ENERGY MATERIALS COORDINATING COMMITTEE (EMaCC)

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Fiscal Year 1994

July 31, 1995



Annual Technical Report

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

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U.S. Department of Energy Office of Energy Research

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Office of Basic Energy Sciences Division of Materials Sciences Washington, D.C. 20585

TABLE OF CONTENTS

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Page

Introduction	1
Membership List	2
Organization of the Report	5
FY 1994 Budget Summary Table for DOE Materials Activities	6

PROGRAM DESCRIPTIONS

OFFICE OF ENERGY EFFICIENCY AND RENEWABLE ENERGY	10
Office of Building Technologies	13
Office of Building Energy Research	14
Buildings Systems and Materials Division	14
Office of Industrial Technologies	17
Office of Waste Reduction Technologies	21
Industrial Energy Efficiency Division	21
Waste Material Management Division	24
Waste Utilization and Conversion	24
Solar Materials Research	26
Office of Industrial Processes	27
Advanced Industrial Materials Program	27
Office of Transportation Technologies	40
Office of Transportation Materials	45

TABLE OF CONTENTS (Continued)

	Page
OFFICE OF ENERGY EFFICIENCY AND RENEWABLE ENERGY (continued)	
Office of Propulsion Systems	70
Advanced Propulsion Division	70
Electric and Hybrid Propulsion Division	73
Office of Alternative Fuels	85
Office of Utility Technologies	87
Office of Solar Energy Conversion	89
Photovoltaic Energy Technology Division	89
Office of Renewable Energy Conversion	91
Geothermal Technology Division	91
Office of Energy Management	94
Advanced Utility Concepts Division	94
Superconductivity Systems Program	94
Thermal Energy Storage Program	. 101
·	
OFFICE OF ENERGY RESEARCH	. 103
Office of Basic Energy Sciences	. 120
Division of Materials Sciences	. 121
Division of Chemical Sciences	. 124
Division of Engineering and Geosciences	. 126
Engineering Sciences Research	. 127
Geosciences Research	. 147
Division of Advanced Energy Projects	. 157
Office of Fusion Energy	. 170

Page

TABLE OF CONTENTS (Continued)

OFFICE OF ENERGY RESEARCH (continued)	
Small Business Innovation Research Program 1	79
Small Business Technology Transfer Program 19	93
OFFICE OF ENVIRONMENTAL MANAGEMENT 19	95
Office of Waste Management 19	98
High Level Waste Division 19	98
Office of Environmental Restoration	03
Office of Technology Development	04
OFFICE OF NUCLEAR ENERGY 2	13
Office of Uranium Programs	15
Office of Space and Defense Power Systems	16
Radioisotope Power Systems Division	16
Space Reactor Power Systems Division 22	18
Thermoelectric Space Nuclear Power System Technology	19
Thermionic Space Nuclear Power System Technology	20
Office of Naval Reactors	22

TABLE OF CONTENTS (Continued)

	<u>Page</u>
OFFICE OF DEFENSE PROGRAMS	226
The Weapons Research, Development and Test Program	238
Sandia National Laboratories	238
Lawrence Livermore National Laboratory	277
Los Alamos National Laboratory	301
OFFICE OF FOSSIL ENERGY	332
Office of Advanced Research	336
Fossil Energy AR&TD Materials Program	336
DIRECTORY	365
KEYWORD INDEX	415

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 intraand interagency compilations.

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

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

Membership in 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.

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 1994 and describes the materials research programs of various offices and divisions within the Department.

The Chairman of EMaCC for FY 1994 was Brian G. Volintine. The compilation of this report was performed by Debbie Haught, EMaCC Executive Secretary for FY 1995, with the assistance of FM Technologies, Inc.

Dr. Cynthia Carter Office of Energy Research Chair of EMaCC, FY 1995

1

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 Waste Materials Management Materials Processing Division Advanced Industrial Materials Separation Division	Scott Richlen, EE-221 Kurt D. Sisson EE-222 Matthew McMonigle, EE-234 Charles Sorrell, EE-232 Brian Volintine, EE-233	202/586-2078 202/586-6750 202/586-2082 202/586-1514 202/586-1739
Transportation Technologies		
Advanced Transportation Materials	Sidney Diamond, EE-34 Jim Eberhardt, EE-34 Debbie Haught, EE-34	202/586-0832 202/586-1694 202/586-2211
Utility Technologies		
Wind/Hydro/Ocean Technologies Geothermal Technology Photovoltaic Technology Advanced Utility Concepts	William Richards, EE-121 Raymond LaSala, EE-122 Richard King, EE-131 James Daley, EE-142 Chris Kang, EE-142	202/586-5410 202/586-4198 202/586-1693 202/586-1165 202/586-4563

ORGANIZATION	REPRESENTATIVE	PHONE NO.
ENERGY RESEARCH		
Basic Energy Sciences		
Materials Sciences	Iran L. Thomas, ER-10 Robert J. Gottschall, ER-13	301/903-3081 301/903-3427
Metallurgy and Ceramics	Alan Dragoo, ER-131 Yok Chen, ER-131 Helen Kerch, ER-131 John Mundy, ER-131	301/903-4895 301/903-3428 301/903-3428 301/903-4271
Solid State Physics and Materials Chemistry	W. Oosterhuis, ER-132 Jerry Smith, ER-132 Richard Kelly, ER-132	301/903-3426 301/903-3426 301/903-3426
Chemical Sciences Engineering and Geosciences Advanced Energy Projects Safety and Health	Stephen A. Butter, ER-142 Oscar P. Manley, ER-15 Cynthia Carter, ER-16 Albert Evans, ER-13 Michael Teresinski, ER-13	301/903-2367 301/903-5822 301/903-5995 301/903-3427 301/903-5155
Laboratory Management		
Laboratory Technology Transfer	Ted Vojnovich, ER-80	202/586-2343
Fusion Energy		
Fusion Technologies	F. W. (Bill) Wiffen, ER-543	301/903-4963
NUCLEAR ENERGY		
Space and Defense Power Systems		
Defense Energy Projects Radioisotope Power Systems	John W. Warren, NE-52 William Barnett, NE-53	301/903-6491 301/903-3097
Naval Reactors	David I. Curtis, NE-60	703/603-5565
Nuclear Safety Self-Assessment		
Nuclear Quality Assurance	John Dowicki, NE-84	301/903-7729

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Membership List

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ORGANIZATION	REPRESENTATIVE	PHONE NO.
DEFENS	E PROGRAMS	
Research and Advanced Technology		
Research and Technology Development	Bharat Agrawal, DP-11	301/903-2057
Inertial Confinement Fusion	Carl B. Hilland, DP-28	301/903-3687
ENVIRONMENTAL RESTORA	TION AND WASTE MANAGER	MENT
Waste Operations		
Waste Management Projects	Mark Frei, EM-34	301/903-7201
Technology Development		
Transportation Management Research and Development	Michael Conroy, EM-561 Stanley M. Wolf, EM-54	301/903-7967 301/903-7962
FOSSIL ENERGY		
Advanced Research	David J. Beecy, FE-72 James P. Carr, FE-72	301/903-2787 301/903-6519
CIVILIAN RADIOACTIVE WASTE MANAGEMENT		
Analysis and Verification	Alan Berusch, RW-2	202/586-9362

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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 1994 budget summary table for DOE Materials Activities in each of the programs is presented on pages 6-9.

FY 1994 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.)

	<u>FY 1994</u>
Office of Building Technologies	\$ 650,000
Office of Building Energy Research	650,000
Buildings Systems and Materials Division	650,000
Office of Industrial Technologies	\$29,083,000
Office of Waste Reduction Technologies	21,593,000
Industrial Energy Efficiency Division Waste Material Management Division	18,485,000 3,108,000
Office of Industrial Processes	7,490,000
Office of Transportation Technologies	\$31,935,000
Office of Transportation Materials	18,233,000
Office of Propulsion Systems	12,977,000
Advanced Propulsion Division Electric and Hybrid Propulsion Division	7,998,000 4,979,000
Office of Alternative Fuels	725,000

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FY 1994 BUDGET SUMMARY TABLE FOR DOE MATERIALS ACTIVITIES (Continued)

	<u>FY 1994</u>
Office of Utility Technologies	\$31,454,000
Office of Solar Energy Conversion	18,100,000
Photovoltaic Energy Technology Division	18,100,000
Office of Renewable Energy Conversion	600,000
Geothermal Division	600,000
Office of Energy Management	12,754,000
Advanced Utility Concepts Division	12,754,000
Superconductivity Systems Program Thermal Energy Storage Program	12,300,000 454,000
Office of Energy Research	\$348,260,033
Office of Basic Energy Sciences	297,371,424
Division of Materials Sciences	277,125,000
Division of Chemical Sciences	5,300,000
Division of Engineering and Geosciences	7,406,424
Engineering Sciences Research Geosciences Research	4,836,821 2,569,603
Division of Advanced Energy Projects	7,540,000
Office of Fusion Energy	14,488,000
Small Business Innovation Research Program	35,030,124
Small Business Technology Transfer Program	1,370,485

FY 1994 BUDGET SUMMARY TABLE FOR DOE MATERIALS ACTIVITIES (Continued)

	<u>FY 1994</u>
Office of Environmental Management	\$37,914,500
Office of Waste Management	14,766,500
High Level Waste Division	. 14,766,500
Office of Environmental Restoration	2,874,000
Office of Technology Development	20,274,000
Office of Nuclear Energy	\$55,265,000
Office of Space and Defense Power Systems	12,265,000
Radioisotope Power Systems Division Space Reactor Power Systems Division	2,425,000 9,840,000
Office of Naval Reactors	43,000,000 [*]
Office of Civilian Radioactive Waste Management	\$ 2,200,000

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^{&#}x27;This excludes \$54 million for the cost of irradiation testing in the Advanced Test Reactor (ATR).

FY 1994 BUDGET SUMMARY TABLE FOR DOE MATERIALS ACTIVITIES (Continued)

	<u>FY 1994</u>
Office of Defense Programs	\$ 78,279,848
The Weapons Research Development and Test Program	78,279,848
Sandia National Laboratories Lawrence Livermore National Laboratory Los Alamos National Laboratory	\$ 32,222,000 19,030,848 27,027,000
Office of Fossil Energy	\$ 8,628,000
Office of Advanced Research	8,628,000
Fossil Energy AR&TD Materials Program	8,628,000
TOTAL	\$623,669,381

OFFICE OF ENERGY EFFICIENCY AND RENEWABLE ENERGY

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

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

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			<u>FY 1994</u>
1.	<u>Of</u>	fice of Building Technologies	\$ 650,000
	a.	Office of Building Energy Research	650,000
		(1) Buildings Systems and Materials Division	650,000
2.	<u>Of</u>	fice of Industrial Technologies	\$29,083,000
	a.	Office of Waste Reduction Technologies	21,593,000
		 Industrial Energy Efficiency Division Waste Material Management Division 	18,845,000 3,108,000
	b.	Office of Industrial Processes	7,490,000
3.	<u>Of</u>	fice of Transportation Technologies	\$31,935,000
	a.	Office of Transportation Materials	18,233,000
	b.	Office of Propulsion Systems	12,977,000
		(1) Advanced Propulsion Division	7,998,000
		(2) Electric and Hybrid Propulsion Division	4,979,000
	c.	Office of Alternative Fuels	725,000

11

Office of Energy Efficiency and Renewable Energy

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4.	Of	fice of Utility Technologies	\$31,454,000
	a.	Office of Solar Energy Conversion	18,100,000
		(1) Photovoltaic Energy Technology Division	18,100,000
	b.	Office of Renewable Energy Conversion	600,000
		(1) Geothermal Division	600,000
	c.	Office of Energy Management	12,754,000
		(1) Advanced Utility Concepts Division	12,754,000

OFFICE OF BUILDING TECHNOLOGIES

E E E E E E E E E E E E E E E E E E E	<u>FY 1994</u>
Office of Building Technologies - Grand Total \$	\$650,000
Office of Building Energy Research \$	650,000
Building Systems and Materials Division \$	\$650,000
Materials Properties, Behavior, Characterization or Testing \$	650,000
Development of Non-CFC Foam Insulations	100,000
Evacuated Powder Panel Insulation	300,000
Gas-Filled Reflective Insulation Panel	100,000
Accelerated Lifetime Test Procedure Development	150,000

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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; 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 1994 \$100,000

DOE Contact: Peter Scofield, (202) 586-9193 ORNL Contact: Ken Wilkes, (615) 574-5931

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

Keywords: CFC, Foam Insulation, Insulation Sheathing, Roofs

2. Evacuated Powder Panel Insulation

DOE Contact: Peter Scofield, (202) 586-9193 ORNL Contact: Ken Wilkes, (615) 574-5931

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

Keywords: Insulation, Vacuum, Heat Transfer

3. <u>Gas-Filled Reflective Insulation Panel</u>

FY 1994 \$100,000

FY 1994 \$300.000

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. Accelerated Lifetime Test Procedure Development

<u>FY 1994</u> \$150,000

DOE Contact: Peter Scofield, (202) 586-9193 ORNL Contact: Ken Wilkes, (615) 574-5931

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

Keywords: Thermal Resistance, Test Procedures

OFFICE OF INDUSTRIAL TECHNOLOGIES

	<u>FY 1994</u>
Office of Industrial Technologies - Grand Total	\$29,083,000
Office of Waste Reduction Technologies	\$21,593,000
Industrial Energy Efficiency Division	\$18,485,000
Materials Properties. Behavior. Characterization or Testing	\$ 2,857,000
Advanced Heat Exchanger Material Technology Development Ceramic Fiber Residue Measurement Continuous Fiber Ceramic Composites (CECC) Supporting	1,132,000 20,000
Technologies	1,705,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	\$ 6,492,000
CFCC Program - Industry Tasks	6,492,000
Device or Component Fabrication, Behavior or Testing	\$ 9,136,000
Ceramic Composite Heat Exchanger for the Chemical Industry HiPHES System Design Study for Energy Production	363,000
from Hazardous Wastes	623,000
HiPHES System Design Study for an Advanced Reformer Ceramic Components for Stationary Gas Turbines in	350,000
Cogeneration Service	7,200,000
Long-Term Testing of Ceramic Components for Stationary Gas Turbines	600,000

