped Contact Layers

FY 1993
$50,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Michael L. Lovejoy, (505) 844-6814

The 2-D electron density in the quantum well of strained quantum well FETs (SQWFETs), or equivalently pseudomorphic HEMTs (PHEMTS), is an important parameter for device performance. Figures of merit such as the source-drain current and transconductance are proportional to the carrier concentration (n_{2D}) in the well, hence, accurate n_{2D} data are needed for structure optimization and reliable device modeling. Measurement of n_{2D} is complicated by two factors. First, high-performance SQWFETs require heavily doped contact layers that presents a conduction path parallel to the 2-D gas conduction channel in the SQW. In general, Hall effect and Shubnikov-de Haas (SdH) responses of the 2 layers are different; consequently, the measured Hall and longitudinal voltages are intermediate values which don't accurately characterize either layer. Second, high-performance also requires high carrier concentrations which results in multiple subbands being occupied; SdH oscillations from individual subbands are superimposed which makes data analysis difficult. We have developed a hybrid analysis technique to extract the n_{2D} where severe parallel conduction occurs with multiple subband occupation.

Keywords: Semiconductor, Compound, Electronic Structure

474. <u>Matrixed Field Emitter Arrays</u> <u>FY 1993</u> $40,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: James G. Fleming, (505) 844-9158

Project summary withheld because information is CRADA sensitive.

Keywords: Semiconductor, Silicon, Ceramics, Electronic

475. <u>Midwave (4 μm) Infrared Emitters with Biaxially Compressed InAsSb Active Regions</u> <u>FY 1993</u> $200,000

DOE Contact: Maurice Katz, (202) 586-5799
SNL Contact: Robert M. Biefeld, (505) 844-1556

Strained InAsSb heterostructures offer the promise of new III-V based, infrared detectors and emitters. As-rich InAsSb heterostructures may display unique electronic properties that are beneficial to infrared emitter performance. Changes in the heavy-hole ground state in a biaxially compressed InAsSb layer should increase the threshold energy of the dominant Auger process. With this improvement, the wavelength of diode lasers operating at room temperature may be extended from recently demonstrated 2.1-2.3 μm devices in unstrained InGaAsSb to the 3-5 μm range where devices are presently limited by Auger processes. Metal-organic chemical vapor deposition is being used to prepare InAsSb/InGaAs strained-layer superlattices for use in 3-5 μm lasers and light emitting diodes.

Keywords: Semiconductor, Compound, CVD, Laser

476. Phosphorus-Containing Precursors for III-V Semiconductors FY 1993
$50,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Neal D. Shinn, (505) 844-5457

Phosphorus-containing III-V semiconductors are attractive materials for electronic and optoelectronic devices. Phosphine (PH_3) is the usual source of atomic phosphorus in organometallic chemical vapor deposition. However, the inordinate quantities of this toxic gas required for phosphorus incorporation present significant health and environmental risks. Using synchrotron-based Soft X-ray Photoelectron Spectroscopy (SXPS), we have studied the surface chemistry of PH_3, PF_3, and PCl_3 in order to guide the design of alternate, phosphorus-containing precursor molecules. These results show that PF_3 is more stable than either PH_3 or PCl_3 on Ru(0001) at 150K. Using this and other temperature-dependent data, a thermochemical analysis allows important energetic parameters to be extracted, thereby yielding insights into the chemistry of these isostructural molecules.

Keywords: Semiconductor, Deposition

477. Rapid Methods for Calculating Reflectance Spectra of Growing Semiconductor Films for Applications in Process Control FY 1993
$100,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: William G. Breiland, (505) 844-7029

Modern semiconductor electronic and optoelectronic devices require very stringent control over a wide variety of materials properties such as thickness, composition, strain, doping level, and interface abruptness. We are currently exploring the use of normal-incidence reflectance to serve as an in situ monitor and to develop model-based active control of thin film growth. To be successful as an active control, a model-based control strategy must be able to rapidly compute the reflectance spectra expected for a given semiconductor multi-layer film under processing conditions such as elevated temperature. Advances in sensor technology place heavy demands on such computations. It is now possible to collect a 2048-point reflectance spectrum every quarter-second during a growth run. This data must be analyzed and materials-properties extracted in real time in order to provide a basis for control. An efficient method for calculating the reflectance (or ellipsometry) spectrum of an arbitrarily complex multi-film structure for any incidence angle and polarization has been devised, with particular emphasis on calculating the spectral reflectance of a growing film.

Keywords: Semiconductor, CVD, MBE, Process Control

Instrumentation and Facilities

478. Real Time Control of MBE by Optical Based Flux Monitoring (OFM) FY 1993
$200,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Kevin P. Killeen, (505) 844-5164

We have developed and demonstrated a new method for controlling molecular beam epitaxy (MBE) of compound semiconductors based on the vapor-phase optical absorption of group III elemental sources (i.e., Al, Ga and In). Angle resolved, high resolution laser excitation and absorption experiments were conducted on Ga and Al to measure the spectral overlap between the Doppler shifted beam absorbance and hollow cathode lamp emissions of these elements. A monitor was then designed and implemented on the CSRL's Riber 32P MBE system with the lamp probe light passing parallel and adjacent to the GaAs substrate. The absorbance signal was scaled by a beam velocity correction factor to yield an instantaneous reading proportional to the beam flux. Since the sticking coefficients for the group III sources are essentially unity, this relative flux signal can be used to directly determine growth rates and group III lattice composition once calibrations to material properties are established.

Keywords: Semiconductor, Compound, MBE, Process Control

479. Semiconductor Wafer Cleaning FY 1993
$810,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Carol L. J. Adkins, (505) 845-9119

Project summary withheld because information is CRADA sensitive.

Keywords: Semiconductor, Cleaning

480. Sensors for Process Control FY 1993
$30,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Raymond P. Goehner, (505) 844-9200

Project summary withheld because information is CRADA sensitive.

Keywords: Semiconductor, Sensors, Organic

481. Shallow Zn Ion Implantation for GaAs Junction Field Effect Transistors

FY 1993
$200,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: John C. Zolper, (505) 845-9709

To realize high performance n-channel GaAs junction field effect transistors (JFETs) a shallow, abrupt, highly doped p-layer is required. This can be achieved with ion implantation if the ion species has a shallow projected range, does not exhibit significant channeling, and does not diffuse during the high temperature activation anneal. Zn is known to meet the first two criteria but was generally thought to be a fast diffuser at elevated temperatures. We have demonstrated that the use of a capless rapid thermal anneal along with P co-implantation minimizes Zn diffusion thus making Zn ion implantation an excellent choice for GaAs JFET fabrication. In fact, GaAs JFET fabricated in our lab showed a two-fold increase in performance over previous JFETs made using Mg implantation.

Keywords: Semiconductor, Compound, Ion Implantation

482. Surface Science of Compound Semiconductor Epitaxy

FY 1993
$300,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: J. Randall Creighton, (505) 844-3955

Organometallic and hydride compounds are widely used as precursors for epitaxial growth of GaAs and other compound semiconductors. We are investigating the surface chemical and physical properties of these precursors on compound semiconductors in order to develop a fundamental understanding of the epitaxial deposition processes (e.g., MOCVD). This project uses a surface science approach which employs a wide variety of diagnostics. The use of trimethylgallium (TMGa) as a precursor during GaAs epitaxy often leads to high levels of carbon incorporation. Using a variety of surface science diagnostics we have identified a likely carbon incorporation pathway initiated by methyl group dehydrogenation. Methyl group dehydrogenation is evidenced by a small amount of hydrogen evolution around 430°C during temperature programmed desorption. Extended TMGa exposures in this temperature regime yield substantial coverages of methylene (CH_2) adsorbate which is detected by vibrational spectroscopies (HREELS and FTIR). The CH_2 adsorbate completely dehydrogenates at higher temperatures and leaves a strongly bound form of carbon on the GaAs surface that is ultimately responsible for doping.

Keywords: Semiconductor, Compound, CVD, Surface Chemistry

483. Theory and Computer Simulation of Low-Temperature, rf-Driven Plasmas Relevant to Plasma Processing

FY 1993
$150,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Merle E. Riley, (505) 844-3141

Radio-frequency-driven plasmas are widely used in the processing and manufacture of microelectronics devices. These plasmas are of great current interest to researchers. They are difficult to analyze and model in a predictive fashion because of the computational difficulty associated with the description of extremely stiff multi-dimensional problems, and also because of unknown atomic and kinetic data in the reactive species. The theoretical plasma simulation effort at Sandia has concentrated on the development and benchmarking of numerical methods as well as theoretical models of the basic atomic processes in simple plasmas. We have developed two new acceleration schemes for the solution of the time-dependent Poisson-Boltzmann equation describing the rf-driven plasmas. There are two major areas of significance to this work as it exists thus far. The first is that, for the first time, we have benchmarked theory against experiment for these rf-driven, capacitively-coupled, low-temperature plasmas. The second is that we have participated in an international effort, started at the 1992 Gaseous Electronics Conference, to compare many computational descriptions of a model plasma in order to assess the accuracy and validity of the theories.

Keywords: Semiconductor, Plasma, Microelectronics, Boltzman, Kinetics, Processing

484. Analytical Capabilities

FY 1993
$4,500,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Robert J. Eagan, (505) 845-8943

Advanced analytical techniques are a critical element of meeting DP needs for characterizing materials and processes used to produce and dismantle weapons. This project supports the maintenance and improvement of analytical capabilities required to develop and characterize materials and processes used to produce or dismantle weapons. Typical tasks include software upgrades, retrofitting equipment, and development of broadly applicable analytical techniques.

Keywords: Analysis, Capabilities

485. Analysis of Crystalline Silicotitanate (CST) for Cs-Extraction from Radwaste

FY 1993
$112,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Thomas J. Headley, (505) 844-4787

Project summary withheld because information is patent sensitive.

Keywords: Analysis, Chemical, Microscopy, Spectroscopy, X-ray

486. Beam Characterization of a Materials Processing CO_2 Laser

FY 1993
$12,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Marcelino Essien, (505) 844-2838

In the interaction of metals with powerful light fluxes, it has been shown that the absorption of laser energy by metals is intensity dependent. As a result, processes such as laser cutting and drilling which require removal of material through evaporation, and soldering and welding which require melting, depend strongly on the characteristics of the materials processing laser. Consequently, characterization of the propagation and focusability of a laser beam is essential in the laser materials processing application. In many cases, the required intensity threshold for a material may be reached by focusing the laser radiation. In this application, one should therefore ask (1) what parameter determines the intrinsic limit to which a laser can be focused, (2) what limits the focusing ability of a high-quality laser lens, and (3) how does this limitation vary among different types of lenses? These questions may be answered by measuring four important parameters that characterize a laser for materials processing—mainly, minimum spotsize, beam quality, minimum spotsize location, and depth of focus.

Keywords: Analysis, Laser

487. Booster for Tandem

FY 1993
$1,200,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: H. Schone, (505) 844-2598

Extremely high-energy microfocused heavy-ions have not been readily available for applications such as (1) the simulation of high Linear Energy Transfer (LET) particles to test the response of modern solid state devices, or (2) the enhancement of flux pinning in high temperature super conductors by the production of ion tracks. We have just finished the design stage for a radio frequency quadrupole (RFQ) booster addition to the tandem in the Ion Beam Materials Research Lab (IBMRL) that will provide 1.9 MeV/amu ions (i.e., 1.9 MeV protons or ~400 MeV Pb-208). The tandem+RFQ combination will be capable of opening these new research areas to the Physical and Chemical Sciences Center.

Keywords: Analysis, Ion Beam

488. Characterization of Quartz Resonators FY 1993 $40,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Vicki E. Granstaff, (505) 844-8789

Quartz resonators are used in a variety of applications, including sensors based on mass changes or liquid property changes, and studies of electrodeposition, corrosion, and electroactive polymers. Many of these applications use a polymer-coated resonator in contact with a liquid. When polymer losses and polymer-liquid interactions are significant, existing mass measurement techniques are inaccurate. We have developed a new physically-based analysis method that predicts the electrical impedance vs. frequency of a quartz resonator having any number of nonpiezoelectric layers of arbitrary thickness and complex shear modulus. The predictions can be fit to experimental data to extract the physical properties of the layers in contact with the quartz resonator.

Keywords: Analysis, Resonance, Organic, Polymer

489. Chemometrics Methods Developments FY 1993 $220,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: David M. Haaland, (505) 844-5292

Project summary withheld because information is patent sensitive.

Keywords: Analysis, Chemometric, Spectroscopy

490. Diagnostics for Supercritical Water Oxidation of Hazardous Wastes FY 1993 $70,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Bernice E. Mills, (510) 294-3230

We are integrating chemical and physical diagnostics with process control for supercritical water oxidation (SCWO) destruction of hazardous wastes. We have performed some preliminary experiments using non-dedicated reactors to study corrosion of SCWO reactors handling the complex molecules in realistic wastes. These experiments have shown that on-line diagnostics will facilitate these experiments and can be expected to permit better control of the pilot-scale reactor now being designed. They should also help us to predict the lifetime of the material in such a reactor. A reactor to test the diagnostics and use them to perform corrosion and solids handling experiments is nearing completion. Diagnostics have been evaluated for use on this system and most of them have been obtained through purchase or, if possible, on loan pending proof of efficacy. Calibration curves for integration into monitoring software have been obtained for those that require them. A gas-liquid separator with a minimum volume has been designed and manufactured to deliver a gas-free liquid and a liquid-free gas stream for analysis with a minimum of time lag. We expect the engineering evaluation reactor (EER) to be on-line for the first experiments in January 1994.

Keywords: Analysis, Supercritical, Metals, Corrosion

491. Helium Leak Testing of Integrated Circuit Packages — FY 1993 $12,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Steve M. Thornberg, (505) 844-8710

Some integrated circuits must be hermetically sealed for some applications and MIL specifications. A method for measuring the helium leak rates of small integrated circuit packages was developed which is capable of discriminating between leakage from defects (cracks, separation from pins, etc.) and permeation through the potting compounds. The helium leak testing method successfully tested integrated circuit packages. Helium permeation through the sealing O-ring was distinguishable from true leaks in the package using this technique. The devices were tested to 10^{-9} atm cc/s.

Keywords: Analysis, Spectroscopy, Semiconductor, Packaging

492. Ion Induced Roughening and Smoothing of SiO_2 Films — FY 1993 $80,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Thomas M. Mayer, (505) 844-0770

The morphology that surfaces acquire during processing is a result of the microscopic dynamics of growth and removal. The evolution of this surface morphology into the micro- and macrostructure of the fabricated material makes the dynamics of the process important with regard to the properties and performance of the material. For this reason, much recent effort has focused on the relationship between dynamics and material structure, particularly in thin film deposition and etching processes. Ion bombardment of surfaces is a common phenomenon in many film processing environments, including sputter etching and deposition, ion beam assisted growth, reactive ion etching, and plasma assisted chemical vapor deposition. It is important to understand the nature of ion bombardment, the dynamic surface processes that occur as a result, and the evolution of surface structure during material processing. We have demonstrated that surface topography development during sputtering processes can be understood quantitatively within the framework of a model which contains measurable dynamic surface processes.

Keywords: Analysis, Surface

493. Massively Parallel Quantum Chemistry Code Development FY 1993
$100,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Mark P. Sears, (505) 845-7194

A massively parallel computer code, MSLAB, has been developed for the purpose of computing the electronic structure of large molecule systems and periodic systems with large unit cells. The challenge is to develop a method that scales well with large number of atoms, and runs effectively on the most powerful computers available. The method employs the local density functional approximation to the quantum chemical equations, and uses first principles pseudopotentials to remove the chemically inert core electrons. Linear combinations of contracted gaussians are used to represent the orbitals, in a linear combination of atomic orbitals, or LCAO, approach. Taking advantage of the local representation of the basis set, a subtraction scheme due to Feibelman is implemented which reduces, in principle, the computational effort associated with the construction of the Hamiltonian (the atom interaction matrix) scales linearly with the size of system. Except for very large systems, this constitutes the majority of the computational effort.

Keywords: Analysis, Electronic Structure

494. Mechanism of Lithium Ion Production from the PBFA II Anode FY 1993
$100,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Robert A. Anderson, (505) 844-7676

The PBFA II machine in organization 1200 accelerates an intense burst of lithium ions toward a target in order to study controlled fusion. Ions are obtained from a half-micron thick coating of lithium fluoride (LiF) on the anode in the accelerator diode. The long-standing presumption has been that a flashover discharge on the LiF surface is responsible for the ion production, although the absence of intense fluorine line emission which is expected with a surface flashover discharge has been puzzling. This project had the objective of comparing the existing spectroscopic evidence with the flashover hypothesis to test for consistency or to develop alternate hypotheses.

Keywords: Analysis, Electrical Properties, Theoretical, Breakdown

495. Noninvasive Alcohol Monitor FY 1993
$35,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: David M. Haaland, (505) 844-5292

Chemometric multivariate calibration methods have the potential to be used with near-infrared spectra obtained through the finger of humans for noninvasive monitoring of alcohol. If successful, noninvasive alcohol monitoring can be used to monitor blood-alcohol levels of sensitive DOE security personnel involved in the transport or protection of nuclear material. A noninvasive monitor could also be used to decrease problems associated with DWIs. We have earlier shown that monitoring glucose noninvasively is feasible. We are now evaluating spectrometer and sampling configurations to define the optimal conditions for noninvasive blood–University of New Mexico School of Medicine (UNM SOM) with encouraging results.

Keywords: Analysis, Chemometric, Spectroscopy

496. Optical Diagnostics for Process Control in Steelmaking FY 1993
$315,000

DOE Contact: Robert Trimberger, (208) 526-1807
SNL Contact: David K. Ottesen, (510) 294-3567, Robert R. Hurt, (510) 294-3707

Real-time optical sensing methods are being developed for optimizing carbon content and final temperature of the molten bath in Basic Oxygen Furnace (BOF) steelmaking. Activities in FY93 included laboratory development of two line-of-sight infrared spectroscopic methods for measurement of BOF exit gas temperature and composition; and video-imaging and thermographic measurements of the molten bath. Optical measurement methods for CO, CO_2, and H_2O in the BOF off-gas employed infrared absorption near 4.7 μm wavelength using a tunable diode laser, and infrared emission in the same wavelength region using a multiplexed detector array. Feasibility of these methods was demonstrated using the hot exhaust stream of a pilot-scale combustor at Sandia. A prototype imaging thermographic sensor was designed and fabricated for extracting video images and temperatures of the molten bath. This device was tested in the laboratory using a high-temperature blackbody source. Both sensor systems will be field-tested at a Bethlehem Steel pilot-scale BOF early in FY 94.

Keywords: Analysis, Spectroscopy, Metals, Manufacturing, Organic, Laser, Sensors

497. Parallel Numerical Libraries for Materials Modeling Programs FY 1993
$201,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Mark P. Sears, (505) 845-7194

Project summary withheld because information is CRADA sensitive.

Keywords: Analysis, Electronic Structure

498. Phase Identification in the Scanning Electron Microscopy by Backscattered Electron Kikuchi Patterns FY 1993
$60,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Joseph R. Michael, (505) 844-9115

The microstructural characterization of materials is essential to understand and improve their properties. The identification of microconstituents from their crystallography is typically accomplished using transmission electron microscopy (TEM). The development at Sandia National Laboratories of a CCD array-based detector for backscattered electron Kikuchi patterns has permitted crystallographic phase identification to be performed in the scanning electron microscope much more quickly than in TEM due to the reduced specimen preparation requirements. The objective of this project is to add to our understanding of BEKPs and to develop a new routine tool for microstructural characterization The applicability of this technique is being expanded by applying it to various materials problems and by performing specific experiments to further our understanding of the origin of these patterns.

Keywords: Analysis, Diffraction, Microscopy, Microstructure

499. Porous Silicon Photoluminescence and K-Map X-ray Diffraction FY 1993
$100,000

DOE Contact: Maurice Katz, (202) 586-5799
SNL Contact: J. Charles Barbour, (505) 844-5517

Visible light photoluminescence (PL) from electrochemically prepared porous silicon (PS) has excited technical interest because of its potential use in optical displays requiring light from blue to red (400 to 800 nm). Scientifically, interest in PS stems from the desire to understand the luminescence mechanism and its possible relationship to sample microstructure (which is also not well understood). One of the leading mechanisms proposed for luminescence assumes the PS contains a microstructure of small Si columns or possibly particles which act as quantum wells causing carrier confinement. The modification of band structure from quantum size effects is thought to produce an optical bandgap (~2 eV) suitable for visible light emission. This work examined several categories of PS and related the PL signal to distributions of particle sizes measured by K-map X-ray diffraction.

Keywords: Analysis, Microstructure, Porosity, Spectroscopy, X-ray

500. Quantitative Materials Characterization by Nuclear Microprobe Analysis FY 1993 $770,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Arthur E. Pontau, (510) 294-3159

Nuclear microprobe techniques using focused MeV ions provide nondestructive materials characterization for applications ranging from analyzing the elemental and isotopic composition of particulates to determining uniformity in microporous materials. For example, analysis of overtly- or covertly-collected particles on collection media to identify *in situ* uranium or plutonium provides critical intelligence information for assessing source material origin and processing history. Inhomogeneity and internal flaw detection can lead to improved processing and machining of microporous materials which are of increasing interest in the areas of catalysts or catalyst supports, capacitors, batteries and gas or liquid separators. For elemental composition, characteristic X-rays are measured using particle-induced X-ray emission (PIXE) while isotopic information is collected using Coulomb excitation (CE) measurements of characteristic g-rays. This project includes developing the capabilities to perform these ion microanalysis measurements on samples, and to nondestructively identify and quantify elemental and isotopic information with micron-scale resolution in a timely manner.

Keywords: Analysis, Ion Beam, Microscopy, Microstructure, Spectroscopy

501. Resonant Ionization Detection of Atomic H from Surfaces FY 1993 $70,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Alan R. Burns, (505) 844-9642

H_2 and H-containing molecules are always present as background gases, even in ultra high vacuum systems. H-containing molecules that are used in critical technologies include metal organics for MOCVD, precursors for diamond growth, and NH_3 for nitridation. Thus it is highly desirable to detect and monitor the H removal and to explore the direct channel for H removal by electron or photon induced dissociation. We have successfully demonstrated the ability to use resonance-enhanced multiphoton ionization (REMPI) to probe the electronically-induced (non-thermal dissociation) of adsorbed NH_3 on Pt(111). The primary reaction that has been monitored is $NH_3(a) \rightarrow NH_2(a) + H(g)$, although H(g) from $NH_2(a)$ and NH(a) also occurs. The detection scheme is a (2+1) process, where two uv photons (243 nm) promote the ground-state ($1^2S_{1/2}$) H atoms to the first excited state ($2^2S_{1/2}$), which is subsequently ionized by a third photon of the same color. The ability to monitor with high sensitivity the production of gas-phase H from technologically-important surface processes provides valuable information with regard to rate-limiting steps in surface modification or film growth. Of particular significance are detailed studies of electron-driven, non-thermal removal of H from passivated Si surfaces.