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OFFICE OF INDUSTRIAL TECHNOLOGIES

	<u>FY 1994</u>
Office of Waste Reduction Technologies (continued)	
Waste Material Management Division	\$ 3,108,000
Waste Utilization and Conversion	\$ 2,308,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	\$ 2,308,000
Wood Wastes to Adhesives Waste Tire Composite Silicon Oxide Recovery-Conversion Bioconversion of Food Wastes to Lactic Acid	638,000 1,000,000 0 670,000
Solar Materials Research	\$ 800,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	\$ 800,000
Photocatalysts Based on Titanium Dioxide Solar Materials Processing	250,000 550,000
Office of Industrial Processes	\$ 7,490,000
Advanced Industrial Materials Program	\$ 7,490,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	\$ 2,825,000
Advanced Methods for Processing Ceramics Synthesis and Design of Intermetallic Materials Development of Weldable, Corrosion Resistant	60,000 490,000
Iron-Aluminide Alloys	180,000

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OFFICE OF INDUSTRIAL TECHNOLOGIES (Continued)

]	FY_1994
Office of Industrial Processes (continued)		
Advanced Industrial Materials Program (continued)	\$:	3,108,000
Materials Preparation, Synthesis, Deposition, Growth or Forming (continued)		
Composites Through Reactive Metal Infiltration Magnetic Field Processing of Inorganic Polymers Development of New Composite Aerogel Materials Microwave Processing of Continuous Ceramic Oxide Filaments Conducting Polymers: Synthesis and Industrial Applications Microwave Assisted Chemical Vapor Infiltration High Deposition Rate Ceramic Synthesis		325,000 225,000 275,000 350,000 325,000 270,000 325,000
Materials Properties, Behavior, Characterization or Testing	\$	500,000
Three Dimensional X-ray Tomography of Crack-Resistant Composites Characterization of Three-Way Automotive Catalysts Materials Structure and Composition	\$ 2	200,000 300,000 2,590,000
High-Temperature Precipitate-Strengthened Iron-Aluminide	Ψ-	_,,
Alloys Metallic and Intermetallic Bonded Ceramic Composites Advanced Ordered Intermetallic Alloy Development Superior Metallic Alloys Through Rapid Solidification		260,000 430,000 165,000
Processing by Design Polymerization and Processing of Organic Polymers		225,000
in a Magnetic Field Microwave Joining of SiC		300,000 80,000
Microwave Processing of Materials: Glass-Ceramics Characterization of CVI Densification of Ceramic		85,000
Composites Biomimetic Thin Film Synthesis		120,000 325,000
Composites and Blends from Biobased Materials		300,000 300,000

OFFICE OF INDUSTRIAL TECHNOLOGIES

FY 1994

Office of Industrial Processes (continued)

Advanced Industrial Materials Program (continued)	
Device or Component Fabrication. Behavior or Testing	\$ 1,575,000
Ni ₃ Al Technology Transfer	750,000
Advanced Microwave Processing Concepts	240,000
Selective Inorganic Thin Films	425,000
Chemical Vapor Infiltration of TiB ₂ Composites	160,000

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	<u>FY 1994</u>
		\$1,132,000

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. <u>Ceramic Fiber Residue Measurement</u>

FY 1994 \$20,000

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

7. <u>Continuous Fiber Ceramic Composites (CFCC) Supporting Technologies</u> <u>FY 1994</u> \$1,705,000 DOE Contact: S. Richlen, (202) 586-2078

ORNL Contact: S. Kichlen, (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

8. <u>CFCC Program - Industry Tasks</u>

<u>FY 1994</u> \$6,492,000

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

9. <u>Ceramic Composite Heat Exchanger for the Chemical Industry</u>

<u>FY 1994</u> \$363.000

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

10. <u>HiPHES System Design Study for Energy Production from Hazardous</u> <u>Wastes</u> <u>F</u>

<u>FY 1994</u> \$623,000

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 (HiPHES) 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

11.HiPHES System Design Study for an Advanced ReformerFY 1994\$350,000

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

12. Ceramic Components for Stationary Gas Turbines in Cogeneration Service

<u>FY 1994</u> \$7,200,000

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

13. Long-Term Testing of Ceramic Components for Stationary Gas Turbines FY 1994 \$600,000

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

14.	<u>Wood</u>	Wastes to	<u>Adhesives</u>
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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

15. <u>Waste Tire Composite</u>

DOE Contact: Stuart Natof, (202) 586-2370 Composite Particles, 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

16. <u>Silicon Oxide Recovery-Conversion</u>

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

<u>FY 1994</u> \$638,000

<u>FY 1994</u> \$1.000.000

> <u>FY 1994</u> \$0

17. Bioconversion of Food Wastes to Lactic Acid

<u>FY 1994</u> \$670,000

<u>FY 1994</u> \$250,000

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 lactide polymers.

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

18. <u>Photocatalysts Based on Titanium Dioxide</u>

DOE Contact: Frank Wilkins, (202) 586-1684 NREL Contact: Daniel M. Blake, (303) 275-3702

The objectives of this work are to develop materials that are more active photocatalysts for the oxidation of organic compounds in air or aqueous phases, determine the characteristics of titanium dioxide and modified forms that influence the activity, and test the catalysts in laboratory and pilot scale reaction systems. 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

19. Solar Materials Processing

FY 1994 \$550,000

DOE Contact: Frank Wilkins, (202) 586-1684 NREL Contact: Allan Lewandowski, (303) 275-3672

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, synthesis, production and processing of advanced ceramic powders, solar assisted chemical vapor deposition of thin films on various substrates, rapid thermal heat treating and cladding, solar production of Fullerenes, and other surface modification techniques. The project seeks to explore a wide range of technologies, assess those with commercial potential and develop the most promising technologies in conjunction with industry. Several technologies have demonstrated significant technical success and are now being explored more fully through Cooperative Research and Development Agreements.

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

Office of Industrial Processes

Advanced Industrial Materials Program

The Advanced Industrial Materials program mission is to unite National Laboratory/ industry/university teams to commercialize materials 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

20.	Advanced Methods for Processing Ceramics	<u>FY 1994</u>
		\$60,000
DOE	Contact: Charles A. Sorrell, (202) 586-1514	
Georg	gia Institute of Technology Contact: W. B. Carter and J. K. Cochran, (40)4) 894-6762

Advanced methods for processing ceramic materials, such as Combustion Chemical Vapor Deposition and Rapid Polymerization of Aqueous Slurries are providing potential solutions for improved thermal insulation and thermal barrier coatings. Combustion chemical vapor deposition (CCVD) is a chemical vapor deposition (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. Rapid Polymerization of Aqueous Slurries is a process to form polycrystalline fibers from polymerized aqueous solution. Results have demonstrated the deposition of several materials via CCVD including YSZ, SiO₂, BaTiO₃, and yttrium iron garnet.

Keywords: Combustion Chemical Vapor Deposition, Coatings, Ceramic Fibers

21.	Synthesis and Design of Intermetallic Materials	<u>FY 1994</u>
		\$490,000

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

The objective of this project is to develop $MoSi_2$ -based composites that will combine good room temperature fracture toughness with excellent oxidation resistance and hightemperature strength for industrial applications. Plasma spraying has proved to be very successful for fabricating $MoSi_2$ -based gas burner nozzles. In addition, development of laminated composites of $MoSi_2$ with Al_2O_3 interlayers has shown promising results for advanced burner nozzles. A new development has been in the synthesis of Si_3N_4 - $MoSi_2$ composites where the minority silicide phase provides conductivity for electro-discharge machining and ductile reinforcement at high temperatures. Future efforts will focus on developing microstructurally realistic models of toughening for materials with combined reinforcements such as SrO_2 and SiC and fabricating novel composites with silicides.

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

22. Development of Weldable, Corrosion Resistant Iron-Aluminide Alloys FY 1994 \$180,000 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 considerably improve room-temperature ductility and hightemperature tensile and creep strength relative to binary alloy systems. The objectives of this project are to complete alloy development efforts to maximize weldability and properties improvements in FeAl alloys for structural applications, and to develop the potential for weldable FeAl alloys for use in weld-overlay cladding applications. Several new modifications of the FeAl/FA-385 base alloys compositions were found to have good weldability and mechanical behavior. These FeAl alloys are nearly as weldable as 300 series austenitic stainless steels. Weld-clad deposits of these weldable FeAl alloys have been made into type 30L austenitic stainless and 2¼ Cr-1 Mo bainitic/martensitic steel substrates, and with proper preheat and post-weld heat treatments. Such weld-deposits are crack-free.

Keywords: Iron Aluminides, Coatings, Claddings, Thermophysical Properties

23.	Composites Through Reactive Metal Infiltration	<u>FY 1994</u>
		\$325,000
DOE	Contact: Charles A. Sorrell, (202) 586-1514	
Sandi	a National Laboratories Contact: R. E. Loehman, (505) 844-2222	

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

Keywords: Metal Matrix Composites, Reactive Metal Infiltration, Ceramics

24.	Magnetic Field Processing of Inorganic Polymers	FY 1994
		\$225,000
DOE	Contact: Charles A. Sorrell, (202) 586-1514	-
Idaho	National Engineering Laboratory Contact: D. C. Kunerth, (208) 526-0103	

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

Keywords: Polymers, Magnetic Field Processing

25.	Development of New Composite Aerogel Materials	<u>FY 1994</u>
		\$275,000

DOE Contact: Charles A. Sorrell, (202) 586-1514 Lawrence Berkeley Laboratory Contact: A. Hunt, (415) 486-5370

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

Keywords: Thermal Insulation, Sol-Gel, Aerogels

26.	Microwave Processing of Continuous Ceramic Oxide Filaments	<u>FY 1994</u>
DOF	Contract: Charles & Sorrell (202) 586 1514	\$350,000

Los Alamos National Laboratory Contact: G. J. Vogt and J. D. Katz, (505) 665-1424

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

Keywords: Microwave Processing, Filaments

27. <u>Conducting Polymers: Synthesis and Industrial Applications</u>

<u>FY 1994</u> \$325,000

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

The process of separating pure components out of a mixture of gases is of great industrial importance. Current gas separation technologies have major shortcomings, including poor energy efficiency and the generation of secondary pollution. The objective of this project is to (1) demonstrate new conducting polymer materials for electrochemical capacitors and (2) establish new activity on conducting polymer membranes for gas separation. Current efforts are devoted to developing and characterizing electronically conducting polymers, with eventual goal of demonstrating the technology at the semi-industrial level. In addition, the high solubility of oxygen was measured in the polyaniline membranes and identified it as an important element of the exceptionally high O_2/N_2 separation factors achieved with polyaniline membranes.

Keywords: Electrically Conducting Polymers, Gas Separation, Capacitors

28.	Microwave Assisted Chemical Vapor Infiltration	<u>FY 1994</u>
· ·		\$270,000
DOF	E Contact: Charles A. Sorrell, (202) 586-1514	

DOE Contact: Charles A. Sorrell, (202) 586-1514 Los Alamos National Laboratory: D. J. Devlin, (505) 667-9914

The use of microwave heating of ceramic fiber preforms is being explored as a means of developing an improved rapid process for the fabrication of composites by chemical vapor infiltration. The volumetric and preferential heating of certain materials by microwaves provides a means of establishing inverted thermal gradients in a preform. The result is the ability to rapidly infiltrate the preform developing the matrix from the inside-out. Using this technique, silicon carbide reinforced silicon-nitride composites have been fabricated. Future efforts will optimize processing to achieve sufficient density for mechanical testing of the composites.

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

29.	High Deposition Rate Ceramic Synthesis	<u>FY 1994</u>
		\$325,000
DOE	Contact: Charles A. Sorrell, (202) 586-1514	
Sand	ia 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. The objective of this project is to develop predictive computational models and other tools for designing, optimizing, and operating new ceramic processing technologies. 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. Future efforts will continue to focus on SiC deposition from chlorinated organosilanes. Results of this research should permit rapid and efficient development of new materials synthesis reactors.

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

Materials Properties, Behavior, Characterization or Testing

30. <u>Three Dimensional X-ray Tomography of Crack-Resistant Composites</u> <u>FY 1994</u> \$200,000 DOE Contact: Charles A Sorrell (202) 586-1514

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. Currently a high resolution, three-dimensional tomography system has been used to quantify microstructural evolution in continuous filament composites during chemical vapor infiltration processing. Microstructural parameters such as the amount of fiber tow consolidation and changes in surface area provide information which is essential for validating process models.

Keywords: X-ray, Tomography, Composites

31.Characterization of Three-Way Automotive CatalystsFY 1994
\$300,000DOE Contact:Charles A. Sorrell, (202) 586-1514\$300,000ORNL Contact:E. A. Kenik, (615) 574-5066574-5066

General Motors-AC Rochester Division Contact: W. LaBarge, (313) 257-0875

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

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

Materials Structure and Composition

32. <u>High-Temperature Precipitate-Strengthened Iron-Aluminide Alloys</u> FY 1994 \$260,000

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

FeAl-type iron-aluminide alloys have outstanding oxidation at >1000°C, but lack strength at 600°C and above, and many lack weldability. The objective of this project is to explore precipitate-strengthening effects for improved high temperature strength while also improving weldability in various intermetallic alloys, starting with FeAl-type (B2 phase) iron-aluminides. New modified FeAl-type alloys have been developed which have better weldability and creep-rupture strength than the base alloys. The modified FeAl alloys have weldability similar to that of type 316 austenitic stainless steel, and creep-resistance similar to that of type 304 stainless steel.