Keywords: Analysis, Chemical, Electronic Structure, Spectroscopy, Surface

502. Scanning Tunneling Microscope for CVD Processes FY 1993
$80,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Brian S. Swartzentruber, (505) 844-6393

In order to better control the growth of overlayers in low-temperature CVD growth processing environments it is of particular interest to understand the atomic-scale details of the nucleation events involved in the initial stages of growth, i.e., whether nucleation occurs at steps or other surface defects, how surface mobilities are affected by the presence of ligands, whether intermixing with the substrate occurs during the initial stages of growth, etc. We have constructed an STM and ultra-high vacuum chamber for investigations of the initial stages of metal nucleation and growth on silicon surfaces. The chamber is equipped with a dosing cell through which metalorganic gas can be introduced. The STM is a variable temperature design which allows for the imaging of the sample surface at elevated temperatures. We have used this instrument in preliminary investigations of the initial stages of Fe nucleation on the Si(001) surface through the decomposition of $Fe(CO)^5$. Because of its inherent resolution the STM has the capability to image nucleation events on the atomic scale. Using this tool we will be able to elucidate the roles that various processes, e.g., diffusion, ligand interactions, have in the details of the nucleation event.

Keywords: Analysis, Microscopy

503. Sorting of Waste Plastics Using Near Infrared Spectroscopy and Neural Networks FY 1993
$254,000

DOE Contact: Maurice Katz, (202) 586-5799
SNL Contact: M. Kathleen Alam, (505) 845-9621

Project summary withheld because information is patent sensitive.

Keywords: Analysis, Chemometric, Spectroscopy, Organic, Polymer

504. Studies on Triboluminescent Materials

FY 1993
$25,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Willard A. Hareland, (505) 844-7758

Project summary withheld because information is patent sensitive.

Keywords: Analysis, Spectroscopy, Organic, Triboluminescent

505. Techniques for Measuring Outgassing Characteristics of Polycarbonate Polymers

FY 1993
$140,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Steve M. Thornberg, (505) 844-8710

Polymer outgassing can adversely affect yields in semiconductor manufacturing by contaminating wafers. Wafers are stored and shipped in containers made of various polymers (typically, polycarbonate). Identifying and locating the sources of these contaminates is the necessary first step to remediating the contamination. Techniques to identify and quantify outgassed volatile organic compounds were developed for thermal desorption, cryofocused gas chromatography/mass spectroscopy (GC/MS). Volatiles from polycarbonate samples were thermally driven out of the polycarbonate and collected in a cold trap. The volatiles are injected into the gas chromatography column by rapidly heating the trap in the helium carrier gas. The polycarbonates outgassed numerous volatile organic compounds, making precise identification of all components difficult. However, the technique for chromatographically separating the many VOCs at the very low concentrations needed (ppb by weight) has been successfully demonstrated. Work continues to expand the list of identified and quantified compounds.

Keywords: Analysis, Chromatography, Spectroscopy, Organic, Polymer, Semiconductor, Packaging

506. Tritium Monitor

FY 1993
$50,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: William R. Wampler, (505) 844-4114

Measurement of tritium is of great interest for many Sandia and DOE programs including nuclear weapons, environmental restoration and fusion energy. Existing methods of detecting tritium, based on the use of wipes and liquid scintillation cocktails, are expensive, do not give real-time information, and do not meet completely the needs of the above programs. Furthermore, wipes can only detect loosely bound surface tritium, and liquid scintillation cocktails generate mixed waste. A new method to monitor tritium is needed which overcomes the limitations and disadvantages of existing methods. As part of our magnetic fusion energy program, we have developed a new method to monitor tritium. Prototypes of the new tritium monitor have been used to measure tritium on components from the TFTR, JET and DIIID tokamaks at levels in the range from 0.3 to 30 nCi/cm^2. The monitor uses a PIN photodiode and low noise pulse amplifier to count tritium betas emitted from surfaces. The present embodiment of the monitor has a probe which is held against the surface to be measured. A lower limit of detection for tritium activity of about 0.1 disintegration per second (3 pico Curie per square centimeter) has been demonstrated.

Keywords: Analysis, Ion Beam

507. <u>Weapon Component Characterization for Disposition</u> <u>FY 1993</u>
$400,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: William B. Chambers, (505) 844-3849

Inductively coupled plasma-atomic emission spectroscopy (ICP-AES) and non-destructive X-ray fluorescent spectrometry (XRFS) have been used to support the disposition of dismantled nuclear weapon hardware. A number of non-nuclear components from different weapon systems and with diverse functions have been analyzed by ICP-AES using the Environmental Protection Agency (EPA) Toxicity Characteristic Leaching Procedure (TCLP). The majority of the electronic and electro-mechanical components tested exhibit the Toxicity Characteristic for lead (Pb) and/or cadmium (Cd) and would be regulated as hazardous solid waste under EPA. However, many of these components contain significant quantities of precious and recyclable metals. We have been investigating the use of XRFS as a rapid, non-destructive method for semiquantitative determination of toxic contaminants and recoverable metals in excess weapon hardware. The objective is to be able to sort materials on-line by chemical composition thereby minimizing the quantity of hazardous waste generated by the dismantlement processes.

Keywords: Analysis, Spectroscopy, Chemical, X-ray

508. <u>X-ray Reflectivity Characterization of Thin Film Structures</u> <u>FY 1993</u>
$100,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Eric H. Chason, (505) 844-8951

In situ, non-destructive characterization is important to the development of advanced thin film structures and processing techniques. We have developed in situ X-ray reflectivity as a technique for measuring thin film thickness and interfacial roughness with high resolution (0.3 nm in thickness and 0.04 nm in surface roughness) and reasonably short acquisition time

(<500 s per spectrum). We have used this technique to study two different thin film structures: SiGe heterostructures grown by CVD and metal films deposited on quartz substrates.

Keywords: Analysis, Surface, X-ray, Ceramics, Metallization, Semiconductors, CVD

509. Microstrain in Diamond Films — FY 1993 $20,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Michael O. Eatough, (505) 844-7761

Project summary withheld because information is CRADA sensitive.

Keywords: Ceramics, Diamond, Analysis, X-ray

510. Scattering Center Development — FY 1993 $150,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Thomas Rieker, (505) 272-7611

In a joint venture with the University of New Mexico, a unique scattering facility has been established at UNM's Farris Hall to serve the Sandia and UNM materials science communities. A number of specialized X-ray and light scattering instruments were brought to working order by the dedication of the Scattering Center on August 17, 1993. Together these instruments constitute a state-of-the-art capability for structural characterizations over nearly five decades in length scale. This facility is used for a wide range of materials studies with dual-use, Defense Programs and Energy Programs, applications including porous materials of all kinds, thin films, and sol-gel precursors.

Keywords: Ceramics, Modeling, Preparation, Sol Gel, Solution

511. Beam Quality Measurements and the Proposed ISO Standard — FY 1993 $100,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Phillip W. Fuerschbach, (505) 845-8877

Laser beam-quality can indicate the maximum power density that can be obtained with a specific laser and serves as a figure-of-merit when comparing lasers, calibrating lasers, and in assessing a laser's operating condition. Directly related to beam-quality is the laser power density. The magnitude of the incident laser power density is a fundamental characteristic in laser beam welding that affects the weld penetration, the shape of the weld pool, and the overall energy transfer efficiency of the process. Because measuring laser power density is a difficult task, few researchers report values of power density in the welding literature, the performance of several types of focusing lenses is unproved, and the transfer of welding schedules from one laser to another is not feasible.

Keywords: Metals, Intelligent Processing, Manufacturing, Modeling, Weld

512. High Energy, High Flux Pulsed Ion Beams for Surface Modification — FY 1993 $300,000

DOE Contact: Maurice Katz, (202) 586-5799
SNL Contact: Regan W. Stinnett, (505) 845-7488

Project summary withheld because information is patent sensitive.

Keywords: Metals, Surface

513. Medical Applications of Ion Beam Induced Radiation — FY 1993 $250,000

DOE Contact: Maurice Katz, (202) 586-5799
SNL Contact: Kevin M. Horn, (505) 845-7944

Radiation therapy is a commonly used tool in the clinical treatment of malignant cancer tumors. However, established techniques and equipment utilizing radioactive sources (brachitherapy), cyclotron-produced, high energy proton beams (proton radiotherapy and radiosurgery), and laser treatments are often not applicable in certain situations. Medical clinicians claim that the development of a radiation source that could be handled like a radiation "air-brush" to deliver relatively large doses of radiation to specific areas with hand-held control would provide an ease of use and flexibility that currently does not exist in traditional radiation therapies. The micro-radiosurgery technique is based upon the concept that low energy ion-induced nuclear reactions can be used to produce high energy protons directly at a tumor site.

Keywords: Organic, Biomedical

514. Photoluminescence Analysis of Tetragonal Mercuric Iodide — FY 1993 $30,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Richard J. Anderson, (510) 294-3258

Mercuric iodide, used as a room temperature X-ray and gamma-ray detector material, is seriously impaired by the presence of impurities. Photoluminescence is used as an analytical technique to probe for these harmful defects. However, until now the mechanism whereby the photoluminescence spectrum is altered by the presence of impurities has not been well understood. Using time-resolved photoluminescence of highly pure, single-crystalline mercuric iodide after excitation by absorption of one photon (surface excitation) or two photons (bulk excitation), at temperatures from 4.6 K to 100 K, we have shown that the structure in the exciton photoluminescence spectrum arises only from radiative recombination of the free exciton. The lifetime of the free exciton increases nearly one hundredfold from 4.6 K to 100 K because radiative decay, caused by cooling and transport to the surface, is blocked by the presence of thermally populated phonons. Changes in the spectrum due to the presence of impurities, quenching certain spectral features, we can identify as caused by radiative decay short-circuited to traps rather than to photoluminescence; spectral features once felt to be impurity-related are instead characteristic of the purity of the sample.

Keywords: Analysis, X-ray Detector, Gamma-ray Detector, Optical Diagnostics, Impurities

515. Radiation Microscopy — FY 1993 — $200,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
SNL Contact: Barney L. Doyle, (505) 844-7568

The deposition of charge resulting from the passage of ions through integrated circuits (IC) scan cause a memory bit to change state, i.e. from a 1-0 or 0-1. These malfunctions are called Single Event Upsets (SEUs), and it has been well documented that such upsets, caused by solar flair and cosmic ray particles, routinely plague advanced ICs in satellites and spacecraft. For example Voyager, Magellan, INSAT, and GOES/TRDS series satellites have all suffered such problems. While space and nuclear weapon applications currently require the most radiation resistant ICs, with the continued shrinkage of both feature size and stored charge of microelectronic devices, even terrestrial applications of ICs are now starting to be effected by SEUs, We have developed two techniques to study SEU microscopically: Single Event Upset (SEU) imaging and Ion Beam Induced Charge Collection (IBICC) microscopy. Both techniques utilize scanned nuclear microprobes at Sandia and the University of Melbourne.

Keywords: Semiconductor, Ion Beam, Analysis

516. Time-of-Flight Heavy Ion Backscattering Spectroscopy — FY 1993 — $300,000

DOE Contact: Maurice Katz, (202) 586-5799
SNL Contact: James A. Knapp, (505) 844-2305

With new generations of electronic devices reaching ever smaller dimensions, substantially decreased contamination levels are required in both materials and processes. Reliably quantifying the required cleanliness is straining the capabilities of available diagnostics. Heavy Ion Backscattering Spectrometry (HIBS), invented and patented at Sandia, is an analysis tool for measuring surface contamination which has already demonstrated sensitivity better than Total-reflection X-ray Fluorescence (TXRF) for most elements. Furthermore, HIBS is standardless and has no matrix effects, measuring all elements above Ar with sensitivity increasing with atomic number. HIBS uses relatively low-energy, heavy ions for backscattering analysis, taking advantage of the increased yield which can be obtained by using high Z ion beams at lower energy. Background due to increased yield from the substrate is eliminated by a thin carbon foil in front of the detector, with a thickness chosen to range out ions scattered from the substrate and allow only ions scattered from impurities heavier than the substrate to reach the detector. We have now developed a new time-of-flight detector for HIBS which gives more sensitivity and better mass resolution.

Keywords: Semiconductor, Silicon, Analysis, Ion Beam, Surface

Lawrence Livermore National Laboratory

Materials Preparation, Synthesis, Deposition, Growth or Forming

517. Inorganic Aerogels — FY 1993 $100,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
LLNL Contact: L. W. Hrubesh, (510) 423-1691

The objective of this project is to develop the chemistry and procedures for processing monolithic metal oxide aerogel materials.

The approach is to perform a controlled hydrolysis of metal alkoxides such that the partially hydrolyzed chemical can be limited from further condensing reactions by using an appropriate solvent diluent. Subsequently, this pre-hydrolyzed compound can either be further diluted to make very low density sol-gels, or gelled directly for higher densities. Aerogels are obtained by super-critical solvent extraction of the wet gels.

Aerogels have unusual optical, thermal, and acoustic properties due to the ultrafine porous microstructure. Applications for these materials include target material for direct drive laser fusion experiments, thermally insulated windows and skylights, and as collector material for hyper-velocity microparticle capture.

We have synthesized new pure zirconia and tantala aerogels at densities lower than previously achieved for these mid-Z metals. We have achieved monolithic zirconia aerogels at densities as low as 38 kg/m^3, although they are extremely weak. Tantala aerogels have been made to densities as low as 60 kg/m^3, which is within a factor of four of the theoretical limit. We have also synthesized new rare earth metal oxide aerogels of erbia, and neodymia, and praseodymia, both pure and mixed with silica. These are used as a starting material to make very pure full density glasses at temperatures well below the melting temperature of the glass.

In addition to our synthesis efforts, we have completed the characterization of the rare earth metal oxide aerogels, and published the results.

We also have completed studies to determine the microstructures which control the thermal and acoustic transport in aerogels. We have developed a model, applicable to all varieties of aerogels, which accurately predicts the optimum density for minimizing the thermal conductivity. Measurements of the thermal conductivity of ultralow-density (i.e., <50 kg/m^3) silica aerogels have been completed and the data were successfully compared with the model. We have also completed an analysis of the frequency dependence of sound attenuation by aerogels and we have completed sound absorption measurements at ultrasonic frequencies.

Keywords: Inorganic Aerogels, Sol Gel Chemistry, Laser Fusion Targets

518. Organic Aerogels

FY 1993
$325,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
LLNL Contact: R. W. Pekala, (510) 422-0152

The aqueous polycondensation of (1) resorcinol with formaldehyde or (2) melamine with formaldehyde are two proven synthetic routes for the formation of organic aerogels. The former materials can also be pyrolyzed in an inert atmosphere to give vitreous carbon aerogels. The structure and properties of organic aerogels are analogous to their inorganic (e.g., silica) counterparts. In general, these materials have continuous porosity, an ultrafine cell/pore size (<50 nm), high surface area (400-100m^2/g), and a solid matrix composed of interconnected colloidal-like particles or fibrous chains with characteristic diameters of 10 nm.

A major advantage of organic aerogels is their low Z (atomic number) composition. Recently, we showed that resorcinol-formaldehyde aerogels are even better insulators than silica aerogels when measured under ambient conditions. A record low thermal conductivity of 0.012 W/m-K was obtained at a density of 0.16 g/cc.

Carbon aerogels are of particular importance because they are the first electrically conductive aerogels to be synthesized. The low resistivity of the aerogel network and the large surface areas per unit volume are being exploited in supercapacitors that have both high power (7.5 kW/kg) and energy densities (4-20 Whr/kg). Carbon aerogels are also being investigated as candidates for the storage of hydrogen and methane.

Keywords: Organic Aerogels, Sol-Gel, Supercapacitors, Thermal Insulation

519. Engineered Nanostructure Laminates

FY 1993
$330,000

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 500μm 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: ultra-high strength materials; high performance tribological coatings; coatings for aircraft gas turbine engines; high performance capacitors for energy storage; capacitor structures for industrial applications; integrated circuit interconnects; magnetic transducers/GMR; and EUV, soft X-ray and X-ray optics spectroscopy and imaging.

Keywords: Thin Films, Multilayer Technology

520. Sol Gel Coatings

FY 1993
$325,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
LLNL Contacts: I. M. Thomas, (510) 423-4430 and J. Britten, (510) 423-7653

We continue to investigate the preparation of multilayer sol-gel 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

521. KDP Growth Development FY 1993
$600,000

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 (1-2 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.

In FY93 we 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 15cm on a side and have shown that crystals grown by this method are of exceptionally high quality. We are currently constructing a station for the growth of $50x50x50cm^3$ crystals in FY94. We will continue to grow crystals at the 10-15cm scale in order to determine optimum hydrodynamic and regeneration conditions.

Keywords: KDP, Nonlinear Crystals, Crystallization

522. Advanced Finishing Development FY 1993
$850,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
LLNL Contact: J. S. Taylor, (510) 423-8227

Advanced optical fabrication methods will almost certainly be utilized to finish optical surfaces in advanced ICF laser architectures. We are working to understand the effect of finishing parameters on optical surface characteristics, including subsurface damage and resulting damage threshold. We are also developing rapid grinding and polishing methods which will simultaneously reduce the cost of fabricating optical surfaces while maintaining the high quality necessary for high power laser applications.

In FY93 we began experiments on a newly installed double-sided grinder/polisher. Large versions of this machine can potentially reduce costs for the initial grinding and polishing of flat ICF components. We hope to complete and experimentally verify a model of the fundamental sources of flatness errors for this machine tool. Our model will provide performance predictions of machines that are not commercially available, thus enabling us to evaluate vendor proposals for machine development.

Keywords: Optical Finishing, Laser Glass, Cost Reduction, Manufacturing, ICF

523. Synthesis and Scale-up

FY 1993
$250,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
LLNL Contact: C. Coon, (510) 422-6311

We have synthesized several interesting energetic materials in FY93 which derived from two areas of research; neo-inositol and pryidazine-1-oxide derivatives.

1,4-Dideoxy-1,4-dinitro-neo-inositol (NNI) is readily formed by the condensation of nitroform and glyoxal. NNI is a useful intermediate for a wide range of energetic materials including high energy oxidizers and energetic binders. The 2,5-dinitrate derivative (LLM-101) is especially interesting because it approaches HMX in energy content and may act as an energetic binder ingredient through its two reactive hydroxyl groups.

3-Hydroxy-4,6-dinitropyridazine-1-oxide and 3-amino-4,6-dinitropyridazine-1-oxide were synthesized from a common precursor, 3-ethoxypyridazine-1-oxide. These materials are interesting because of their energy content and possible shock insensitivity.

Pyridazine-N-oxides were initially investigated as anti-cancer agents in the 1960s. An interesting pyridazine-1-oxide intermediate, which may have some clinical applications, is 3-ethoxy-4-nitro-6-(5 amino-3-nitro-1,2,4-triazoyl) pyridazine-1-oxide. This compound has the same molecular structure as a nucleoside.

Keywords: Energetic Materials, Pyridazine

524. Doped Polymers for ICF

FY 1993
$200,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
LLNL Contacts: R. Cook, (510) 422-3117 and G. E. Overturf III, (510) 422-7280

This program is developing covalently doped polystyrene derivatives for use as spectroscopic tracers in direct drive laser fusion experiments. The doped polymers are formed into small spherical shells that serve as the mandrel around which the ICF capsule is constructed. The dopant atoms should be atomically dispersed and thus must be covalently incorporated into the structure of the polymer. We have succeeded in producing soluble polystyrene derivatives doped with Cl, Br, I, Fe, and Cr at levels up to 3 atom percent. Current work focuses on a Ti-doped polymer.

Keywords: Polymers, Dopants, Laser Fusion Targets

525. Plasma Polymer Coating Development FY 1993
$900,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
LLNL Contacts: S. Letts, (510), 422-4373, R. Brusasco, (510) 422-3111 and R. Cook, (510) 422-3117

This program is developing the capability to produce ultra-smooth plasma polymer coatings on plastic microshells for use as targets in ICF experiments. These coatings are formed by reacting trans-2-butene monomer and hydrogen gas in an RF plasma created by a helical resonator reactor operating at 40 MHz. This coating technology has demonstrated the ability to prepare coatings with surface roughness of the order of 5 nm RMS. Our goal is to make coatings of this quality a routine procedure by determining the fundamental mechanisms of surface roughening. Recent efforts on process characterization have addressed the effects of the helical resonator and process variables on the quality of the polymer coating. An impedance model for the helical resonator was developed that allowed us to determine the distribution of magnetic field strength. A series of experiments investigated the effect of gas flow rates, substrate temperature, and total coating thickness on coating roughness. From these experiments the scaling behavior of coating roughness was determined. We found that coating roughness is controlled by surface relaxation processes such as surface diffusion. This has provided a better understanding of the coating process and has given us the ability to calculate surface roughness based on deposition conditions and coating thickness.

Keywords: Plasma Polymer, Laser Fusion Targets, Surfaces, Coatings

526. Polymer Films by RF Sputtering FY 1993
$125,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
LLNL Contact: E. Hsieh, (510) 422-0753

After experimenting with the RF sputtering technique to deposit various polymer films, including Acrylic, Polypropylene, Polystyrene, Parylene-N and PTFE (Teflon), we have concentrated our efforts on two types of polymers, the TPX and PTFE, which are of interest to the Laser Fusion community. The sputtering rates have been improved to more than 1 μ/hour. Both the density and composition of the sputtered films have been determined. Various metal dopants have been tried in a co-deposition configuration and we are proceeding to accurately determine the doping levels. The solution to the adhesion problem encountered when metal films are deposited onto the polymer films is close on hand. Both sputtered polymer films have been used in the Laser Fusion Targets at our NOVA Laser Facility.

Keywords: RF Sputtering, Polymer Films, Laser Fusion Targets

527. Excimer Laser Micromachining — FY 1993 $468,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
LLNL Contact: R. Wallace, (510) 423-7864

This program is developing methods of using pulsed UV excimer laser photoablation techniques to micromachine plasma polymer coatings. Surface perturbations on microshells result in growth of Rayleigh-Taylor (RT) instabilities during the acceleration phases of an ICF implosion. To test current theories of RT growth and its effects on target performance, we are investigating methods of applying known perturbations, depth and mode distribution, to smooth capsules. Due to very high RT growth rates, excimer laser ablation etch rates in the range of a few hundred Ås are required. Micromachining at this level pushes the limits of excimer laser ablation due to low absorbtivity and incubation processes in polymer coatings.

Keywords: Excimer Laser Ablation, Plasma Polymer, Laser Fusion Targets

Materials Properties, Behavior, Characterization or Testing

528. Advanced Synchrotron Radiation Study of Materials — FY 1993 $365,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
LLNL Contacts: Joe Wong, (510) 423-6385

The objective of this materials science program is to advance and develop state-of-the-art synchrotron radiation (SR) methods to investigate and elucidate the role of atomic and electronic structures in determining the physico-chemical properties of materials and their processing. The activities defined in this program take advantage of the various unique characteristics of synchrotron radiation such as high intensity, high collimation, high polarization and broadband tunability from VUV to soft and hard X-ray to probe the structure of matter on an element-selective basis in real-time down to the second and sub-second time scale as well as in real space. The research areas consist of both an expansion of our existing SR capabilities in materials characterization using these powerful photon sources and development of new capabilities (a) to investigate the phase transformation *in situ* in fusion welds; (b) to develop and implement a novel quick-scanning EXAFS capability on our PRT X-ray beamline at SSRL to study time-dependent phenomena, and (c) to develop new soft X-ray capabilities to study low-Z materials containing Si, Al and Mg that are of technological importance.

Keywords: Synchrotron, TR-XRD, Fusion Welds, Phase Transformation, QEXAFS, YB_{66} Soft X-ray Monochromator

529. <u>Structural Transformations and Precursor Phenomena</u> <u>FY 1993</u> $200,000

DOE Contact: C. B. Hillard, (301) 353-3687
LLNL Contact: P. E. A. Turchi, (510) 422-9925

A new class of alloys for which local order *alone* indicates a near-degeneracy between phase decomposition and order was identified. Our first-principles study showed that, for such alloys prepared in the high temperature disordered state and subsequently quenched inside the miscibility gap, an ordered phase spontaneously forms before evolving, as time progresses, toward phase separation. The microstructural evolution has been fully analyzed. Codes based on modern alloy theory have been developed to study the doping effect on the formation of complex phases. Application to Fe-Ti-V has shown the important role played by atomic orbital directionality in the stability of complex phases.