Keywords: Iron Aluminide, Nickel Aluminides, Physical Properties

33. <u>Metallic and Intermetallic Bonded Ceramic Composites</u> FY 1994

DOE Contact: Charles A. Sorrell, (202) 586-1514 ORNL Contacts: T. N. Tiegs and K. B. Alexander, (615) 574-0631 Lawrence Berkeley Laboratory Contact: R. O. Ritchie, (415) 642-0417

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

33

\$430,000

identified and composites have been fabricated with properties comparable to, or better than, commercial ceramic composites at a lower raw material cost.

Keywords: Ceramics, Composites, Nickel Aluminide

34. Advanced Ordered Intermetallic Alloy Deve	lopment FY 1994
	\$165,000
DOE Contact: Charles A. Sorrell, (202) 586-1514	
ORNL Contact: C. T. Liu, (615) 574-4459	

Many ordered intermetallics possess unique properties and have the potential to be developed as new materials for energy related applications. The objective of this project is to develop low-density, high-strength ordered intermetallic alloys for high-temperature structural use in advanced heat engines, energy conversion systems, and other industrial systems. Current efforts are focused on (1) the development of NiAl and TiAl alloys, (2) shape memory alloys based on NiAl/Ni₃Al compositions, (3) Ni₃Si alloys, and (4) reaction synthesis of NiAl and Ni₃Al alloys. Evaluations of the microstructure, mechanical properties of the cast NiAl alloys in different environments have been completed. Chromium additions substantially reduce the air oxidation rate of Ni-19% Si alloy at temperatures below 800°C but not above that temperature. Shape-memory alloys based on Ni-Al-Fe-B have been prepared by both conventional and innovative methods. The materials prepared by both methods show thermally activated shape-memory effects at temperatures close to 200°C.

Keywords: Intermetallics, Ordered Alloys, Shape Memory Alloys

35. <u>Superior Metallic Alloys Through Rapid Solidification Processing</u> by Design <u>FY 1994</u> \$225,000

DOE Contact: Charles A. Sorrell, (202) 586-1514 Idaho National Engineering Laboratory Contact: J. E. Flinn, (208) 526-8127

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

materials currently being used with those obtained by RSP. These materials are for high temperature electrical, corrosion and wear, and photovoltaic applications.

Keywords: Rapid Solidification, Alloys, High Temperature Microstructure

36. <u>Polymerization and Processing of Organic Polymers</u> in a Magnetic Field

<u>FY 1994</u> \$300,000

FY 1994 \$80,000

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. Current efforts are focused on polysilanes processed by the magnetic field/shear technique. Of the five novel high molecular weight polysilanes processed on a polysiloxane substrate, samples with unusual infrared and mechanical properties were generated. For the formation of composites, the use of a 4.2 T field was sufficient to orient graphite fibrils in space. A proof-of-principle was demonstrated for 3-D composite formation.

Keywords: Organic Polymers, Magnetic Processing, Mechanical Properties

37. <u>Microwave Joining of SiC</u>

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. The joined reaction bonded silicon carbide tube sections have average mechanical strength of 190 MPa, which is more than adequate for radiant burner and heat exchanger applications.

Keywords: Microwave Processing, Microwave Joining, SiC

38.	Microwave Processing of Materials:	Glass-Ceramics	<u>FY 1994</u>
	•		\$85,000

DOE Contact: Charles A. Sorrell, (202) 586-1514 ORNL Contact: M. A. Janney, (615) 576-5183

Microwave heating represents an emerging technology for high temperature processing of materials. The objective of this research is to provide clear engineering guidelines for using microwave processing in an industrial environment for high temperature applications. Results of this investigation so far indicate that microwave processing lowers the processing temperature for a zirconia-toughened alumina glass ceramic by approximately 100-150°C. Future investigations will focus on including compositions that sinter as glasses and convert to the crystalline state.

Keywords: Microwave Processing, Sintering, Zirconia-Toughened Alumina

39.	Characterization of CVI Densification of Ceramic Composites	<u>FY 1994</u>
		\$120,000

DOE Contact: Charles A. Sorrell, (202) 586-1514

Georgia Institute of Technology Contact: Tom Starr, (404) 583-0579 and S. R. Stock, (404) 894-6882

The objective of this research is to understand the relationship between preform fiber architecture and densification behavior to design preforms for optimum infiltration. In collaboration with Lawrence Livermore National Laboratory, high resolution X-ray tomography will be used to observe the deposition of matrix materials in the pores of ceramic fiber preforms at various stages of the chemical infiltration process (CVI). These observations will relate local deposition rates in various regions of the composite to the surrounding network of porosity and will aid in developing a better model between gas transport and fiber architecture in CVI preforms.

Keywords: Chemical Vapor Infiltration, Ceramic Composites, Preforms

40. <u>Biomimetic Thin Film Synthesis</u>

<u>FY 1994</u> \$325,000

DOE Contact: Charles A. Sorrell, (202) 586-1514 Pacific Northwest Laboratory Contact: G. L. Graff, (509) 375-6786

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

Keywords: Biomimetic, Organic Interfaces, Ceramic Coatings

41. <u>Chemical Recycling of Plastics</u>

<u>FY_1994</u> \$300,000

<u>FY 1994</u> \$300.000

DOE Contact: Charles A. Sorrell, (202) 586-1514 National Renewable Energy Laboratory Contact: R. J. Evans, (303) 231-1384

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

Keywords: Plastics Recycling, Pyrolysis, Waste Streams

42. <u>Composites and Blends from Biobased Materials</u>

DOE Contact: Charles A. Sorrell, (202) 586-1514 National Renewable Energy Laboratory Contact: S. S. Kelley and S. S. Shojaie, (303) 384-6123

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

morphology of the composites or blends. Current efforts are focused on utilizing cellulose esters to prepare novel composites and blends. These materials have improved permeselective and/or compaction properties relative to unmodified cellulose esters.

Keywords: Biobased Materials, Composites, Thermomechanical Testing

Device or Component Fabrication, Behavior or Testing

43. <u>Ni₃Al Technology Transfer</u>

\$750,000 DOE Contact: Charles A. Sorrell, (202) 586-1514 ORNL Contacts: M. L. Santella, (615) 574-4805 and V. K. Sikka, (615) 574-5112

Ductile $Ni_{1}Al$ and $Ni_{2}Al$ -based alloys have been identified for a range of applications. Although significant progress has been made in the melting, casting and near-net-shape forming of nickel aluminides, some issues still remain including the need for (1) highstrength, castable composition for turbochargers, furnace furniture, and hot-die applications; (2) castability (fluidity, hot-shortness, porosity, etc.); (3) weld repairability of castings; and (4) hot fabricability of cast ingots. The objective of this research is to mature the Ni₃Al and the Ni₂Al-based alloy technology for industrial application and commercial manufacturing, and to commercialize the Ni₃Al and the Ni₃Al-based alloys. Significant progress was made in the maturation of nickel aluminide technology and applications including (1) the development of a new alloy for Cummins Engine Company and PCC Airfoils, Inc.; (2) the development of roller assembly for Bethlehem Steel; and (3) the transfer of welding technology to Sandusky International. Future efforts will focus on (1) optimizing alloy composition and process parameters for sand and investment castings of Ni₃Al-based alloys; (2) developing methods for fabricating weld wire and producing weld components; (3) developing fracture toughness and other mechanical property data on prototype components and (4) continuing technology transfer activities.

Keywords: Nickel Aluminides, Processing, Mechanical Properties

44. Advanced Microwave Processing Concepts

FY 1994 \$240,000

FY 1994

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

The purpose of this project is to explore the feasibility of several advanced microwave processing concepts to develop new energy-efficient materials and processes as well as to reduce consumption of strategic metals. The project includes three tasks: (1) microwave sintering of multilayer ceramic capacitors; (2) commercialization of the variable frequency

microwave furnace; and (3) microwave curing of polymer composites. Efforts to date have shown uniform curing of neat resin samples with no evidence of overheating.

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

45. <u>Selective Inorganic Thin Films</u>

<u>FY 1994</u> \$425,000

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

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

Keywords: Coatings, Sol-Gel Processing

46.	Chemical Vapor Infiltration of TiB ₂ Composites	<u>FY 1994</u>
		\$160,000

DOE Contact: Charles A. Sorrell, (202) 586-1514 Oak Ridge National Laboratory Contact: T. Besmann, (615) 574-6852

This program is designed to develop a Hall-Heroult aluminum smelting cathode with substantially improved properties. The carbon cathodes in current use require significant anode-to-cathode spacing in order to prevent shorting, causing significant electrode inefficiencies. A fiber reinforced-TiB₂ matrix composite would have the requisite wettability, strength, strain-to-failure, cost, and lifetime to solve this problem. The approach is to fabricate a cathode material through chemical vapor infiltration (CVI). Current efforts are focused on preparing specimens for the licensee, Advanced Innovative Technologies, Inc., and for testing at Alcoa Technical Center. The results were promising in that aluminum was produced and did flow, albeit not uniformly.

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

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	<u>FY 1994</u>
Office of Transportation Technologies - Grand Total	\$31,935,000
Office of Transportation Materials	\$18,233,000
Materials Preparation, Synthesis, Deposition, Growth	
or Forming	\$ 8,224,000
Powder Characterization (WBS No. 1118)	110,000
Microwave Sintering (WBS No. 1124)	400,000
Cost Effective Silicon Nitride Powder (WBS No. 1125)	920,000
Cost Effective Sintering of Silicon Nitride	
Ceramics (WBS No. 1127)	462,000
Cost Effective Manufacture of Silicon Nitride	
Components (WBS No. 1128)	0
Advanced Processing (WBS No. 1141)	1,000
Improved Processing (WBS No. 1142)	650,000
Processing of Silicon Based Ceramics (WBS No. 1225)	288,000
In-Situ Toughened Silicon Nitride (WBS No.1226)	300,000
Dispersion Toughened Oxide Composites (WBS No. 1231)	350,000
Low Thermal Expansion Ceramics (WBS No. 1243)	100,000
NZP Components (WBS No. 1245)	541,000
Low Cost Aluminum Titanate/NZP Ceramics (WBS No. 1246)	247,000
Advanced Manufacturing (WBS No. 1520)	397,000
Advanced Ceramic Manufacturing (WBS No. 1521)	1,779,000
Advanced Ceramic Manufacturing (WBS No. 1522)	1,679,000
Materials Properties, Behavior, Characterization or Testing	\$ 3,963,000
Development of Standard Test Methods for	
Evaluating the Wear Performance of Ceramics (WBS No. 2222)	30,000
Advanced Statistics Calculations (WBS No. 2313)	100,000
Microstructural Analysis (WBS No. 3111)	50,000
Microstructural Characterization of Silicon Carbide and	
Silicon Nitride Ceramics for Advanced Heat Engines	
(WBS No. 3114)	200,000
Project Data Base (WBS No. 3117)	240,000
Fracture Behavior of Toughened Ceramics (WBS No. 3213)	290,000

<u>FY 1994</u>

Office of Transportation Materials (continued)

Materials Properties, Behavior, Characterization or Testing (continued)

Cyclic Fatigue of Toughened Ceramics (WBS No. 3214)	220,000
Tensile Stress Rupture Development (WBS No. 3215)	300,000
Life Prediction Verification (WBS No. 3216)	200,000
Toughened Ceramics Life Prediction (WBS No. 3217)	200,000
Life Prediction Methodology (WBS No. 3222)	0
Life Prediction Methodology (WBS No. 3223)	600,000
Environmental Effects in Toughened Ceramics (WBS No. 3314)	383,000
High Temperature Tensile Testing (WBS No. 3412)	250,000
Standard Tensile Test Development (WBS No. 3413)	125,000
Non-Destructive Evaluation (WBS No. 3511)	460,000
Computed Tomography (WBS No. 3515)	120,000
Nuclear Magnetic Resonance (NMR) Imaging (WBS No. 3516)	80,000
Assessment of Magnesium for Automotive Applications	115,000
Technology Transfer and Management Coordination	\$ 1,400,000
Management and Coordination (WBS No. 111)	950,000
International Exchange Agreement (IEA) (WBS No. 4115)	200,000
Standard Reference Materials (WBS No. 4116)	150,000
Mechanical Property Standardization (WBS No. 4121)	100,000
Device or Component Fabrication, Behavior or Testing	\$ 4,646,000
Advanced Coating Technology (WBS No. 1311)	175,000
Coatings to Reduce Contact Stress Damage of	
Ceramics (WBS No. 1313)	28,000
Wear Resistant Coatings (WBS No. 1331)	46,000
Wear Resistant Coatings (WBS No. 1332)	0
Thick Thermal Barrier Coating Systems for Low Heat	
Rejection Diesel Engines (WBS No. 1342)	0

FY 1994

Office of Transportation Materials (continued)

Device or Component Fabrication, Behavior or Testing (continued)

Active Metal Brazing PSZ-Iron (WBS No. 1411)	220,000
Surface Durability of Machined Ceramics (WBS No. 1500)	200,000
Next-Generation Grinding Wheel (WBS No. 1501)	0
Grindability Test (WBS No. 1502)	0
Chemically Assisted Grinding of Ceramics (WBS No. 1503)	150,000
Grinding Consortium (WBS No. 1503)	150,000
High Speed Grinding (WBS No. 1504)	372,000
Laser-Based NDE Methods (WBS No. 1507)	180,000
Development of "Smart" Grinding Wheel (WBS No. 1510)	50,000
Automotive Materials Development	3,000,000
Ultracapacitors for Electric and Hybrid Vehicles	75,000
Office of Propulsion Systems	\$12,977,000
Advanced Propulsion Division	\$7,998,000
Materials Properties, Behavior, Characterization or Testing	\$250,000
Advanced Turbine Supporting Research and Technology	250,000
Device or Component Fabrication, Behavior or Testing	\$7,748,000
Hybrid Vehicle Turbine Engine (HVTE) Technology Support	3,725,000
Ceramic Turbine (CT) Engine Demonstration Project	2,873,000
Advanced Diesel Engine Component Development Project	250,000
Advanced Piston and Cylinder Component Development	300,000
Advanced Piston and Cylinder Component Development	600,000