A time-resolved Auger electron spectroscopy study of statics and kinetics of surface segregation on a (111) FeCr single crystal, with and without C-doping, was performed. From the X-ray grazing incidence diffraction experiments done on FeCr single crystals at the NSLS, a strongly first order transition bcc to σ was observed below the σ-transition temperature although no clear indications for a diffuse intensity build up above this temperature could be detected. Our work provided information on the influence of surface contaminants, like C, on the possible surface-induced formation of the σ phase in FeCr.

Keywords: Electronic Structure, Phase Stability, Short Range Order, Complex Alloys, Surface Properties

530. <u>PALX Low Vulnerability High Explosives for 155mm Artillery Shells</u> <u>FY 1993</u> $200,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
LLNL Contact: D. M. Hoffman, (510) 422-7759

A series of low-vulnerability, low-cost explosive formulations were developed for evaluation as replacements for TNT in 155 mm artillery shells. These formulations were based on available, inexpensive solids (RDX, aluminum and sodium nitrate); non migrating, energetic liquids (TMETN and TEGDN); and a low modulus, compatible polyurethane binder based on Desmondur N100 polyisocyanate and a blend of Tone polycaprolactone polyols. Extended potlife is achieved through the use of a latent mercaptotin catalyst that can be masterbatched with the polyols and energetic plasticizers to form a stable premix. PALX-35-CE survived the 1:1 sympathetic detonation test in 155 mm hardware with separation between rounds comparable to that found in the actual 155 mm pallets. PALX formulations have survived slow cookoff tests and a variety of other vulnerability tests described in a preliminary report.* This research has been completed and will be implemented as current needs within the DOD and the U.S. Army dictate.

Keywords: High Explosives

531. Very High Energy Density Materials — FY 1993 $1,350,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
LLNL Contacts: R. L. Simpson, (510) 423-0379 and M. Hoffman, (510) 422-7559

B-Program/Surety Program ($650K): We have investigated the synthesis of Transferable Insensitive Explosives (TIE) based on mixtures of 1,3,5-Triamino-2,4,6-trinitrobenzene (TATB) and bis (2-fluoro-2,2-dinitroethyl) formal (FEFO). These mixtures are high viscosity liquids which were formulated as both curable and non-curable systems and have a variety of applications.

Office of Munitions ($700K): We are preparing a variety of explosive formulations to serve in hard structure munitions which are principally comprised of an explosive, oxidizer, aluminum and an energetic binder. They are being evaluated with respect to their performance, safety characteristics, and vulnerability.

Keywords: Transferable Insensitive Explosives (TIE), Hard Structure Munitions

532. Interfaces, Adhesion, and Bonding — FY 1993 $300,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
LLNL Contact: Wayne E. King, (510) 423-6547

We have developed a unique capability for calculation of the electronic structure at interfaces, where symmetry is reduced compared with the bulk. Specifically, the method, called the real-space multiple-scattering theory (RSMST), can treat interfaces and include the effect of atomic relaxation at the interface. We have coupled this method with the semi-empirical embedded atom method (EAM), which uses modified two-body potentials with molecular dynamics, molecular statics, or Monte Carlo techniques to determine atomic rearrangements.

*UCRL-UR-110363 Internal Report (June 1, 1992).

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

533. Laser Damage: Modeling and Characterization — FY 1993 $400,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
LLNL Contact: M. R. Kozlowski, (510) 294-5637

We have been working to understand the damage mechanism in thin film coatings used on Nova for a number of years, with the ultimate goal of improving the damage threshold in coatings for future laser systems. In recent years, we have utilized atomic force microscopy (AFM) to characterize laser damage as well as the laser conditioning process which allows coatings to sustain higher laser fluences. We have shown that damage threshold correlates with the density of pre-existing defects, and that nodular defects often damage but that the craters (produced by nodules "popping" out prior to laser irradiation) do not damage.

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. Previously, it was thought that defects had to be absorbing (either carbonaceous or non-stoichiometric material) to produce the large field enhancements which produce damage. We will use these results to help modify the coating process to avoid the formation or incorporation of these defects into the coating, thereby improving the damage threshold.

Keywords: Coatings, Atomic Force Microscopy, Laser Damage

534. KDP Characterization FY 1993
$300,000

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. The level of internal strain is the single most important factor 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 in KDP and DKDP, understand how these defects are generated and how to avoid them during the growth process.

Using optical, X-ray topographic and crystal growth methods, we have shown that the primary sources of strain are dislocations formed during seed regeneration or following solvent inclusion. Using atomic force microscopy (AFM) we have been able to correlate macroscopic defects associated with regions of strain to the size of the Burgers vectors of dislocation bunches. We are now using AFM to determine how the strength of the dislocation sources depend on the regeneration regime.

Keywords: KDP, Strain, Crystal

535. Damage Testing FY 1993
$730,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
LLNL Contact: F. Rainer, (510) 422-4376

We maintain four facilities to measure laser damage thresholds and characterize damage morphologies of optical materials at pulse durations of 3 and 10 ns. We can conduct measurements at the first four fundamental wavelengths of Nd:YAG (1064, 532, 355 and 266 nm). We are developing automated techniques to (1) detect laser damage, (2) condition optics to higher thresholds with gradual increases in laser fluence, and (3) monitor laser parameters. These techniques can be applied to small witness samples as well as full-sized optics up to 1 m in size. We test and document several hundred samples per year, including coatings, crystals, glasses, and the effect of finishing processes on surfaces. This information is in turn utilized to help make important decisions in the development of these materials for ICF laser systems. The ICF Program maintains one of the world's largest databases of damage results for optical materials.

Keywords: Laser Damage, ICF

536. Energy Transfer Dynamics in Energetic Materials

FY 1993
$308,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
LLNL Contact: A. Ruggiero, (510) 423-1020

When an energetic material is shocked, optical phonon energy is up-converted to intramolecular vibron modes which ultimately leads to molecular dissociation. The anharmonic potential and energy transfer rate determines, in part, a materials sensitivity. These dynamics are being probed using LLNL's unique femtosecond laser capability and are being modeled using a molecular dynamics approach.

Keywords: Explosive, Laser, Dynamics

537. Processing-Structure-Property Correlation in Laminated Metal Composites

FY 1993
$160,000

DOE Contact: C. B. Hilland, (301) 353-3687
LLNL Contact: Chol K. Syn, (510) 534-8226

Alternating layers of metals (e.g., Al 5182) and metal matrix composites (e.g., Al 6061-25 vol.% SiC) are to be press-bonded with heavy deformation to form laminated metal composites with strength, toughness, and other properties far superior to those of the constituent materials. Interfacial bonding strength and microstructure will be correlated with the processing parameters and mechanical properties and the mechanical properties will be modelled using the Laboratory's finite element codes.

Keywords: Laminated Metal Composites, Deformation Bonding

Instrumentation and Facilities

538. Scanning Tunneling Microscopy (STM) and Atomic Force Microscopy (AFM)

FY 1993
$546,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
LLNL Contact: W. Siekhaus, (510) 422-6884

A large stage scanning probe microscope that can perform scanning tunneling as well as contact and non-contact atomic force microscopy on the surface of objects as large as 6" in diameter has been acquired and used to study (a) the relationship between surface morphology and laser damage threshold of antireflection and high-reflection optical coatings, and (b) the quality and degradation of large gratings used in the optical and X-ray experiments. Scanning probe technology has been developed to measure the roundness of laser fusion targets. A small-stage non-contact AFM has been acquired and used to study (a) thermally induced degradation (void formation) in TATB (explosive) and (b) surface damage caused by impact of multiply charged (e.g., U^{70+}) EBIT ions. UHV STM has been used to determine the XeF_2-Si etching mechanism and rate at room temperature. A new technique, nanostethoscopy, has been developed to locate and to monitor nm-scale emitters of acoustic energy in materials and biological sciences.

Keywords: NDE, Laser Damage, Optical Coatings, Ion Surface Damage, High Explosive Degradation, Nano-Lithography, Chemical Reaction, XeF_2, Etching, Roundness, Nano-Stethoscope

539. Pyrochemical Technology Development | FY 1993 | $5,000,000

DOE Contact: Lori Myers, (510) 422-3483
LLNL Contact: Mark C. Bronson, (510) 422-3061

The scope of this activity is the development and demonstration of pyrochemical processes for the recovery, purification, and conversion to metal of actinides (plutonium, americium, and uranium). This is being carried out in support of the Reconfiguration Program and the Environmental Restoration/Waste Minimization Program. The Reconfiguration Program entails the design of the next generation plutonium storage, processing, and fabrication facility in the reconfigured nuclear weapons complex. Development emphasis is on waste minimization, worker dose reduction, and construction costs.

During FY93, development efforts were carried out in plutonium component disassembly, Pu recovery by hydride/dehydride, separation of Am from Pu, electrorefining, pyrochemical salt scrub, Pu purification by chloride volatility, materials to contain liquid actinides, and treatment of Idaho National Engineering Laboratory (INEL) calcine waste.

Keywords: Pyrochemical, Plutonium Processing, Plutonium Recovery, Waste Treatment

540. Thermoelectric Materials with Exceptional Figures of Merit | FY 1993 | $325,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
LLNL Contact: J. C. Farmer, (510) 423-6574

The relative efficiency of a thermoelectric material is measured in terms of the dimensionless figure of merit, ZT. The best known thermoelectric materials are heavily doped, mildly degenerate semiconductors and have $ZT \leq 1$. If materials with $ZT \geq 3$ could be found or developed, thermoelectric devices could be made that would have thermodynamic efficiencies close to that of an ideal Carnot engine.

Keywords: Thermoelectric Materials

541. Capacitive Deionization as an Alternative to Ion Exchange

FY 1993
$795,000

DOE Contact: Douglas Gish, DP 42, (202) 586-1741
LLNL Contact: J. C. Farmer, (510) 423-6574

A *capacitive deionization* process is being developed for the efficient removal of ionic contaminants from aqueous streams. Ions will be held in electric double layers formed at the surfaces of porous electrodes. This new process could replace ion exchange systems and associated secondary waste. Given the high cost of disposal in mined geological repositories, there is tremendous incentive for reducing the volume of waste that must be dealt with. The *mode of operation* and the *electrode material* used in the LLNL capacitive deionizer are entirely new. Ultimately, the system will consist of two multistage capacitors in parallel. One capacitor will be regenerated (discharged) while the other purifies (charges). Since current produced during regeneration will be used for purification, the system will be energy efficient. This mode of operation, *potential-swing ion adsorption*, is analogous to *pressure-swing gas absorption*. In addition to conventional porous carbon electrodes (250 m^2/gm), carbon aerogel electrodes have been developed and are being used (800 m^2/gm). This work is being funded by DOD SERDP (Strategic Environmental Research and Development Program).

Keywords: Capacitive Deionization

542. Trilayer Josephson Junctions (Technology Transfer Initiative)

FY 1993
$250,000

DOE Contact: W. T. Chernock, (301) 586-7590
LLNL Contact: M. J. Fluss, (510) 423-6665

This TTI activity is focused on the development of the knowledge base to mature the technology of heteroepitaxial growth of planar tri-layer high-temperature superconducting Josephson junctions. The JWS calls out milestones at 6-month intervals. Milestones to be accomplished by the end of the first half year for this project are to manufacture trilayers (Varian) and pattern devices (Varian) with candidate materials, to characterize device quality by basic transport measurements (Varian/LLNL), to begin microscopic investigations of interface quality and layer characteristics (LLNL), to identify techniques and begin testing chemical homogeneity and surface regularity (LLNL) and to begin developing a processing database with LLNL quality assured substrates. LLNL is making good progress towards accomplishing all of the specified first 6-month period milestones.