	<u>FY 1994</u>
Office of Propulsion Systems (continued)	
Electric and Hybrid Propulsion Division	\$4,979,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	\$1,200,000
Electrochemical Properties of Solid-State Sodium Polymer Cells	260,000
Corrosion Resistant Coatings for High-Temperature High-Sulfur-Activity Applications	0
Improved Container Electrode Coatings for Sodium/Sulfur Battery Systems	100,000
The Performance of New Materials for Polymer Electrolyte Batteries	140,000
Batteries Novel Solid Polymer Electrolytes for Advanced Secondary	160,000
Batteries Sol Col Electrolytes in Lithium Batteries	130,000
New Cathode Materials	110,000
Sodium/Polymer Cells	170,000
Materials Properties, Behavior, Characterization or Testing	\$2,675,000
Surface Morphology of Metals in Electrodeposition/	240.000
Battery Materials Structure and Characterization	100,000
In Situ Spectroscopic Applications to the Study of Rechargeable Lithium Batteries	135,000
Polymer Electrolyte for Ambient Temperature Traction Batteries: Molecular Level Modeling for Conductivity	
Optimization	160,000
Heat Transport and Thermal Management in Advanced Batteries	240,000
Electrode Surface Layers	125,000

<u>FY 1994</u>

Office of Propulsion Systems (continued)

Electric and	Hybrid	Propulsion	Division	(continued)
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Materials Properties, Behavior, Characterization or Testing (continued)

Electrode Kinetics and Electrocatalysis		100,000
Effect of Electrocatalyst and Electrolyte Composition on		
Methanol/Air Fuel Cell Performance		215,000
Poisoning of Fuel Cell Electrocatalyst Surfaces:		
NMR Spectroscopic Studies		200,000
Fuel Cells for Renewable Applications		1,000,000
Electrocatalysis of Fuel Cell Reactions		0
Device or Component Fabrication, Behavior or Testing	\$	1,104,000
Zn/NiOOH Cell Studies		250,000
Applied Research on Secondary Zn/NiOOH Battery Technology		200,000
Development of a Thin-Film Rechargeable Lithium Battery for		
Electric Vehicles		150,000
Na/SRPE Electric Vehicle Batteries		200,000
Lithium-Ion Battery Testing		200,000
Novel Concepts for an Oxygen Electrode in Secondary		,
Metal-Air Batteries		104,000
	•	505 000
Office of Alternative Fuels	\$	725,000
Materials Properties, Behavior, Characterization or Testing	\$	725,000
Cold-start Assist Materials		50,000
CNG Adsorbents Demonstration		300,000
Improved Catalyst Materials and Emissions Control Systems		375,000
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The Office of Transportation Technologies (OTT) 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 overall goal of the Materials Technology Program is to develop, in concert with the United States-based industry, an industrial technology base in cost-effective, advanced transportation-related materials and associated processing of these materials. The timely availability of these materials and processing techniques will enable the development of more energy-efficient transportation technologies capable of utilizing alternative fuels and electricity. Research and development activities focus on (a) propulsion system materials (specifically cost-effective ceramics which are critical to the development of more efficient advanced heat engines for transportation propulsion); (b) vehicle system materials (specifically lightweight materials that could aggressively reduce the weight and improve the fuel economy of vehicles without compromise to passenger comfort and safety); and (c) operation of the High Temperature Materials Laboratory.

The primary focus of the Propulsion System Materials Program is the development of reliable, cost effective ceramics to facilitate their commercial introduction in propulsion systems. After an aggressive 10-year effort that clearly demonstrated the feasibility of producing reliable engine components, the program is now focused on reducing the cost of ceramic components and improving their performance. A majority of the research is conducted by industry. The Ceramic Technology Program is managed by the Oak Ridge National Laboratory (ORNL). The DOE contact is Robert Schulz, (202) 586-8051.

The Vehicle System Materials Program is focused on the development of costeffective processing and manufacture of advanced lightweight material components that will, in the near term, continually improve the fuel economy of current production vehicles, and in the long term, allow aggressive weight reductions needed by hybrid and purely electric vehicles. Lightweight materials will be increasingly important in achieving the energy, economic, and environmental goals for the transportation sector. The DOE contact is Sidney Diamond, (202) 586-8032. The High Temperature Materials Laboratory (HTML) at the Oak Ridge National Laboratory is a state-of-the-art research and user facility which supports advanced materials research conducted by the Department of Energy, as well as by industry, universities, and other research and development laboratories. The HTML currently includes six user centers (equipped primarily for characterizing materials), namely materials analysis, high temperature mechanical properties, high temperature x-ray diffraction, physical properties, ceramic specimen preparation, and residual stress measurements. A seventh center includes instrumentation for conducting sophisticated research on machining of advanced ceramic materials with the goal of working directly with industrial teams to achieve cost effective manufacturing. The DOE contact is Debbie Haught, (202) 586-2211.

Materials Preparation, Synthesis, Deposition, Growth or Forming

47. Powder Characterization (WBS No. 1118)	<u>FY 1994</u>
	\$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

FY 1994

\$400,000

48. <u>Microwave Sintering (WBS No. 1124)</u> 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, or (5) contribute to cost effectiveness of silicon nitride materials.

46

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

Keywords: Microwave Sintering, Silicon Nitride

49.	Cost Effective Silicon Nitride Powder (WBS No. 1125)	<u>FY 1994</u>
	· · · · · · · · · · · · · · · · · · ·	\$920,000
DOF	E Contact: Robert B Schulz (202) 586-8051	

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 highquality, 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

50.Cost Effective Sintering of Silicon Nitride Ceramics (WBS No. 1127)FY 1994\$462,000\$462,000DOE 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 the densification, microstructure, and properties of silicon nitride 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. In addition, a prototype belt furnace will be designed and constructed.

Keywords: Cost Effective Ceramics, Silicon Nitride, Sintering

51. <u>Cost Effective Manufacture of Silicon Nitride Components (WBS No. 1128)Y 1994</u> \$0

DOE Contact: Robert B. Schulz, (202) 586-8051 ORNL Contact: R. L. Beatty, (615) 574-4536 Golden Technologies Contact: Jack Sibold, (303) 271-7164

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 (SRBSN) 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

52. Advanced Processing (WBS No. 1141)

<u>FY 1994</u> \$1,000

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

53. Improved Processing (WBS No. 1142)

<u>FY 1994</u> \$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. The process chosen for initial consideration is gelcasting, a process developed at ORNL.

Keywords: Powder Processing, Silicon Nitride, Gel Casting

54. Processing of Silicon Based Ceramics (WBS No. 1225)

<u>FY 1994</u> \$288,000

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 -Si₃N₄ 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

55. In-Situ Toughened Silicon Nitride (WBS No. 1226)

DOE Contact: Robert B. Schulz, (202) 586-8051 ORNL Contact: T. N. Tiegs, (615) 574-5173 AlliedSignal Ceramic Components Contact: H. C. Yeh, (213) 618-7449

The purpose of this effort is to develop compositions and processes to obtain high fracture toughness and strength for silicon nitride (Si_3N_4) -based ceramic materials through microstructure control. Under Phase I, an in situ reinforced silicon nitride material (AS800) with elongated grain microstructure was developed. The objective of this follow-on effort (Phase II) is to expand the AS800 material property database to meet the requirements for heat engine applications and to build on Phase I results to further improve material properties and processing.

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

56. Dispersion Toughened Oxide Composites (WBS No. 1231) FY 1994

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 whiskerreinforced 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

57. Low Thermal Expansion Ceramics (WBS N	<u>(0, 1243)</u> <u>FY 1994</u>
• • • • • • • • • • • • • • • • • • •	\$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 coordinate efforts regarding the application of lowexpansion ceramics in advanced heat engines. Contracts have been placed with Golden

<u>FY 1994</u> \$300,000

\$350,000

Technologies, Inc., and LoTEC, Inc., to develop cost effective processes for the fabrication of portliners. Golden is investigating Al_2TiO_5 and $Ca_{1-x}Mg_xZr_4P_6O_{24}$ (CMZP), while LoTEC is working with NZP materials $Ba_{1+x}Zr_4P_{6-2x}Si_{2x}O_{24}$ (BaZPS) and $Ca_{1-x}Sr_xZr_4P_6O_{24}$. ORNL is assisting Golden Technologies and LoTEC with the characterization and evaluation of their compositions.

Keywords: Aluminum Titanate, NZP, CMZP, Physical/Mechanical Properties, Structural Ceramics, Ultra-low Expansion

58. NZP Components (WBS No. 1245)

<u>FY 1994</u> \$541,000

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

Keywords: Structural Ceramics, Ultra-low Expansion, Zirconia

59. Low Cost Aluminum Titanate/NZP Ceramics (WBS No. 1246) FY 1994

\$247,000

DOE Contact: Robert B. Schulz, (202) 586-8051 ORNL Contact: D. P. Stinton, (615) 574-4556 Golden Technologies, Inc. Contact: D. Coors, (303) 271-7217

The objective of this work is to develop a low-thermal-conducting, high-thermalshock-resistant, ceramic portliner which can survive casting in grey iron and diesel engine operation. Golden will be developing their own aluminum titanate material and, in addition, will scale up production of a unique CMZP material developed at Virginia Polytechnic Institute and State University.

Keywords: Structural Ceramics, Ultra-Low Expansion, Aluminum Titanate, CMZP

60. Advanced Manufacturing (WBS No. 1520)

DOE Contact: Robert B. Schulz, (202) 586-8051 ORNL Contact: D. R. Johnson, (615) 576-6832 Kyocera Contact: E. Kraft, (206) 750-6147

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

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

61.	Advanced Ceramic Manufacturing (WBS No. 1521)	
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DOE Contact: Robert B. Schulz, (202) 586-8051 ORNL Contact: A. E. Pasto, (615) 574-4956 Norton Contact: Eric Bright, (203) 653-8071

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

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

<u>FY 1994</u> \$397,000

<u>FY 1994</u> \$1,779,000

62. Advanced Ceramic Manufacturing (WBS No. 1522)

<u>FY 1994</u> \$1,679,000

DOE Contact: Robert B. Schulz, (202) 586-8051 ORNL Contact: R. L. Beatty, (615) 574-4536 Golden Technologies, Inc. Contact: Jack Sibold, (303) 271-7164

The objective of this program is to develop a cost-competitive, viable manufacturing process for advanced ceramic engine components. To achieve this goal, two components, utilizing two materials, for two engine companies, were selected. Both components share simple, right-circular geometries and similar manufacturing processes. Key challenges in this program are to meet tight tolerances and yet maintain high yields required to meet cost objectives. Three major activities will occur in parallel: (1) Detroit Diesel Corporation component design/development, (2) Cummins component design/development, and (3) intelligent processing and statistical process control development/implementation.

Keywords: Components, Cost Effective Ceramics, Process Control

Materials Properties, Behavior, Characterization or Testing

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

<u>FY 1994</u> \$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

64. Advanced Statistics Calculations (WBS No. 2313)	FY 1994
	\$100,000
DOE Contact: Robert B. Schulz, (202) 586-8051	
ORNL Contact: M. K. Ferber, (615) 576-0818	
GE Contact: C. A. Johnson, (518) 387-6421	

The design and application of reliable load-bearing structural components from ceramic materials requires a detailed understanding of the statistical nature of fracture in brittle materials. The overall objective 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, confidence and tolerance bounds on predictions that use the Weibull distribution and function, strength distributions in multiaxial stress fields, and goodness-of-fit-tests for the Weibull model of strength. The studies 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

65.	Microstructural Analysis (WBS No. 3111)	<u>FY 1994</u>
		\$50,000
DOE	Contact: Robert B. Schulz, (202) 586-8051	
ORN	L 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,	Failure	Mechanism,	Structural	Ceramics,	Silicon	Carbide,	Creep,
	SiAlON, S	ilicon N	itride					

66.	Microstructural Characterization of Silicon Carbide and Silicon			
	Nitride Ceramics for Advanced Heat Engines (WBS No. 3114)	<u>FY 1994</u>		
		\$200,000		
DOT	Contacts Dahart D. Sahula (202) 596 9051			

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 Advanced Turbine Technology Applications Project (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

 67.
 Project Data Base (WBS No. 3117)
 FY 1994

 \$240,000
 \$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

68.	Fracture Behavior of Toughened Ceramics (WBS No. 3213)	FY 1994
DOE ORN	Contact: Robert B. Schulz, (202) 586-8051 L. Contact: D. R. Johnson (615) 576-6832	\$290,000
ONI	E Contact. D. R. Johnson, (013) 570-0852	

ORNL Contact: P. F. Becher, (615) 574-5157

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

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

69.	Cyclic Fatigue of Toughened Ceramics (WBS No. 3214)	<u>FY 1994</u>
DOE	Contact: Robert B. Schulz. (202) 586-8051	\$220,000
ORN	L Contact: D. R. Johnson, (615) 576-6832	
ORNI	L 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

70.	Tensile Stress Rupture Development (WBS No. 3215)	<u>FY 1994</u>
		\$300,000

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

71. Life Prediction Verification (WBS No. 3216)

<u>FY 1994</u> \$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 objective of this effort is to systematically verify life prediction methodologies appropriate for structural ceramic engine components. An emphasis will be to achieve predictability at a level acceptable to end users, in particular, those users associated with the manufacturing of internal combustion engine valves. This effort is comprised of four tasks: (1) characterization of material/mechanical performance, (2) life prediction analysis, (3) test of simulated engine valves, and (4) verification of life prediction methodology. A second objective is to complete the Rotor Database Generation program. The three central goals of that effort are: (1) hightemperature mechanical testing, (2) microstructural characterization of failure phenomena, and (3) the modeling of high temperature deformation in candidate silicon nitrides.