Varian Associates has delivered to LLNL researchers 11 trilayer wafers for evaluation, two of which were specially prepared for this TTI project. LLNL staff have completed preliminary Auger electron spectroscopy, X-ray fluorescence spectroscopy, transmission electron microscopy, atomic force microscopy and Rutherford backscattering spectroscopy measurements on these samples. In addition, LLNL has performed optical interferometry measurements and atomic force microscopy measurements on strontium titanate substrate materials from competing vendors. Results have been transmitted on a weekly basis to Varian participants through technical meetings.

Keywords: Superconductors, High Transition Temperature, Josephson Junction, Tri-Layers, Heteroepitaxy

543. Critical Parameters of Superconducting Materials LDRD (Departmental)

FY 1993
$427,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
LLNL Contact: M. J. Fluss, (510) 423-6665

As practical applications of high temperature superconducting (HiT_c) materials near, there remain significant gaps in our understanding of the superconducting phenomenon. We have been investigating basic physical phenomena such as electron structure, the role of atomic defects, and synthesis methods in HiT_c materials. Previously, we have performed experiments to determine the Fermi surface of $YBa_2Cu_3O_{7-x}$ using angular correlation of the annihilation radiation of electron-positron pairs (ACAR). Now we have used ACAR to deduce the electronic structure of $La_{2-x}Sr_xCuO_4$ over a range of Sr (carrier) concentration. Comparison with theory shows critical features of the Fermi surface along with a "smearing" resulting from electron correlations.

We have measured and calculated the structure/property effects of cation defects and oxygen stoichiometry on the magnetic and transport properties of high-quality electrodeposited crystals of $Ba_{1-x}K_xBiO_3$, a copper-free superconducting oxide with a transition temperature above 31 K. Due to the lack of magnetic ions in the structure and its high onset temperature, it is believed to hold much promise in technological applications.

The solid state of C_{60} (Fullerene), a molecule composed of 60 carbon atoms arranged in a "geodesic" structure, forms an insulator with a wide band gap. This material can be doped with alkali atoms to become metallic and a superconductor with a transition temperature as high as 33 K. We have synthesized large grains (2mm) by developing a novel, open-tube growth technique. Magnetic, transport and pressure studies have all been initiated to further determine the superconducting properties. Also, tunneling investigations are being initiated at LLNL to determine values of the superconducting gap of these novel materials for possible device applications.

Keywords: Superconductors, Electronic Structure, Defects, Fullerenes, Positron Annihilation

544. Lithium Cell Development

FY 1993
$500,000

DOE Contact: Andre Cygleman, (202) 586-8814
LLNL Contact: John R. Kolb, (510) 422-6424

We are working 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 being 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 and eliminates hazards associated with chlorine evolution and lithium withdrawal. ES&H analyses indicate a much-improved process from the standpoint of worker safety.

Keywords: Lithium, Bipolar, Electrolytic Cell Development

545. High Explosives Lead Laboratory Program

FY 1993
$1,000,000

DOE Contact: Andre Cygleman, (202) 586-8814
LLNL Contact: John R. Kolb, (510) 422-6424

We are working vigorously to support the Department of Energy in its design of an ideal high explosives operation of the future. Joint and close cooperation with our colleagues at Los Alamos and the Mason and Hanger Pantex Production Plant have yielded technologies and processes compatible with the construction of an efficient, environmentally sound manufacturing facility for conventional and insensitive high explosives for the future. Integration of the Lead Laboratory design for an ideal High Explosives Operation of the future—from basic research and development through production and surveillance of HE components—with the Fluor Daniel effort on conceptual designs for a "Greenfield" approach to a new manufacturing facility are in process. We in HE at LLNL design in environmentally conscious technologies wherever possible. Currently, we are overseeing the investigation—complex-wide—of upgrading existing capabilities at Livermore, Los Alamos and Pantex in lieu of constructing a new facility.

Keywords: High Explosive, Manufacturing, Upgrade-in-Place

546. <u>Environmentally Safe Disposal of Explosive Wastes: SERDP Project</u> FY 1993 $1,800,000

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. 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, supercritical water oxidation, base hydrolysis and bioremediation as the 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. We will downselect to a single technique or a suite of techniques in early calendar 1994. We will then be in position to design a pilot-scale plant to accommodate environmentally benign treatment of energetic wastes.

Keywords: SERDP, Environmentally Benign High Explosive Waste Destruction

547. <u>Laminated Metal Composites for Aerospace Applications</u> FY 1993 $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

548. Fatigue of Metal Matrix Composites FY 1993
$300,000

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

549. Molecular Dynamics Simulation Studies of Radiation Effects in Solids FY 1993
$60,000

DOE Contact: F. W. Wiffen, (301) 903-4963
LLNL Contacts: T. Diaz de la Rubia, (510) 422-6714 and M. W. Guinan, (510) 422-5776

The objective of this program is to develop and apply advanced computational tools to the study of radiation effects in solids. The aim of the program is to understand, at the atomistic level, the manner in which a material responds in a high radiation environment, such as that present at the first wall of a fusion reactor. We apply molecular dynamics computer simulation methods and this allows us to understand the mechanisms of formation of the primary state of damage in a material. From our simulations, we derive a fundamental understanding of the dynamics of the displacement cascade generated by primary recoils along the path of an irradiating beam of energetic particles, such as neutrons. Our results provide information on the number and geometry of the defects induced in the material by the irradiation as well as on the amount of atomic relocation. This atomistic approach represents a fundamental step critical to the development of a complete picture of the microstructural evaluation of a material under irradiation. Ultimately, the insight gained by these studies will lead to understanding and predicting the macroscopic response and changes in the mechanical properties of irradiated materials.

Keywords: Radiation Damage, Magnetic Fusion, Computer Simulation

550. Fundamental Studies of Particle-Solid Interactions FY 1993
$180,000

DOE Contact: Maury Katz, (202) 586-5799
LLNL Contact: T. Diaz de la Rubia, (510) 422-6714

The objective of this program is to develop and apply computational tools to the study of ion implantation and ion beam modification of semiconductor materials. Despite over

20 years of active research devoted to understanding radiation effects and defect properties in silicon, many questions remain as to the manner in which damage is created and accumulates in this material during irradiation. It is the aim of this program to provide atomistic insight into these phenomena. Our molecular dynamics computer simulation methods provide a unique picture and understanding of the response of silicon to energetic ion beams. From our results we are able to understand the mechanisms of amorphization of the silicon lattice during irradiation as well as the form in which Frenkel pairs are produced. The detailed dynamics of the damage process are explored and this provides insight into the evaluation of the stress state of the crystal and the amount of atomic relocation that occur during irradiation. Ultimately, the knowledge gained by these studies will allow us to make predictions that will enable true physical process modeling of semiconductor manufacturing, a critical issue in the development of 0.1 μm technology.

Keywords: Ion Implantation, Semiconductor Processing, Dopant Diffusion, Computer Simulation

551. <u>Radiation Effects in Materials for Inertial Confinement Fusion</u> <u>FY 1993</u>
$50,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
LLNL Contacts: T. Diaz de la Rubia, (510) 422-6714 and M. Tobin, (510) 423-1168

The objective of this program is to apply advanced computational tools to analyze the feasibility of using certain low activation hazard materials, such as ceramics, in the first wall of inertial fusion energy power plants. We apply molecular dynamics computer simulation methods and this allows us to understand the mechanisms of formation of the primary state of damage created in the high radiation environment present in an IFE plant. From our simulations, we derive a fundamental understanding of the dynamics of the displacement cascade generated by primary recoils along the path of a slowing down neutron in the first wall. Our results provide information on the number and geometry of the defects induced in the material by the irradiation as well as on the amount of atomic relocation. This atomistic approach represents a fundamental step critical to the development of a complete picture of the microstructural evolution of a material under irradiation. Ultimately, the insight gained by these studies will lead to understanding and predicting the macroscopic response and changes in the mechanical properties of irradiated ceramics and oxides. This knowledge will allow a physics-based selection of materials for use as structural components in IFE reactors.

Keywords: Radiation Damage, Inertial Fusion Energy, Low Activation Materials, Computer Simulation

552. Novel Materials for Optoelectronics and Photonics FY 1993
$500,000

DOE Contact: G. J. D'Alessio, (301) 903-6688
LLNL Contact: Howard W. H. Lee, (510) 423-5877

The objective of this program is 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, fullerenes, and aerogels. We have developed a type of nanocrystalline silicon (fabricated from porous silicon) that photoluminesces in the red, green, and blue regions of the visible spectrum (RGB). This nanocrystalline silicon is particularly easy to fabricate and can potentially serve as an efficient and inexpensive phosphor for flat panel displays. Nanocrystals of other materials are also being studied. We have also succeeded in fabricating arrays of miniature junction diodes from porous silicon that emit in the visible and near infrared. Silicon-based emitters are desirable because they integrate well with standard silicon-based microelectronic devices. Furthermore, we found the figures of merit of thin film fullerenes to be very competitive with optical fibers for all-optical switching and have demonstrated a fullerene-based all optical switch. Thin films of materials such as fullerenes allow for an integrated optics approach which greatly minimizes the latency problem inherent with fiber optics. Other thin film materials are also being pursued for these applications. Finally, we are studying doped aerogels for flat panel and three-dimensional displays.

Keywords: Optoelectronics, Photonics, Nanocrystals, Porous Silicon, Fullerenes, Aerogels

553. Uranium Manufacturing Lead Lab Program FY 1993
$3,900,000

DOE Contact: Andre Cygleman, (202) 586-8814
LLNL Contact: Jeff N. Kass, (510) 422-4831

We are working with the DOE, Los Alamos National Laboratory, Sandia National Laboratories and Y-12 Plant to improve the processing technology for depleted alloy and enriched uranium. The new technology is aimed at reducing waste generated in manufacturing weapons components. Improved melting methods, near net shape forming and machining, and inspection of near net shape parts are the areas of primary interest. Funding for this effort is coming from SERDP, WRD&T and process development resources.

Keywords: Manufacturing, Depleted Uranium, Uranium Alloy, Enriched Uranium, Waste Minimization

554. Plutonium Manufacturing Lead Lab Program FY 1993 $5,000,000

DOE Contact: Andre Cygleman, (202) 586-8814
LLNL Contact: J. L. Robbins, (510) 422-7060

We are working with DOE, Los Alamos National Laboratory, Savannah River Plant and Rocky Flats Plant to develop improved manufacturing methods for producing plutonium weapons components. The new technology is aimed at reducing and eliminating waste generated in the manufacturing operations. The LLNL program includes efforts in net shape casting, laser welding, and alternate assembly methods. Funding for this effort is coming from SERDP, WRD&T and process development resources.