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

72.	Toughened Ceramics Life Prediction (WBS No. 3217)	<u>FY 1994</u>
		\$200,000

DOE Contact: Robert B. Schulz, (202) 586-8051 ORNL Contact: D. R. Johnson, (615) 576-6832 NASA - Lewis Research Center Contact: John P. Gyekenyesi, (216) 433-3210

The purpose of this research is to understand the room-temperature and hightemperature 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 hightemperature 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

73. Life Prediction Methodology (WBS No. 3222)

FY 1994

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 data base, 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,
	Nondes	tructive E	Evaluation,	Silicon Ni	itride			

74. Life Prediction Methodology (WBS No. 3223)

DOE Contact: Robert B. Schulz, (202) 586-8051 ORNL Contact: C. R. Brinkman, (615) 574-5106 AlliedSignal Engines Contact: Dave Wu, (602) 231-1206

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

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

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- FY 1994 \$600,000

75. Environmental Effects in Toughened Ceramics (WBS No. 3314) FY 1994

\$383.000

DOE Contact: Robert B. Schulz, (202) 586-8051 ORNL Contact: M. K. Ferber, (615) 576-0818 University of Dayton Contact: N. L. Hecht, (513) 229-4341

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

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

76.	High Temperature Tensile	Testing (WBS No. 3412)	<u>FY 1994</u>
			\$250,000
DOE	Contact: Dobert B. Schulz	(202) 586 8051	

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 Si₃N₄ 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 electron microscopy (TEM), and energy-dispersive spectral analysis (EDS) is an integral part of this effort.

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

77. Standard Tensile Test Development (WBS No.	3413) FY 1994
	\$125,000
DOE Contact: Robert B. Schulz, (202) 586-8051	· · · · · · · · · · · · · · · · · · ·
ORNL Contact: D. R. Johnson (615) 576-6832	

ontact: D. R. Jonnson, (013) 370 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 data base for use in the structural design of heat engines for vehicular applications.

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

78. Non-Destructive Evaluation (WBS No. 3511)

<u>FY 1994</u> \$460,000

<u>FY 1994</u> \$120,000

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. Those materials that have been seriously considered for application in advanced heat engines are all brittle materials whose fracture is affected by structural features whose dimensions are on the order of the dimensions of their microstructure. This work seeks to characterize those features using high frequency ultrasonics and radiography to detect, size, and locate critical flaws and to measure nondestructively the elastic properties of the host material.

Keywords: NDE, Radiography, Structural Ceramics, Ultrasonics

79. Computed Tomography (WBS No. 3515)

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 Advanced Turbine Technology Applications Project (ATTAP) rotors supplied by AlliedSignal Ceramic Components. AlliedSignal 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

80. <u>Nuclear Magnetic Resonance (NMR) Imaging (WBS No. 3516)</u>

FY 1994 \$80,000

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 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				-		

81.	Assessm	ent of Magnesium for Automotive Applications	<u>FY 1994</u>
			\$115,000
DOE	Contact:	Sidney Diamond, (202) 586-8032	
ANL	Contact:	Frank Stodolsky, (202) 488-2431	

An assessment is being performed at ANL to determine the feasibility and technical potential of using magnesium alloys in automotive structural and sheet applications in efforts to enhance the lightweighting and energy efficiency of conventional and advanced passenger vehicles. Magnesium alloys will be identified that have promise to meet vehicle performance requirements such as stiffness, crush behavior, corrosion resistance, fatigue resistance, flammability, and explosiveness. The ability of magnesium to respond to various forming methods will also be assessed and production cost barriers will be identified.

Keywords: Magnesium Alloys, Forming, Structural and Sheet Applications

Technology Transfer and Management Coordination

82. Management and Coordination (WBS No. 111)

FY 1994 \$950.000

<u>FY 1994</u> \$150.000

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

83. <u>International Exchange Agreement (IEA) (WBS No. 4115)</u>	<u>FY 1994</u>
	\$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 purpose of this effort is to organize, assist, and facilitate international research cooperation on the characterization of advanced structural ceramic materials. A major objective of this research is the evolution of voluntary measurement standards for determining mechanical, physical, and structural properties for these materials. Participants in Annex II are the United States, Germany, Sweden, and Japan.

Keywords: IEA, Powder Characterization, Mechanical Properties

84.	Standard Reference	Materials	(WBS No. 4116)	
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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.

Keywords: IEA, Reference Material, Powder Characterization

85. Mechanical Property Standardization (WBS No. 4121)

<u>FY 1994</u> \$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 mechanical test standards in support of the Ceramic Technology Project and the Advanced Turbine Technology Applications Program.

Keywords: Mechanical Properties, Test Procedures

Device or Component Fabrication, Behavior or Testing

86. <u>Advanced Coating Technology (WBS No. 1311)</u>

<u>FY 1994</u> \$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

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

Keywords: Coatings, Chemical Vapor Deposition, Engines, Silicon Carbide, Silicon Nitride, Structural Ceramics, Corrosion 87. <u>Coatings to Reduce Contact Stress Damage of Ceramics (WBS No. 1313) FY 1994</u> \$28,000

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. Current work involves the CVD deposition of multilayered Al_2O_3/SiO_2 coatings on SiC and Si_3N_4 to form mullite.

Keywords:	Adherence,	Coatings,	Mullite,	CVD,	Oxidation,	Modeling,	Corrosion
-	Resistance,	Structural C	Ceramics				

88. Wear Resistant Coatings (WBS No. 1331)

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

89. <u>Wear Resistant Coatings (WBS No. 1332)</u>

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:

<u>FY 1994</u> \$0

<u>FY 1994</u> \$46,000

- low wear as measured in laboratory rig tests which simulate the piston ringcylinder liner environment near the top ring reversal in a heavy duty diesel engine
- lower friction coefficients than for the conventional system under all test conditions
- high adherence and compatibility with substrate materials
- good thermal shock resistance
- high uniformity and reproducibility
- Keywords: Adherence, Coatings, Engines, Friction, Metals, Structural Ceramics, Thermal Conductivity, Wear

90. <u>Thick Thermal Barrier Coating Systems for Low Heat Rejection</u> <u>Diesel Engines (WBS No. 1342)</u>

<u>FY 1994</u> \$0

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

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

<u>FY 1994</u> \$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 current emphasis is on studying the brazing characteristics of silicon nitride and silicon carbide. The techniques of direct brazing as well as vapor coating ceramics to circumvent wetting problems are being applied
to these materials. Work includes continuing the study of both the high temperature brazing of silicon nitride and the mechanical behavior of braze joints. The work will encompass further evaluation and application of an analysis package and approach developed specifically for silicon nitride-to-metal braze joints, and evaluating nonmetallic bonding materials for joining silicon nitride.

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

92. Surface Durability of Machined Ceramics (WBS No. 1500)

FY 1994 \$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. This effort is conducted by industry, other national laboratories, and in-house at ORNL. The ORNL research concerns two technical areas: (1) investigating the effects of machining practices on the durability of ceramics for valve and valve-set applications, (2) understanding and characterizing the detailed nature of machining-induced surface and subsurface damage and their evolution in advanced ceramic materials using a range of analytical tools.

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

JJ. <u>INCAL-</u>	Ovingiation Offi	iung wheel	TWDS NO. 1	<u>.501)</u>	<u>r i 1994</u>
		·			\$0

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 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

Office of Transportation Technologies

94. Grindability Test (WBS No. 1502)

<u>FY 1994</u> \$0

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 program is to develop a cost-effective method to determine the grindability of ceramics leading to cost-effective methods for machining those materials. Phase I efforts will be directed towards a review of literature related to ceramic grinding, development of a variable definition of grindability, design of grindability test experiments, and design of a ceramics grindability test system. The grindability study underway also includes establishment of correlation between the grindability number and conventional grinding practices.

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

95.	Chemically Assisted Grinding of Ceramics (WBS No. 1503)	<u>FY 1994</u>
		\$150,000
DOE	E Contact: Robert B. Schulz, (202) 586-8051	

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 materials such as SiAlON and SiC may be examined for comparison.

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

96. Grinding Consortium (WBS No. 1503)

<u>FY 1994</u> \$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 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

97. High Speed Grinding (WBS No. 1504)

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

70. Lasel-Daseu INDE Methous (WDS NO. 130/	98.	Laser-Based	NDE Me	thods (WBS	No. 1507
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DOE Contact: Robert B. Schulz, (202) 586-8051 ORNL Contact: D. R. Johnson, (615) 576-6832 Argonne National Lab Contact: J. S. Steckenrider, (708) 252-5169

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

Keywords: Machining, Nondestructive Evaluation, Structural Ceramics

99.	Development of "Smart" Grinding Wheel (WBS No. 1510)	<u>FY 1994</u>
		\$50,000
DOE (Contact: Robert B. Schulz, (202) 586-8051	
ORNL	Contact: D. R. Johnson, (615) 576-6832	

Industry Contact: TBD

The objective of this new effort is to produce a commercially viable, "smart grindingwheel" system which is suitable for both grinding research and production use. This project

<u>FY 1994</u> \$372,000

<u>FY 1994</u> \$180,000 will be comprised of three tasks: (1) producing a grinding-wheel design which incorporates sensors and the means to transmit key process parameters to a computer, (2) construction of a prototype grinding-wheel system to be tested on a full-size commercial cylindrical grinder and, finally (3) demonstration of the prototype system. Acquisition cost for commercial versions of the smart-wheel system, truing and dressing practices, and handling and calibration shall also be addressed.

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

100. Automotive Materials Development

FY 1994 \$3,000,000

DOE Contact: Sidney Diamond, (202) 586-8032 ORNL Contact: Philip S. Sklad, (615) 574-5069

This major activity in the Lightweight Materials Program is a collaborative effort between the US Automotive Materials Partnership (USAMP) and the DOE. Development of cost-effective lightweight materials and the processes needed to form or manufacture them reliably and competitively in the required quantities and production rates are addressed through focused research conducted by technical teams. The teams are selected by the technical representatives from Ford Motor Company, Chrysler Corporation, and General Motors Corporation to USAMP from among DOE's National Laboratories, suppliers to the automobile companies, private research organizations, and members of academia. Current topics of interest include advanced metal forming technology, adhesive bonding of polymers and dissimilar materials, metal matrix composites, rapid prototyping, and the utilization of modeling and simulation for optimizing materials and processes. Elements of the projects are being performed at INEL, LANL, ORNL, PNL, SNL, and the University of Texas.

Keywords: Advanced Metal Forming, Metal Matrix Composites, Rapid Prototyping, Adhesive Bonding

101.	<u>Ultracap</u>	acitors for Electric and Hybrid Vehicles
DOE	Contact:	Sidney Diamond, (202) 586 8032 Pat Davis (202) 586 8061
LLNI	Contact:	Dennis O'Brien, (510) 422-5593

The purpose of the present work is to develop deposition techniques for dielectric and conductor films that can ultimately be used in nanostructured multilayer capacitor panels. In the current work being carried out at the LLNL, it is intended that films will be first developed, deposited, and characterized and that then an effort will be made to

FY 1994 \$75,000 synthesize a simple prototype capacitor. The Electric and Hybrid Propulsion Division of OTT has the project lead for this activity. The Office of Transportation Materials is providing partial funding of this work based on the possibility of substantially reducing the weight of electric and hybrid vehicles through the development of small, highly efficient energy storage devices.

Keywords: Nanophase Materials, Ultracapacitors

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 programs: (1) Light Duty Engine Technologies Program focused on Turbine Engine Technologies and Advanced Automotive Piston Engine Technologies; and (2) Heavy Duty Engine Technologies Program focused on Advanced Diesel Engine Technology. Materials activities supported by the Advanced Propulsion Division 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) 586-8012 for Turbine Engine Technologies; Patrick Sutton, (202) 586-8058 for Advanced Automotive Piston Engine Technologies; and John Fairbanks, (202) 586-8066 for Advanced Diesel Engine Technologies.

Materials Properties, Behavior, Characterization or Testing

102. Advanced Turbine Supporting Research and Technology

<u>FY 1994</u> \$250,000

DOE Contact: Thomas Sebestyen, (202) 586-8012 NASA Contact: Thomas Strom, (216) 433-3408

The objective of this program is to evaluate commercially available structural and glass ceramic material specimens exposed to combustion products at temperatures up to 2500°F for periods up to 3,500 hours. Activities include development of design codes for structural component evaluation; research on non-destructive evaluation of ceramic

components to improve reliability; and examination of the effects of corrosive sea salts and other adverse environments on the durability of ceramics.

Keywords: Structural Ceramics, Non-Destructive Evaluation, Silicon Carbide, Silicon Nitride, Gas Turbine Engines

Device or Component Fabrication. Behavior or Testing

103. Hybrid Vehicle Turbine Engine (HVTE) Technology SupportFY 1994\$3,725,000

DOE Contact: Thomas Sebestyen, (202) 586-8012 NASA Contact: Paul Kerwin, (216) 433-3409 Allison Engine Company Contact: Steve Berenyi, (317) 230-6971

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

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

104. <u>Ceramic Turbine (CT) Engine Demonstration Project</u>	<u>FY 1994</u>
	\$2,873,000
DOE Contact: Thomas Sebestyen, (202) 586-8012	
NASA Contact: Thomas Strom, (216) 433-3408	
AlliedSignal Engine Contact: Jay Smyth, (602) 231-4306	

, This project will provide early ceramic turbine field experience by demonstrating the reliability and durability of ceramic components in actual engine application. In support of gas turbine auxiliary power unit (APU) development for the DOE Hybrid Vehicle Program, AlliedSignal began introducing ceramic first stage turbine nozzles and blades into its proven (all-metal) GTCP 331-200 gas turbine APU engine. Laboratory and field testing is continuing to address remaining critical design and production concerns related to structural ceramics in gas turbine engines. In addition, efforts are intensified to scale-up and

demonstrate commercial engine ceramic component manufacturing in coordination with ceramic suppliers and the Propulsion System Materials element of DOE's Materials Technology Program.

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

105. Advanced Diesel Engine Component Development Project

<u>FY 1994</u> \$250,000

DOE Contact: John W. Fairbanks, (202) 586-8066 NASA Contact: J. C. Wood, (216) 433-3419 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

106.	Advanced Piston and C	Vlinder Component	Development	<u>FY 1994</u>

\$300,000

DOE Contact: John W. Fairbanks, (202) 586-8066 NASA Contact: J. C. Wood, (216) 433-3419 Caterpillar Inc. Contact: G. L. Waltz, (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. Zirconia coatings are being used on piston crowns and composite pistons are being tested.

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

107. Advanced Piston and Cylinder Component Development

<u>FY 1994</u> \$600,000

DOE Contact: John W. Fairbanks, (202) 586-8066 NASA Contact: M. J. Valco, (216) 433-3717 Cummins Engine Contact: T. Yonushonis, (812) 377-7078

The objective of the project is to develop advanced technology diesel engine components and integrate these into a test bed engine to demonstrate reduced emissions and improved fuel economy. Advanced ceramic and metallic materials are being investigated and used in structural, insulative and tribological component applications. Castin-place titanium nitride exhaust port liners are emerging with improved reliability. Several powder metallurgy parts are being tested and mullite coatings are being used on piston crowns.

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

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 Program Manager is Kenneth Heitner, (202) 586-2341 for Battery Development; Robert Kost, (202) 586-2334 for Fuel Cells Development; and Albert Landgrebe, (202) 586-2480 for Exploratory Research in support of Batteries and Fuel Cells.

Materials Preparation, Synthesis, Deposition, Growth or Forming

108.Electrochemical Properties of Solid-State Sodium Polymer CellsFY 1994\$260,000\$260,000

DOE Contact: JoAnn Milliken, (202) 586-2480 Lawrence Berkeley Laboratory Contact: L. C. De Jonghe, (510) 486-4881

The objective of this project is to investigate the viability of all-solid-state cells based on Na or Na alloy negative electrodes, polymeric electrolytes, and metal oxide positive electrodes. Emphasis is placed on developing a suitable cathode material not only in terms of performance but also in terms of cost and environmental impact. The approach is to synthesize and characterize manganese oxides for use as a cathode in Na/polymer cells and employ AC and DC techniques (e.g., galvanostatic charging and discharging, four probe techniques, and pulse testing) to characterize solid state batteries, as well as the properties of the individual components and interfaces. Results have shown that Na_{0.44}MnO₂ cathodes in a Na/polymer cell can insert 0.55Na/Mn over a voltage range of 3.4-2.0 V at 0.1 mA/cm², corresponding to a capacity of 160 mAh/g, a theoretical specific energy of 440 Wh/kg and a theoretical energy density of 1450 Wh/L. Future effort will focus on the synthesis, characterization and testing of manganese oxides with large tunnels to accommodate Na ions, measurement of transport properties in Na/polymer cells, and Na/polymer cell testing to optimize its performance.

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

109.Corrosion Resistant Coatings for High Temperature High-Sulfur-ActivityFY 1994Applications\$0

DOE Contact: JoAnn Milliken, (202) 586-2480 Illinois Institute of Technology Contact: J. R. Selman, (312) 567-6914

The objective of this research is to develop corrosion-resistant coatings for cell components that are exposed to high-sulfur-activity environments in Na/S and Li/FeS₂ cells. This research is intended to assist in developing the technology for the production of Mo and molybdenum carbide coatings. Such coatings can be utilized to produce low-cost containers and current collector materials in non-aqueous, alkali/sulfur, and other moltensalt cells. Plasma-enhanced chemical vapor deposition (CVD) was employed as the new technique for the preparation of thin protective films at much lower temperatures than by thermally driven CVD. Theoretical studies were conducted to understand the deposition process. Results to date have shown that the evaporation and deposition rate are correlated with the equilibrium pressure of $Mo(CO)_6$ and other process variables. This project has been completed.

Keywords: Corrosion, Plasma-Enhanced CVD, Kinetic-Gas Theory

110.	Improved Container Electrode Coatings for Sodium/Sulfur	
	Battery Systems	<u>FY 1994</u>
		\$100,000
DOE	Contact: JoAnn Milliken. (202) 586-2480	

Environmental Research Institute of Michigan Contact: T. K. Hunt, (313) 667-2113

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

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

111.The Performance of New Materials for Polymer Electrolyte BatteriesFY 1994\$140,000

DOE Contact: JoAnn Milliken, (202) 586-2480 Northwestern University Contact: D. F. Shriver, (708) 491-5655

The objective of this project is to synthesize polymer electrolytes based on aluminosilicate-polyether hybrid polyelectrolyte with improved low-temperature performance and high cation transport number. These polymer electrolytes should be useful in rechargeable Li/polymer batteries. Initial efforts have focused on cell testing with simple polymer-salt electrolytes. This includes cycling with a cathode consisting of 85% Li_xMnO_2 , 10% carbon, 5% binder, and a Li-metal anode. The data from these cells will provide a baseline for comparison with more advanced polyelectrolytes such as aluminosilicate-polyether hybrid polyelectrolyte.

Keywords: Polymer Electrolytes, Electrochemical Cells

112.	Novel Polymer Electrolytes for Recha	argeable Lithium Batteries	<u>FY 1994</u>
			· · · ·

\$160,000

DOE Contact: JoAnn Milliken, (202) 586-2480 Case Western University Contact: M. Litt, (216) 368-4174

The objective of this research is to develop advanced polymeric electrolytes for rechargeable Li batteries. Thin polymeric films will be cast and characterized by spectroscopic, nuclear magnetic resonance, thermal and electrochemical techniques. Two types of polymer materials are under investigation sulfonated and phosphonated polybenzimidazole polymers, and novel poly (4,5-dimethyleneimidazole and hydroxy imidazole) polymers. Currently, efforts are focused on preparing the polymer electrolytes. Once the electrolytes have been synthesized and evaluated electrochemically, efforts will be expanded to include sulfonated PEEK, sulfonated and phosphonated PPE and soluble polyphenylenes.

Keywords: Polymeric Electrolytes, Li Batteries

Office of Transportation Technologies

Novel Solid Polymer Electrolytes for Advanced Secondary Batteries FY 1994

\$130,000

FY 1994 \$130,000

DOE Contact: JoAnn Milliken, (202) 586-2480 University of Dayton Contact: D. G. Glasgow, (513) 229-2517

The objective of this research program is to synthesize and characterize new polymer electrolytes that contain crown ethers which could improve the Li-ion transport. The systems proposed are doped polymers with side chains having the ability to form liquid crystalline mesophases. Synthesis of the three polymers required for this program has been initiated. Future efforts will focus on completing synthesis of polymer electrolytes and characterization of the polymers with respect to ionic conductivity, dimensional stability, and interfacial stability.

Keywords: Polymeric Electrolytes, Li Batteries, Ion Transport

114.	Sol-Gel	Electroly	rtes in Li	<u>thium l</u>	<u>Batteries</u>		
DOF	Comto atr		A:11:1-0-	(202) 6	06 0400		

DOE Contact: JoAnn Milliken, (202) 586-2480 Rutgers University Contact: L. C. Klein, (908) 932-2096

The objective of this research project is to optimize the synthesis of polymer electrolytes by sol-gel processing of alkali/silicate components, which involves combining the components in liquid form prior to chemically reacting the solution with water to form a gel. These materials should produce solid electrolyte compositions that can be applied directly to electrode materials for rechargeable Li batteries. The approach used in this investigation is to select oxide components that are Li-ion conductors and are thermodynamically stable. Calculations will be conducted to determine the thermodynamic stability of the various oxide materials. Compositions that are predicted to have increased stability will be selected from this analysis and prepared for evaluation.

Keywords: Sol-Gel Electrolytes, Li Batteries, Polymer Electrolytes

115. New Cathode Materials FY 1994 \$110,000

DOE Contact: JoAnn Milliken, (202) 586-2480 State University of New York Contact: M. S. Whittingham, (607) 777-4623

The objective of this project is to synthesize and evaluate oxides of tungsten, molybdenum, and first-row transition metals for alkali-metal intercalation electrodes which are useful as positive electrodes in advanced nonaqueous rechargeable batteries. Mild hydrothermal techniques will be used for the synthesis of molybdenum oxides, or, in cases where the hydrothermal technique does not lead to compounds with the highest oxidation state, electrochemical oxidation from an aqueous alkaline solution will be used to drive the cations to their highest oxidation state. Once completed, research will be expanded to synthesize and test vanadium and manganese oxides.

Keywords: Intercalation Electrodes, Rechargeable Batteries

116. <u>Development of High Energy Density Cathodes for Sodium/Polymer CellsFY 1994</u> \$170,000 DOE Contact: JoAnn Milliken, (202) 586-2480

SRI International Contact: S. Smedley, (415) 859-6173

The major objective of this research is to develop high-performance organic polydisulfide positive electrodes for use in low-temperature (ambient to 100°C) Na/polymer cells. This will be achieved by the synthesis and characterization of hexathiobenzene-based compounds and their derivatives for positive electrodes. Specific parameters under investigation include the nature of any heteroatoms or side chains added to the base polymer, the structure of the polymer, the cathode thickness, the voltage stability window of the cathode, the degree of loading of the positive electrode material, the electrode construction technique, and the operating temperature of the cell. Electrodes will be judged on the basis of capacity density, energy density, discharged rate capability, and cyclability. Current efforts are concentrated on synthesis of electrode materials and on cell design and electrode construction techniques.

Keywords: Cathodes, Na/polymer Cells, Electrochemical Analysis

Materials Properties. Behavior, Characterization or Testing

117.	Surface Morphology of Metals in Electrodeposition/	
	Carbon Electrochemistry	FY 1994
		\$240,000
DOE	Contact: JoAnn Milliken, (202) 586-2480	
Lawre	nce Berkeley Laboratory Contact: K. Kinoshita and C. Tobias, (510) 486-	4260

The objective of this project is to develop a pragmatic understanding of the component processes and their interactions in the macrocrystallization of metals necessary for the design and optimization of rechargeable galvanic cells. This project involves investigation of: (1) the role of electric field and solution-side mass transport in the electrocrystallization of metals, mechanisms of initiation, growth and propagation of imperfections, and development of surface textures; (2) the characterization of gases at electrodes with emphasis on their effect on ohmic resistance and mass transfer; and (3) the role of physicochemical properties of carbonaceous materials on their ability to reversibly intercalate Li. Results have shown that a hemispherical protrusion as small as 50 micron radius can be attached to the surface of a micromosaic electrode. In addition a

mathematical model has been completed to understand the hydrodynamics of flow over protrusions. Future efforts will extend the numerical modeling to study mass transport for flows in a turbulent region and evaluate the dynamics of bubble phenomena in electrolytic gas evolution.

Keywords: Macrocrystallization of Metals, Galvanic Cells, Li Batteries

118.	Battery Materials Structure and Characterization	<u>FY 1994</u>
		\$100,000

DOE Contact: JoAnn Milliken, (202) 586-2480 Brookhaven National Laboratory Contact: J. McBreen, (516) 282-4071

The objective of this research is to elucidate the molecular aspects of materials and electrode processes in batteries and to use this information to develop electrode and electrolyte structures with good performance and long life. Current efforts have included *in situ* extended x-ray absorption fine structure (EXAFS) studies of Bi-doped manganese oxides and *ex situ* studies of lithium manganese oxides and nickel oxide electrodes that were cycled in Zn/NiOOH cells. Results have shown that doping of manganese oxides with Group VIB metal oxides improved the rate capabilities of the electrode in an electrolyte consisting of LiClO₄/PC-DME. Future efforts will focus on EXAFS studies of additives in nickel oxide and zinc electrodes as well as studies of molybdenum and tungsten oxide electrodes.

Keywords: Electrodes, Batteries, EXAFS

119. <u>In Situ Spectroscopic Applications to the Study of Rechargeable</u> <u>Lithium Batteries</u>

<u>FY 1994</u> \$135,000

DOE Contact: JoAnn Milliken, (202) 586-2480 Case Western Reserve University Contact: D. A. Scherson, (216) 368-5186

The purpose of this project is to use *in situ* spectroscopic techniques to investigate the electrochemical phenomena that occur at Li/electrolyte interfaces during charge/discharge cycling. Two cell technologies are being investigated Li/polymer electrolyte and Li/FeS₂. The approach is to conduct experimental studies under ultrahigh vacuum conditions to examine the reactivity of Li at the Li/polymer and Li/liquid electrolyte interfaces. To date, temperature programmed desorption studies have shown that ultra-clean Li exposed to PC produces alkyl carbonate and lithium hydride and Fourier Transform Infrared Spectroscopy (FTIR) indicates that no reaction occurs at the Li/PEO interface. Efforts will continue to investigate the interfacial reactions at the Li/electrolyte interfaces and develop a high-vacuum environmental chamber to conduct ATR/FTIR measurements of the Li/polymer interface.

Keywords: Spectrographic Analysis, Electrochemical Phenomena, Electrolytes

120. <u>Polymer Electrolyte for Ambient Temperature Traction Batteries:</u> <u>Molecular Level Modeling for Conductivity Optimization</u>

<u>FY 1994</u> \$160,000

DOE Contact: JoAnn Milliken, (202) 586-2480 Northwestern University Contact: M. A. Ratner, (708) 491-5371

The goal of this research is to apply molecular dynamics and Monte Carlo simulations to understand the conduction process in polymer electrolytes, and its modification by such parameters as temperature, density, ion species, polymer chain basicity, and interionic correlations. The results of this study should be beneficial in the development of improved polymer electrolytes for rechargeable Li batteries for electric vehicle applications.

Keywords: Batteries, Electric Vehicles, Polymeric Electrolytes

121. Analysis and Simulation of Electrochemical Systems

<u>FY 1994</u> \$240,000

DOE Contact: JoAnn Milliken, (202) 586-2480 University of California, Berkeley Contact: J. Newman, (510) 642-4063

The objective of this program is to improve the performance of electrochemical cells used in the interconversion of electrical energy and chemical energy by identifying the phenomena which control the performance of a system. These phenomena are incorporated into a mathematical model which can predict system behavior. The models aid in the recognition of important parameters that are crucial to the optimization of a given electrochemical system. Computer techniques with electrochemical engineering principles permit the calculation of complex interactions without gross mathematical and physical approximations. Results have identified the physical process taking place in the galvanostatic charge and discharge of a Li/polymer/insertion cell. In addition, a mathematical model has been developed that elucidates the dynamic changes in the secondary cell. Future efforts will continue to focus on modeling the behavior of electrochemical capacitors and metal hydride cells.