Keywords: Plutonium, Manufacturing, Casting, Machining, Waste Minimization

Los Alamos National Laboratory

Materials Preparation, Synthesis, Deposition, Growth or Forming

555. Actinide Processing Development FY 1993 $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

556. Plutonium Oxide Reduction FY 1993 $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

557. Low Density Microcellular Plastic Foams

FY 1993
$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

558. Physical Vapor Deposition and Surface Analysis

FY 1993
$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

559. Chemical Vapor Deposition (CVD) Coatings

FY 1993
$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)

560. Polymers and Adhesives — FY 1993 $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

561. Tritiated Materials — FY 1993 $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

562. Salt Fabrication FY 1993 $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

563. Slip Casting of Ceramics FY 1993 $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

564. Plasma-Flame Spraying Technology FY 1993 $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

565. Rapid Solidification Technology FY 1993
$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

566. Bulk Ceramic Processing FY 1993
$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

567. Synthesis of Ceramic Coatings FY 1993
$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

568. Actinide Surface Properties FY 1993
$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

569. Neutron Diffraction of Pu and Pu Alloys and Other Actinides FY 1993
$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

570. Surface, Material and Analytical Studies FY 1993
$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

571. Mechanical Properties of Plutonium and Its Alloys FY 1993
$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

572. Phase Transformations in Pu and Pu Alloys FY 1993
$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

573. Plutonium Shock Deformation FY 1993
$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

574. Non-Destructive Evaluation FY 1993
$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

575. Powder Characterization FY 1993
$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

576. Shock Deformation in Actinide Materials FY 1993
$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

577. Dynamic Mechanical Properties of Weapons Materials FY 1993
$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

578. Target Fabrication FY 1993
$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

579. Filament Winder FY 1993 $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

580. High Energy Density Welding in Hazardous Environments FY 1993 $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

581. Uranium Scrap Conversion and Recovery FY 1993 $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

582. Electronically Correlated Materials at Ambient and Extreme Conditions

FY 1993
$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

583. Organometallic Chemical Vapor Deposition

FY 1993
$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

584. Polymer Sorbents for Hazardous Metal Uptake

FY 1993
$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

585. Microscopic Materials Modeling: Textures and Dynamics — FY 1993 $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

586. Surface Modification of Materials — FY 1993 $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

587. Integration of Fundamental Knowledge in Plasticity and Textures to Provide Technical Tools for Microscopic Applications

FY 1993
$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

588. High Resolution Electron Microscopy of Materials

FY 1993
$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

589. Nano-Fabrication — FY 1993 $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

590. Thin Film Micro-Electrochemical Sensor Development — FY 1993 $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

591. Liquid Crystal Thermosets — FY 1993 $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

592. Neutron and Resonant X-ray Scattering by Materials FY 1993 $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

593. Structural and Electronic Competitions in Low-Dimensional Materials FY 1993 $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

594. Fundamental Aspects of Photoelectron Spectroscopy in Highly Correlated Electronic Systems

FY 1993
$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

595. Development of High Strength High Conductivity Materials for High Magnetic Field Devices

FY 1993
$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

596. Low Temperature STM for Structural and Spectroscopic Studies of High Temperature Superconductors and Other Electronic Materials

FY 1993
$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

597. Materials with Fine Microstructures

FY 1993
$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

598. Ion Beam Materials Research

FY 1993
$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

599. Texture Studies of Highly Deformed Composite Materials — FY 1993 $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

600. Pressure Dependency of the Structure of High Explosives: Nitromethane — FY 1993 $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

601. Neutron Reflection Studies of Thin Film and Multilayer Structures

FY 1993
$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

602. Neutron Reflectivity Studies of In Situ Corrosion of Metal Surfaces

FY 1993
$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

603. The Dynamics of Amorphous Materials

FY 1993
$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

604. Advanced Material Science Algorithms for Supercomputer Architectures

FY 1993
$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

605. Metal Vapor Synthesis in Organometallic Chemistry

FY 1993
$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

606. Separation Chemistry of Toxic Metals FY 1993
$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

607. Polymers for Integrated Optical Interconnects FY 1993
$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

608. High Temperature Materials Synthesis Without Heat: Oxide Layer Growth on Electronic Materials Using High Kinetic Energy Atomic Species FY 1993
$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

609. Dynamic Deformation of Advanced Materials FY 1993 $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

610. Strain Measurements in Individual Phases of Multi-Phase Materials FY 1993 $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

611. Artificially Structured Nonlinear Optic and Electro-Optic Materials

FY 1993
$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

612. Structural Phase Transitions in Non-Stoichiometric Oxides

FY 1993
$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

613. Strongly Correlated Electronic Materials — FY 1993 $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

614. Plasma Immersion Ion Implantation for Semiconductor Film Growth — FY 1993 $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

615. Analysis of Structure and Orientation of Adsorbed Polymer in Solution Subject to Dynamic Shear Stress

FY 1993
$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 power, 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

616. Development of Pair Distribution Function Analysis of Mesostructural Details in Single Crystal Perovskites and Nanocrystalline Materials

FY 1993
$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

617. Neutron Scattering as a Probe of the Structure of Liquid Crystal Polymer-Reinforced Composite Materials

FY 1993
$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

618. Strain Measurements in Individual Phases of Multi-Phased Materials During Thermomechanical Loading: LANSCE Neutron Scattering Experiment Support

FY 1993
$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

619. A New Approach to Texture Measurements: ODF Determination by Rietveld Refinement

FY 1993
$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

620. Applications of Fullerenes in Nuclear Technology

FY 1993
$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

621. Ceramic Oxide Foams for Separation

FY 1993
$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

622. Materials Modeling Project — FY 1993 — $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

623. Synthesis and Optical Characterization of Novel Fullerene-Based Composites — FY 1993 — $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

624. A Pilot Program: Chemical Vapor Deposition of Diamond in a Fluidized-Bed for Cutting Tool and Tribological Applications — FY 1993 $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

625. Advanced Beryllium Processing — FY 1993 $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

626. Automated Pulsed Laser Deposition System — FY 1993 $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

627. <u>Plasma Source Ion Implantation for the Automotive Industry</u>

FY 1993
$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

628. <u>Processing Modeling and Control for U.S. Steel Industry</u>

FY 1993
$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 1993
Office of Fossil Energy - Grand Total	$6,739,000
Office of Advanced Research	$6,739,000
Fossil Energy AR&TD Materials Program	$6,739,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$3,150,000
Coating Process Development for Cr-Nb Alloys	80,000
Procurement of Advanced Austenitic and Aluminide Alloys	30,000
Development of Iron Aluminides	400,000
Ultrahigh Temperature Intermetallic Alloys	377,000
Microalloyed Iron Aluminides	78,000
Low-Aluminum Content Iron-Aluminum Alloys	300,000
Technology Transfer - Iron Aluminides	60,000
Investigation of Austenitic Alloys for Advanced Heat Recovery and Hot-Gas Cleanup Systems	150,000
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	130,000
Engineering-Scale Development of the Vapor-Liquid-Solid (VLS) Process for the Production of Silicon Carbide Fibrils	160,000
Ceramic Composite Processing Equipment	20,000
Fabrication of Fiber-Reinforced Composites by Chemical Vapor Infiltration and Deposition (CVID)	200,000
Interfaces and Mechanical Properties of Continuous Fiber-Reinforced Ceramic Composites	150,000
Low-Temperature Fabrication of Transparent Silicon Nitride	180,000
Microwave-Assisted Chemical Vapor Infiltration	121,000
Technology Transfer - Microwave Processing	29,000
Carbon Fiber Composite Molecular Sieves	134,000
Activation of Carbon Fiber Composite Molecular Sieves	46,000

OFFICE OF FOSSIL ENERGY

	FY 1993
Office of Advanced Research (continued)	
Fossil Energy AR&TD Materials Program (continued)	
Materials Preparation, Synthesis, Deposition, Growth or Forming (continued)	
Ceramic Composite Molding Equipment	30,000
Ceramic Composite Adsorption Equipment	30,000
Development of Advanced Fiber Reinforced Ceramics	140,000
Modeling of Fibrous Preforms for CVD Infiltration	50,000
Materials Properties, Behavior, Characterization or Testing	$1,834,000
Investigation of the Weldability of Polycrystalline Iron Aluminides	75,000
Aqueous Corrosion of Iron Aluminides	44,000
Fireside Corrosion Tests of Candidate Advanced Austenitic Alloys, Coatings, and Claddings	157,000
Joining Techniques for Advanced Austenitic Alloys	0
Fatigue and Fracture Behavior of Cr-Nb Alloys	23,000
Corrosion and Mechanical Properties of Alloys in FBC and Mixed-Gas Environments	310,000
Environmental Effects on Iron Aluminides	225,000
Investigation of Moisture-Induced Embrittlement of Iron Aluminides	60,000
Determination of Physical Properties of Iron and Nickel Aluminides	10,000
Corrosion Protection of Ultrahigh Temperature Intermetallic Alloys	220,000
Development of Nondestructive Evaluation Methods and Effects of Flaws on the Fracture Behavior of Structural Ceramics	310,000
Joining of Fiber-Reinforced Silicon Carbide Composites	175,000
Ceramic Catalyst Materials: Hydrous Metal Oxide Ion Exchange Supports for Direct Coal Liquefaction	225,000

OFFICE OF FOSSIL ENERGY

	FY 1993
Office of Advanced Research (continued)	
Fossil Energy AR&TD Materials Program (continued)	
Device or Component Fabrication, Behavior or Testing	$1,320,000
Materials and Components in Fossil Energy Applications (Newsletter)	0
Fabrication of Full-Scale Fiber-Reinforced Hot-Gas Filters by Chemical Vapor Deposition	120,000
Development of Ceramic Membranes for Gas Separation	400,000
Investigation of the Mechanical Properties and Performance of Ceramic Composite Components	100,000
Advanced Materials and Electrochemical Processes in High-Temperature Solid Electrolytes	700,000
Instrumentation and Facilities	$ 435,000
Management of the Fossil Energy AR&TD Materials Program	400,000
General Technology Transfer Activities	35,000

OFFICE OF FOSSIL ENERGY

The Office of Fossil Energy responsibilities include management of the Department's fossil fuels (coal, oil and natural gas) research and development program. This research is generally directed by the Office of Coal Technologies (OCT), the Office of Oil, Gas, Shale and Special Technologies (OGSST) and the Office of Advanced Research in support of the National Energy Strategy (NES) 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 OCT and OGSST technology programs. 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.

The acronym PYF indicates that the work in the designated year was supported by prior-year funds.

Materials Preparation, Synthesis, Deposition, Growth or Forming

629. Coating Process Development for Cr-Nb Alloys FY 1993
$80,000

DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (615) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole, (615) 574-4824
Ohio State University Contact: R. A. Rapp, (614) 292-6178

Cr-Nb alloys are being developed for high temperature service, but they need 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

630. Procurement of Advanced Austenitic and Aluminide Alloys FY 1993
$30,000

DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (615) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole, (615) 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

631. Development of Iron Aluminides FY 1993
$400,000

DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (615) 576-0735
Oak Ridge National Laboratory Contact: C. G. McKamey, (615) 574-6917

The objective of this project is to develop low-cost, low-density intermetallic alloys based on Fe_3Al with an optimum combination of strength, ductility, and corrosion resistance for use as components in advanced fossil energy systems.

Keywords: Alloys, Aluminides, Intermetallic Compounds

632. Ultrahigh Temperature Intermetallic Alloys FY 1993
$377,000

DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (615) 576-0735
Oak Ridge National Laboratory Contact: C. T. Liu, (615) 574-4459

The objective of this project is to develop high-strength, corrosion-resistant intermetallic alloys for use as hot components in advanced fossil energy conversion systems. The successful development of these alloys is expected (1) to improve the thermal efficiency of fossil energy conversion systems, and (2) to increase the service life of hot components exposed to corrosive environments.

Keywords: Alloys, Chromium-Niobium, Corrosion, Intermetallic Compounds

633. Microalloyed Iron Aluminides FY 1993
$78,000

DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (615) 576-0735
Oak Ridge National Laboratory Contact: C. G. McKamey, (615) 574-6917

The objective of this project is to use microalloying techniques to extend the development of those Fe_3Al-based alloys identified as possessing improved room-temperature tensile properties. Emphasis is on low-cost, low-density, precipitation-strengthened Fe_3Al-based alloys with improved high-temperature creep resistance and an optimum combination of good room- and high-temperature tensile properties, weldability, and corrosion resistance.

Keywords: Alloys, Aluminides, Microalloy

634. <u>Low-Aluminum Content Iron-Aluminum Alloys</u> FY 1993
$300,000

DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (615) 576-0735
Oak Ridge National Laboratory Contact: V. K. Sikka, (615) 574-5112

The objective of this project is to develop a conventionally fabricable low-cost, low-density iron-aluminum alloy with a good combination of strength, ductility, weldability, and corrosion resistance for use as components in advanced fossil energy conversion systems.

Keywords: Alloys, Iron-Aluminum

635. <u>Technology Transfer - Iron Aluminides</u> FY 1993
$60,000

DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (615) 576-0735
Oak Ridge National Laboratory Contact: V. K. Sikka, (615) 574-5112

The purpose of this activity is to establish a Cooperative Research and Development Agreement (CRADA) with an industrial partner for the development of corrosion-resistant surface protection for fossil power systems.