Keywords: Electrochemical Phenomena, Galvanostatic Charge/Discharge

122. Heat Transport and Thermal Management in Advanced Batteries

<u>FY 1994</u> \$160,000

DOE Contact: JoAnn Milliken, (202) 586-2480 University of California, Berkeley Contact: J. W. Evans, (510) 642-3807

This project was initiated in FY 1994 to investigate, by mathematical modeling and experimental measurement, heat generation and transport in advanced secondary batteries for EV applications. The objectives of this project are to evaluate the management of the temperature of the battery for optimum performance and avoiding temperature excursions damaging to the battery. Initial investigations will focus on Li/polymer batteries that are under development to operate in the temperature range of approximately 60 to 140°C which is required to obtain sufficient polymer conductivity and to avoid overheating.

Keywords: Thermal Modeling, Advanced Batteries

123.	Electrode	e Surface Layers	<u>FY 1994</u>
			\$125,000
DOE	Contact:	JoAnn Milliken, (202) 586-2480	

Lawrence Berkeley Laboratory Contact: F. R. McLarnon, (510) 486-4260

Advanced *in situ* and *ex situ* characterization techniques are being used to study the structure, composition, and mode of formation of surface layers on electrodes used in rechargeable batteries. The objective of this research is to identify film properties that improve the rechargeability, cycle-life performance, specific power, specific energy, stability, and energy efficiency of electrochemical cells. Sensitive techniques such as ellipsometry, light scattering, Raman spectroscopy and scanning electron microscopy will be utilized to monitor the formation of surface layers on secondary battery electrodes. In addition, foreign ions will be incorporated in porous nickel electrodes to improve the cycle performance in an alkaline electrolyte.

Keywords: Ion Implantation, Electrodes, Rechargeable Batteries

124.	Electrode	Kinetics	and	Electrocatalysis

<u>FY 1994</u> \$100,000

DOE Contact: JoAnn Milliken, (202) 586-2480 Lawrence Berkeley Laboratory Contact: P. N. Ross, Jr., (510) 486-6226

Physically meaningful mechanistic models are essential for the interpretation of electrode behavior and are useful in directing the research on new classes of materials for electrochemical energy conversion and storage devices. The objective of this project is to develop an atomic-level understanding of the processes taking place in complex electrochemical reactions at electrode surfaces. Researchers are employing LEED to study

single crystals; HREM for carbon electrode materials; and EXAFS for organometallic catalysts. LEIS and AES are being utilized to study the composition of sputtered and UHV-annealed polycrystalline Pt-Ru bulk alloys for methanol electrocatalysis. Future efforts will consider methanol electrocatality on Pt-Ru electrocatalyst particles.

Keywords: Spectrographic Analysis, Electrocatalysts, Electrooxidation

125. Effect of Electrocatalyst and Electrolyte Composition on Methanol/Air Fuel Cell Performance FY 1994 \$215,000

DOE Contact: JoAnn Milliken, (202) 586-2480 Lawrence Berkeley Laboratory Contact: E. J. Cairns and P. N. Ross, (510) 486-6226

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

Keywords: Electrooxidation, Fuel Cells

126. <u>Poisoning of Fuel Cell Electrocatalyst Surfaces: NMR Spectroscopic</u> <u>Studies</u>

<u>FY 1994</u> \$200,000

DOE Contact: JoAnn Milliken, (202) 586-2480 Lawrence Berkeley Laboratory Contact: E. J. Cairns, (510) 486-5028

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

Keywords: NMR, Electrooxidation, Fuel Cells

127. Fuel Cells for Renewable Applications

FY 1994 1,000,000

DOE Contact: JoAnn Milliken, (202) 586-2480 Los Alamos National Laboratory Contact: S. Gottesfeld, (505) 667-0853

The primary focus of this program is to develop efficient and cost-effective polymer electrolyte fuel cells (PEFC) for transportation applications. The specific goals of the program are to: (1) reduce the cost of the Pt catalyst and ionomeric membrane, (2) increase the efficiency and power density of the PEFC, (3) optimize the system for operation on reformed organic fuels and air, (4) achieve stable, efficient, long-term operation, and (5) solve key technical issues that impede the development of the DMFC. Two patents have been awarded describing the developments in membrane catalyst layers for fuel cells and the use of the thermoplastic (TBA+) form of the ionomer. Efforts will continue to focus on improving the performance and life of PEM fuel cells and identifying new low-cost components for these fuel cells.

Keywords: Fuel Cells, Proton Exchange Membranes, Methanol Oxidation

128. <u>Electrocatalysis of Fuel Cell Reactions</u>	<u>FY 1994</u>
	\$0
DOE Contact: JoAnn Milliken, (202) 586-2480	
Brookhaven National Laboratory Contact: J. McBreen, (516) 282-4513	

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

Keywords: Fuel Cells, Electrocatalysts, X-Ray Absorption

Device or Component Fabrication, Behavior or Testing

129. Zn/NiOOH Cell Studies

DOE Contact: JoAnn Milliken, (202) 586-2480 Lawrence Berkeley Laboratory Contact: E. Cairns and F. McLarnon, (510) 486-4260

The purpose of this project is to investigate the behavior of Zn electrodes in alkaline Zn/NiOOH cells to improve their lifetime and performance. Zn/NiOOH batteries would provide superior performance and lower life-cycle costs compared to Cd/NiOOH and MH/NiOOH batteries. The approach of this project is to determine the performance and cycle life of alkaline Zn/NiOOH cells using realistic cell components and operating conditions as well as utilize analytical instruments such as X-ray diffraction analysis and XAS to understand changes to cell components resulting from charge/discharge cycling. X-ray photoelectron spectroscopy results have shown that the NiOOH electrode in the Zn/KOH/NiOOH cells do not chemically react with the Zn species under cycling conditions with a KOH-KF-K₂CO₃ electrolyte. Future efforts will focus on: (1) evaluating lightweight low-cost NiOOH electrodes in model Zn/NiOOH cells, (2) evaluating novel separator and wick materials that may provide better wetting characteristics, and (3) establishing a CRADA with Energy Research Corporation to further technology transfer.

Keywords: Electrodes, Batteries, Electric Vehicles

130. Applied Research on Secondary Zn/NiOOH Battery Technology FY 1994

\$200,000

DOE Contact: JoAnn Milliken, (202) 586-2480 Acme Electric Corporation Contact: M. Anderman, (602) 921-0470

The objectives of this project are to evaluate the Lawrence Berkeley Laboratory (LBL) electrolyte composition for extending the cycle life of Zn/NiOOH cells, and to develop these cells for EV applications. Cells containing the LBL electrolyte were fabricated and results have shown that 175 charge/discharge cycles were completed. A visual examination of the electrodes showed a drastic improvement (reduction) in electrode shape change compared to the electrodes cycled in the standard, highly-alkaline electrolyte. Future efforts will be aimed at achieving comparable performance with 20-Ah cells to that obtained by LBL.

Keywords: Electrodes, Batteries, Electric Vehicles

<u>FY 1994</u> \$250,000

131. <u>Development of a Thin-Film Rechargeable Lithium Battery for</u> <u>Electric Vehicles</u>

FY 1994 \$150,000

DOE Contact: JoAnn Milliken, (202) 586-2480 Oak Ridge National Laboratory Contact: J. B. Bates (615) 574-4143

The objective of this research is to identify methods for depositing acceptable thinfilm electrodes for rechargeable Li batteries. These methods are being applied to develop solid-state Li/Li_xMn₂O₄ rechargeable thin-film Li batteries for electric vehicle applications. The batteries are expected to have several important advantages as power sources high specific energy and energy density, long cycle lifetimes, and a wide temperature range of operation. Accomplishments have included fabrication of Li/Li_x/Mn₂O₄ cells in which the cathode was deposited at temperatures below 150°C by rf magnetron sputtering and fabrication of thin-film cells capable of sustaining current densities of several mA/cm², having a specific power of 30 W/g at an 85 C discharge rate. Efforts will focus on improving the performance of Li_xMn₂O₄ cathode films deposited at low temperatures and investigate the performance of a hybrid solid-state Li-Li_xMn₂O₄ cell.

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

132. Na/SRPE Electric Vehicle Batteries

DOE Contact: JoAnn Milliken, (202) 586-2480 PolyPlus Battery Company Contact: May-Ying Chu (510) 841-4313

The purpose of this project is to demonstrate the cycling capability of cells containing Na negative and organosulfur-based positive electrodes, and develop a low-cost highperformance Na/polymer cell that utilizes an organosulfur-based positive electrode. The proposed batteries will be mechanically sturdy, have a reliable electrical performance, operate between 50 and 80°C, and are expected to be immune to thermal cycling. To date, approximately 80 laboratory Na/solid redox polymerization electrode (SRPE) cells have been constructed and testing has been initiated. Future efforts will include formulating a low-cost cell design and demonstrating the performance scaling of cells to 10 times larger than current test cells.

Keywords: Electrodes, Batteries, Electric Vehicles

FY 1994 \$200,000

133. Lithium-Ion Battery Testing

<u>FY 1994</u> \$200,000

DOE Contact: JoAnn Milliken, (202) 586-2480 Lawrence Livermore National Laboratory Contact: S. Mayer, (510) 423-4897

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

Keywords: Li Batteries, Dynamic Stress Testing

134. <u>Novel Concepts for an Oxygen Electrode in Secondary</u> <u>Metal-Air Batteries</u>

<u>FY 1994</u> \$104,000

DOE Contact: JoAnn Milliken, (202) 586-2480 Eltech Research Corporation Contact: E.J. Rudd, (216) 357-4073

The objective of this research is to develop improved bifunctional air electrodes for electrically rechargeable Zn/air cells. The successful development of bifunctional air electrodes depends on selecting electrochemically stable support materials and electrocatalysts for O_2 reduction and evolution, and the fabrication of suitable porous structures that are capable of extended operation. In this program, the properties of corrosion-resistant substrates such as semi-graphitic carbon, graphite or non-carbon materials were investigated. Results show that electrodes with a graphitized acetylene black for the support and NiCo₂O₄ and either CoTMPP or La_{0.6}Ca_{0.4}CoO₃ as electrocatalysts have operated for over 100 cycles in 35% KOH at room temperature.

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

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 biofuels is John Ferrell, (202) 586-6745, and the DOE contacts for alternative fuels are John Russell, Richard Wares, or Steve Goguen, (202) 586-8053.

Materials Properties. Behavior. Characterization or Testing

135. **Cold-start Assist Materials**

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

136. CNG Adsorbents Demonstration

DOE Contact: M. Gurevich, (202) 586-8053 BNL Contact: J. Wegrzyn, (516) 282-7917

This project screens and evaluates materials for their effectiveness in adsorbing natural gas. An adsorbent placed in a storage vessel could hold sufficient compressed natural gas (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

Improved Catalyst Materials and Emissions Control Systems 137. FY 1994

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

This project is being conducted in a CRADA between AC Delco and Oak Ridge National Laboratory. The focus of the effort is to determine deactivation mechanisms in catalysts and thereby propose improvements in materials that will extend catalyst life. The project is co-funded by other DOE offices. Relationships between catalyst microstructure, bench tests, and engine test cell results are being developed.

Keywords: Alternative Fuels, Catalyst, Catalyst Performance

FY 1994 \$50,000

FY 1994

\$300,000

\$375,000

OFFICE OF UTILITY TECHNOLOGIES

	E	<u>Y 1994</u>
Office of Utility Technologies - Grand Total	\$3 2	1,454,000
Office of Solar Energy Conversion	\$18	8,100,000
Photovoltaic Energy Technology Division	\$18	8,100,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	\$13	3,200,000
Amorphous Silicon for Solar Cells Polycrystalline Thin Film Materials for Solar Cells Deposition of III-V Semiconductors for High-Efficiency		4,500,000 7,500,000
Solar Cells	1	1,200,000
Materials Properties, Behavior, Characterization or Testing	\$ 2	2,500,000
Materials and Device Characterization	2	2,500,000
Device or Component Fabrication, Behavior or Testing	\$ 2	2,400,000
High-Efficiency Crystal Silicon Solar Cells	2	2,400,000
Office of Renewable Energy Conversion	\$	600,000
Geothermal Division (GD)	\$	600,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	\$	90,000
Thermally Conductive Composites for Heat Exchangers		90,000
Materials Properties, Behavior, Characterization or Testing	\$	510,000
Advanced High Temperature Geothermal Well Cements Advanced High Temperature Chemical Systems for		390,000
for Lost Circulation Control		20,000
Contosion Mitigation in Highly Acidic Steam Condensates		100,000

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OFFICE OF UTILITY TECHNOLOGIES

	F	<u>Y 1994</u>
Office of Energy Management	\$12	2,754,000
Advanced Utility Concepts Division	\$ 12	2,754,000
Superconductivity Systems Program		
Device or Component Fabrication, Behavior or Testing	\$12	2,300,000
Wire Technology Project Systems Technology Superconductivity Partnership Initiative		5,500,000 5,600,000 1,200,000
Thermal Energy Storage Program	\$	454,000
Materials Properties, Behavior, Characterization or Testing	\$	140,000
High Temperature Composite Phase Change Material		40,000
Water Heating		100,000
Device or Component Fabrication, Behavior or Testing	\$	314,000
Phase Change Thermal Storage for Domestic Water Heating Complex Compound Thermal Energy Storage System		59,000 255,000

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

138. Amorphous Silicon for Solar Cells

<u>FY 1994</u> \$4,500,000

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 cm²) 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 cm². 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

139. Polycrystalline Thin Film Materials for Solar Cells

<u>FY 1994</u> \$7,500,000

DOE Contact: Richard King, (202) 586-1693 NREL Contact: Kenneth Zweibel, (303) 384-6441

This project performs applied research upon the deposition of CuInSe₂ 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 cm²) 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 cm². 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

140.	Deposition of III-V Semiconductors for High-Efficiency Solar Cells	<u>FY 1994</u>
	· · · · · · · · · · · · · · · · · · ·	\$1,200,000
DOE	Contact: Richard King (202) 586-1693	

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 cm² 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

141. <u>Materials and Device Characterization</u>

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

142. High-Efficiency Crystal Silicon Solar Cells

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.