Keywords: Alloys, Iron-Aluminum, Corrosion, Technology Transfer

636. <u>Investigation of Austenitic Alloys for Advanced Heat Recovery and Hot-Gas Cleanup Systems</u> FY 1993
$150,000

DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (615) 576-0735
Oak Ridge National Laboratory Contact: R. W. Swindeman, (615) 574-5108

The purpose of this project is to evaluate austenitic alloys for improved performance in high-temperature components in advanced heat recovery and hot-gas cleanup systems. Factors considered included strength, ductility, corrosion resistance, high-temperature stability, and fabricability.

Keywords: Materials, Mechanical Properties, Austenitics, Hot-Gas

637. Technology Transfer - Advanced Austenitics FY 1993 $80,000

DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (615) 576-0735
Oak Ridge National Laboratory Contact: R. W. Swindeman, (615) 574-5108

The purpose of this activity is to establish a Cooperative Research and Development Agreement (CRADA) with an industrial partner for the development of advanced austenitic alloys for fossil power systems.

Keywords: Alloys, Austenitics, Technology Transfer

638. Influence of Processing on Microstructure and Properties of Aluminides FY 1993 $175,000

DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (615) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole, (615) 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

639. Investigation of Electrospark Deposited Coatings for Protection of Materials in Sulfidizing Atmospheres FY 1993 $130,000

DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (615) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole, (615) 574-4824
Westinghouse Hanford Company Contact: R. N. Johnson, (509) 376-3582

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 superheater alloys. Materials to be deposited may include MCrAl, MCrAlY, highly wear-resistant carbides, and other hardsurfacing materials.

Keywords: Coatings, Materials, Deposition

640. Engineering-Scale Development of the Vapor-Liquid-Solid (VLS) Process for the Production of Silicon Carbide Fibrils

FY 1993
$160,000

DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (615) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole, (615) 574-4824
The Carborundum Company Contact: R. S. Storm, (716) 278-2000

The purpose of this work is to transfer to industry a specific technology developed by DOE under the AR&TD Materials Program for the production of silicon carbide fibrils for the reinforcement of ceramic matrices. The Vapor-Liquid-Solid (VLS) process has been developed at Los Alamos National Laboratory (LANL) 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

641. Ceramic Composite Processing Equipment

FY 1993
$20,000

DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (615) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole, (615) 574-4824

This task provides funds for the procurement of major equipment items necessary for AR&TD Materials Program activities.

Keywords: Equipment

642. Fabrication of Fiber-Reinforced Composites by Chemical Vapor Infiltration and Deposition (CVID)

FY 1993
$200,000

DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (615) 576-0735
Oak Ridge National Laboratory Contact: D. P. Stinton, (615) 574-4556

The purpose of this task is the development of 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 as solid phases to form the matrix of the composite. Modifications to the process which are being explored include controlling the porosity and permeability of the fibrous preforms and variation of the deposition conditions.

Keywords: Composites, Fiber-Reinforced, Ceramics

643. Interfaces and Mechanical Properties of Continuous Fiber-Reinforced Ceramic Composites

FY 1993
$150,000

DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (615) 576-0735
Oak Ridge National Laboratory Contact: D. P. Stinton, (615) 574-4556

The purpose of this task is to optimize the strength and toughness of fiber-reinforced ceramic composites by tailoring the strength of the bonds between the fiber and the matrix. Methods must first be developed to characterize the fiber-matrix bond strengths in fiber-reinforced ceramic composite systems. Coating or pretreatment processes can then be utilized to tailor the fiber-matrix bonding within various composite systems and to optimize the strength and toughness of the composite.

Keywords: Composites, Ceramics, Fiber-Reinforced, Interfaces

644. Low-Temperature Fabrication of Transparent Silicon Nitride

FY 1993
$180,000

DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (615) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole, (615) 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

645. Microwave-Assisted Chemical Vapor Infiltration

FY 1993
$121,000

DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (615) 576-0735
Oak Ridge National Laboratory Contact: M. A. Janney, (615) 574-4281

The purpose of this activity is to explore the feasibility of using microwave heating as a means of fabricating electrode, electrolyte, and interconnect materials having improved electrical properties for monolithic solid oxide fuel cell designs being advanced by DOE. The ultimate goal is to develop the technology (materials and process) for fabricating a complete monolithic fuel cell module in one operation.

Keywords: Ceramics, Microwave Processing

646. Technology Transfer - Microwave Processing | FY 1993 $29,000

DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (615) 576-0735
Oak Ridge National Laboratory Contact: M. A. Janney, (615) 574-4281

The purpose of this activity is to establish a Cooperative Research and Development Agreement (CRADA) with an industrial partner for the development of ceramic composite filters by microwave processing techniques.

Keywords: Ceramics, Microwave Processing,Technology Transfer

647. Carbon Fiber Composite Molecular Sieves | FY 1993 $134,000

DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (615) 576-0735
Oak Ridge National Laboratory Contact: T. D. Burchell, (615) 576-8595

The purpose of this work is to develop carbon molecular sieves starting with porous carbon fiber composites manufactured from petroleum pitch-derived carbon fibers. The carbon fiber composite molecular sieves will be used in pressure swing adsorption units for the efficient recovery of hydrogen from refinery purge gases and for other gas separation operations associated with petroleum refining.

Keywords: Carbon Fibers, Sieves, Composites

648. Activation of Carbon Fiber Composite Molecular Sieves | FY 1993 $46,000

DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (615) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole, (615) 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 ORNL staff and Prof. Frank Derbyshire and Ms. Marrit Jagtoyen at the University of Kentucky Center for Applied Energy Research (UKCAER). 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

649. Ceramic Composite Molding Equipment FY 1993 $30,000

DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (615) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole, (615) 574-4824

This task provides funds for the procurement of major equipment items necessary for AR&TD Materials Program activities.

Keywords: Equipment

650. Ceramic Composite Adsorption Equipment FY 1993 $30,000

DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (615) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole, (615) 574-4824

This task provides funds for the procurement of major equipment items necessary for AR&TD Materials Program activities.

Keywords: Equipment

651. Development of Advanced Fiber Reinforced Ceramics FY 1993 $140,000

DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (615) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole, (615) 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

652. Modeling of Fibrous Preforms for CVD Infiltration | FY 1993 $50,000

DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (615) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole, (615) 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

Materials Properties, Behavior, Characterization or Testing

653. Investigation of the Weldability of Polycrystalline Iron Aluminides | FY 1993 $75,000

DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (615) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole, (615) 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

654. Aqueous Corrosion of Iron Aluminides | FY 1993 $44,000

DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (615) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole, (615) 574-4824
University of Tennessee Contact: R. A. Buchanan, (615) 974-4858

The objective of this project is to investigate the aqueous corrosion of iron aluminides based on Fe_3Al. The effort provides basic corrosion information over a wide range of pH values for each of several experimental iron aluminide compositions and allows comparisons to be made among iron aluminide compositions, as well as with other corrosion-resistant materials of interest to fossil energy systems.

Keywords: Alloys, Aluminides, Corrosion

655. Fireside Corrosion Tests of Candidate Advanced Austenitic Alloys, Coatings, and Claddings

FY 1993
$157,000

DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (615) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole, (615) 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

656. Joining Techniques for Advanced Austenitic Alloys

FY 1993
$0 (PYF)

DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (615) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole, (615) 574-4824
University of Tennessee Contact: C. D. Lundin, (615) 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

657. Fatigue and Fracture Behavior of Cr-Nb Alloys FY 1993
$23,000

DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (615) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole, (615) 574-4824
University of Tennessee Contact: Peter Liaw, (615) 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 shall 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

658. Corrosion and Mechanical Properties of Alloys in FBC and Mixed-Gas Environments FY 1993
$310,000

DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (615) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole, (615) 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

659. Environmental Effects on Iron Aluminides — FY 1993 $225,000

DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (615) 576-0735
Oak Ridge National Laboratory Contact: J. H. DeVan, (615) 574-4451

The purpose of this task is to evaluate the corrosion properties of Fe_3Al-based alloys as they relate to fossil energy applications. A primary objective is to measure the resistance of the alloys to mixed-oxidant [oxygen-sulfur] environments that arise in the combustion or gasification of coal. This includes a determination of the effects of sulfur on oxidation kinetics and oxide microstructures, the effects of rare earth additions on sulfidation and oxidation resistance, and the mechanical behavior of reaction product scales in mixed-gas environments.

Keywords: Corrosion, Aluminides, Mixed-Gas, Scales

660. Investigation of Moisture-Induced Embrittlement of Iron Aluminides — FY 1993 $60,000

DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (615) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole, (615) 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

661. Determination of Physical Properties of Iron and Nickel Aluminides — FY 1993 $10,000

DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (615) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole, (615) 574-4824
Texas A&M University Contact: M. N. Srinivasan, (409) 845-1417

The purpose of this work is to determine the elastic modulus and Poisson's ratio of intermetallic alloys. Elastic modulus and Poisson's ratio measurements will be conducted on nickel-aluminide and iron aluminide alloys. Data analyses will be performed to provide explanations for the observed values of modulus and Poisson's ratio with respect to composition and test temperature variation.

Keywords: Alloys, Aluminides, Properties

662. Corrosion Protection of Ultrahigh Temperature Intermetallic Alloys FY 1993 $220,000

DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (615) 576-0735
Oak Ridge National Laboratory Contact: P. F. Tortorelli, (615) 574-5119

The purpose of this activity is to support the development of high-strength, corrosion-resistant intermetallic alloys by conducting critical experiments and analyses to evaluate the best alloy design and surface treatments to offer protection for environmental degradation at high temperatures.

Keywords: Corrosion, Chromium-Niobium, Mixed-Gas, Scales

663. Development of Nondestructive Evaluation Methods and Effects of Flaws on the Fracture Behavior of Structural Ceramics FY 1993 $310,000

DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (615) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole, (615) 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

664. Joining of Fiber-Reinforced Silicon Carbide Composites FY 1993 $175,000

DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (615) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole, (615) 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.

Keywords: Joining, Ceramics, Composites

665. Ceramic Catalyst Materials: Hydrous Metal Oxide Ion Exchange Supports for Direct Coal Liquefaction — FY 1993 $225,000

DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (615) 576-0735
Oak Ridge National Laboratory Contact: N. C. Cole, (615) 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

666. *Materials and Components in Fossil Energy Applications* (Newsletter) — FY 1993 $0 (PYF)

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The purpose of this task is to publish a periodic (bimonthly) newsletter to address current developments in materials and components in fossil energy applications.

Keywords: Materials, Components

667. Fabrication of Full-Scale Fiber-Reinforced Hot-Gas Filters by Chemical Vapor Deposition FY 1993 $120,000

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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 will be developed.

Keywords: Ceramics, Composites, Filters

668. Development of Ceramic Membranes for Gas Separation FY 1993 $400,000

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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

669. Investigation of the Mechanical Properties and Performance of Ceramic Composite Components FY 1993 $100,000

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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

670. Advanced Materials and Electrochemical Processes in High-Temperature Solid Electrolytes — FY 1993 $700,000

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The objective of this research is (1) to identify, develop, and demonstrate advanced materials for use as alternative electrodes and current interconnections in solid oxide fuel cells, and (2) to develop an understanding of the synergistic effects of materials properties, structures, and compositions on electrochemical processes related to high-temperature solid electrolyte use in electrochemical cells.

Keywords: Fuel Cells, Electrochemical, Electrolytes

Instrumentation and Facilities

671. Management of the Fossil Energy AR&TD Materials Program — FY 1993 $400,000

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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 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

672. <u>General Technology Transfer Activities</u> <u>FY 1993</u>
$35,000

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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

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A

B

C

D

E

F

G

H

I

J

K

L

M

N

O

P

Q

R

S

T

U

V

W

X

Y

Z