<u>FY 1994</u> \$2,500,000

<u>FY 1994</u> \$2,400,000

Materials Preparation, Synthesis, Deposition, Growth or Forming

143. Thermally Conductive Composites for Heat Exchangers

FY 1994 \$90,000

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

This project is investigating thin thermally conductive polymer-based composites for use as corrosion and scale-resistant liner materials on carbon steel tubing used in shell and tube heat exchangers in binary geothermal processes or for bottoming cycles in multi-stage flash plants. Corrosion and scaling on the brine side of carbon steel tubing in shell and tube heat exchangers have been major problems in the operation of geothermal processes. Compared to the cost of high alloy steels, a considerable economic benefit could result from the utilization of a proven corrosion resistant polymer concrete material if sufficient heat transfer and anti-fouling properties can be derived. The work consists of determinations of the effects of compositional and processing variables on the thermal and fouling properties of the composite, and measurements of the physical and mechanical properties after exposure to hot brine in the laboratory and in plant operations. The effects of anti-oxidant additives on the fouling coefficient and scale adherence are also being evaluated. Results to date from field tests performed in FY 1994 with flowing hypersaline brine under heat exchange conditions indicate heat transfer and fouling coefficients similar to those for high alloy stainless steels. Further improvements by the inclusion of anti-oxidants are anticipated.

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

Materials Properties, Behavior, Characterization or Testing

144.	Advanced High Temperature Geothermal Well Cements	<u>FY 1994</u>
		\$390,000
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 CO₂ at temperatures >150°C are also needed. Emphasis is being placed on high temperature rheology, phase chemistry, and the mechanical, physical, and chemical resistance properties of the cured materials. Retarding admixtures required to maintain pumpability during placement operations are also being identified. To date, phosphate bonded calcium aluminate cement formulations containing hollow aluminosilicate microspheres appear to meet the design criteria and preparations for large-scale mixing and field placement are underway.

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

145. <u>Advanced High Temperature Chemical Systems for Lost</u> <u>Circulation Control</u>

<u>FY 1994</u> \$20,000

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 1995.

Keywords: Cement, Pumpable Slurries, Strength, Transformation, Bulk Characterization, Permeability, Hydrothermal Stability

146.	Corrosion Mitigation in Highly Acidic Steam Condensates	<u>FY 1994</u>
		\$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 $\sim 200^{\circ}$ 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

Office of Energy Management

Advanced Utility Concepts Division

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

Superconductivity Systems Program

Device or Component Fabrication, Behavior or Testing

147. <u>Wire Technology Project</u>

<u>FY 1994</u> \$5,500,000

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

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

1. Phase Development - Researchers developed a two-powder process that consists of reacting Pb-doped Bi-2212 with $CaCuO_2$ within an Ag tube. This process yields Bi-2223 with significantly improved phase purity compared to conventional processes, which is important for fabricating long lengths of wire having uniform and reproducible properties.

- 2. Improvement of Transport Current Researchers developed improved techniques to correlate transport properties and microstructure in the same grain boundary. Current-voltage, I(V), measurements can distinguish between flux depinning and weak links, and a single parameter, J_c , which can be compared from sample-to-sample and lab-to-lab, can be extracted from fits to I(V) curves.
 - 3. AC Losses HTS Materials development has matured enough so that prototype construction for applications such as ac fault-current limiters for power utility systems is underway. Low-loss ac downlinks, each consisting of only four sinterforged Bi-2223 bars, were produced for service at 1000 A rms per downlink in a 77-4.2 K gradient to serve a current limiter operated in liquid He.
 - 4. Critical Currents and Microstructure of HTS Materials In collaboration with General Electric, Intermagnetics General, American Superconductor, IBM, and others, a range of HTS materials were irradiated with high energy heavy ions in order to introduce nearly ideal, columnar defects for flux pinning. Splayed columnar defects, resulting from the irradiation, resulted in enhanced current flow in magnetic fields.
 - 5. Characterization of Bi(2223,2212)/Ag tapes In order to determine the limiting factors for J_c in currently available tapes and to help guide further development of these tapes, researchers constructed special equipment to permit detailed measurements of the behavior of the resistive transitions of the tapes under applied magnetic fields at various temperatures, i.e. 4.2, 27, and 54-90 K. Researchers made measurements for a number of Bi(2212, 2223)/Ag tapes fabricated by Intermagnetics General Corporation.
 - 6. Thick Films Researchers processed 10-20 micron thick films generated by screen printing precursor powders of the Pb-, Sr- substituted Tl-1223 material onto both insulating $LaAlO_3$ and metallic Ag foil substrates.
 - 7. Process Development for TI-1223 Wires and Tapes Researchers developed high-current Ag-sheathed tapes containing Pb-, Sr-doped TI-1223 powders, which have excellent performance in magnetic fields at 77K. The TI-free starting powders are chemically prepared using the Sandia co-precipitation process and then fabricated into wires and tapes using either the standard powder in tube method (PIT) or by extrusion techniques.

- 8. TI-1223 Electrodeposition NREL extensively studied the electrodeposition process to improve reproducibility and stoichiometry control. The electrodeposition process produces a precursor film that is extremely reactive and is therefore conducive to rapid production of high quality superconducting films. This improved process produced films on Ag foil with outstanding critical current densities (J_c) : 7 x 10⁴ A/cm² at 77K in zero field and 14 x 10⁴ A/cm² at 0.4 T for H parallel to the c-axis.
- Bi-2223/Bi-2212 Wire Researchers conducted processing studies of tapes containing mixtures of Bi-2223 precursors. Improvements led to J_c (77K) values above 26,000 A/cm² in short length. Processing studies of Bi-2212 wires in collaboration with Oxford Instruments yielded values of J_c (4.2K, 2T) of above 100,000 A/cm².
- 10. Y123 Thin Film Technology Activities extended technology to production of thick films on both ceramic and metal surfaces. Thick Y123 films up to 8 microns were successfully deposited by pulsed laser deposition onto a buffer layer. The associated J_c and I_c were over 800,000 A/cm² and 25 A, respectively, at 77K for Y123 film (1.4 microns) formed on a ceria buffer layer deposited on polycrystalline nickel.
- 11. Characterization of Superconducting Properties of HTS Wire Configurations -Researchers conducted studies of J_c dependence as a function of tape orientation with respect to magnetic field and of the current direction along and normal to the tape axis.
- 12. Experimentation Using Liquid Neon Refrigerant This work enabled the characterization of HTS tapes at 27K and at higher field levels than previously possible. This resource will be further developed to be offered as a national user facility to industry and other collaborators in conjunction with the National High Magnetic Field Laboratory (NHMFL) at Los Alamos. The NHMFL satellite at Los Alamos was used in studying the behavior of HTS tapes subjected to very high magnetic fields up to 18T.
- 13. High Energy Proton Bombardment Proton bombardment of Bi-2212 wire led to substantially improved flux pinning and improved current carrying in magnetic fields. The experiment was conducted with IBM, Oak Ridge, Argonne, and SUNY-Buffalo and used 0.8 GeV protons from Los Alamos'

meson facility. The irreversibility line for Bi-2212 was dramatically increased, resulting in the enhancement of operating temperature from 30 up to 50 K in a magnetic field of 2 telsa.

- Keywords: Phase Development, Transport Current, AC Losses, Microstructure, Thick Film, Electrodeposition, Flux Pinning, Bismuth, Thallium
- 148. Systems Technology

<u>FY 1994</u> \$5,600,000

148. <u>Systems recimology</u>

DOE Contact: Jim Daley, (202)586-1165 Argonne National Laboratory: U. Balu Balachandran, (708) 252-4250 Brookhaven National Laboratory: David Welch, (516) 282-3517 Los Alamos National Laboratory: Dean Peterson, (505) 665-3030 National Renewable Energy Laboratory: Richard Blaugher, (303) 384-6518 Oak Ridge National Laboratory: Robert Hawsey, (615) 574-8057 Sandia National Laboratory: Thomas Bickel, (505) 845-9301 American Superconductor Contact: G. N. Bart Riley, (508) 836-4200 Intermagnetics General Contact: Pradeep Haldar, (518) 782-1122 General Electric Research & Development, J. Eric Tkaczyk, (518) 387-5004 Oxford Instruments, Inc. Contact: Ken R. Marken, (908) 541-1300

The systems technology project includes long length wire and coil manufacture. Some preliminary systems development is also undertaken. Project subtasks are as follows:

- 1. Thallium Conductor Development Work on Tl-based conductors is carried out in cooperation with General Electric, Intermagnetics General, IAP, and on the base program. Microstructural studies of spray-pyrolyzed Tl-1223 deposits focus on correlating flux morphology with current carrying capability.
- 2. Thermo-Mechanical Processing of BSCCO Conductors The effects of oxygen partial pressure in the carrier gas and pyrolysis temperature on the phase content of aerosol powers were measured. The processing of PIT conductor containing aerosol powers is being conducted in cooperation with American Superconductors.
- 3. Development of BSCCO-2212 Composite Conductors Ceramic-silver composite conductors have been fabricated in lengths greater than 100 meters using both powder-in-tube and dip-coated methods.
- 4. Stability and Protection in High-T_c Superconducting Devices Researchers investigated design and operational issues facing HTS magnets and developed design options that make these magnets economically competitive.

- 5. AC Applications of HTS Wires and Coils Activities were conducted in collaboration with American Superconductor. The tasks were: electrical measurements of small HTS coils, theoretical calculations concerning the stability and protection of HTS coils, and design calculations and cryogenic engineering.
- 6. Demonstration of a Magnetic Refrigerator for HTS Electric Power Applications - Oak Ridge developed a prototype 50-W (40K) magnetic refrigerator. Fabrication and component testing activities were completed in coordination with Astronautics.
- 7. Development of Practical HTS Coils for Power Applications Progress was made in resolving limitations on achieving long lengths in the bismuth-and-thallium based tapes as illustrated by increased values of J_c in extended lengths.
- 8. Long-length BSCCO Wire Production The program between Argonne and Intermagnetics General concentrates on producing long, uniform lengths of conductors exhibiting good mechanical and superconducting properties for commercial operation at >35K.
- 9. Development of Tl-1223 Conductors for High-temperature, High-field Applications Researchers made Tl-1223 wire using variants of the two-powder process and have determined the microstructure in tapes made by SUNY-Buffalo, which have the highest J_c in the U.S.
- 10. Resolving Limitations on Achieving Long Lengths in the Bismuth-and-Thalliumbased Tapes as Illustrated by the Increased Values of J_c in Extended Lengths -Los Alamos and Martin Marietta initiated a productive collaboration directed towards development of practical HTS coils for power applications. Several HTS coils were successfully processed and are being evaluated.

Additional Applications:

1. Work on current leads consists of collaborative projects with Superconductivity, Inc., Babcock & Wilcox, and ZerRes Corp. Results indicate a boiloff one-tenth that of the best conventional leads, and a demonstration that DC currents produce essentially the same boiloff as 60Hz AC currents with the same rms amplitude. Researchers developed an intermediate-temperature heat intercept for use with HTS leads that has a low thermal resistance, but very high electrical resistance.

- 2. Superconducting bearing work Research was conducted in a collaborative project with Commonwealth Research Corp. (CRC) and involves substantial CRC funding to ANL. DOE funds are used to develop bulk HTS levitators; CRC funds are used to evaluate the levitation properties, develop HTS bearings, and to test flywheel energy storage using these bearings. In a small bell-jar vacuum chamber, researchers evaluated the performance of HTS bearings with the levitated mass of 400g and measured coefficients of friction for these bearings as low as 3×10^{-7} . In a larger stainless-steel vacuum chamber, researchers up to 12 kg.
- 3. Laboratory-scale conductors have been fabricated with J_c 's of 32,900 A/cm² (77K, self field, 1 micro V/cm). Production-scale wires have been fabricated at ASC's pilot plant with lengths greater than 1 km and J_c 's of 12,700 A/cm² (77K, self field)
- 4. Recent efforts are directed at the development of a continuous fabrication process for TI(1223) tape conductors. Researchers demonstrated the fabrication of 3 micron thick polycrystalline films with high critical current density and strong-linked behavior in applied magnetic fields.
- Keywords: Thallium Conductor, Composite Conductors, Stability and Protection, AC Application, Coils, Long Length Wire

149. <u>Superconductivity Partnership Initiative</u>

<u>FY 1994</u> \$1,200,000

DOE/Golden Field Office Contact: Jeff Hahn, (303) 275-4775 General Electric Co. Contact: Harley Lake, (518) 387-7895 Martin Marietta Contact: Eddie Leung, (619) 974-1166 Reliance Electric Company Contact: Rich Schiferl, (216) 266-6253 Electric Power Research Institute Contact: Don Von Dollen, (415) 855-2679

The Superconductivity Partnership Initiative supports industry development of superconductivity systems. In FY 94, projects are underway for a superconducting 100 MVA generator (General Electric), fault-current limiter (General Dynamics), and 125 HP motor (Reliance, Electric Company). In addition, a transmission cable project, in the past sponsored by the Electric Power Research Institute and Pirelli Cable, is being considered for funding in FY 1994. All of these projects will incorporate high-temperature superconducting wire. Four Department of Energy National Laboratories are currently directly supporting the Superconductivity Partnership Initiative Projects: Argonne, Los Alamos, Oak Ridge, and Sandia.

Project subtasks are as follows:

- 1. Generator Results of the generator project, in FY 94, included generator assessment activities including defining the applications, establishing a conceptual generator design, developing a preliminary generator design and initiating the performance analysis of the generator in the utility system. In addition, wire and coil development activities will be started and include wire development, fabrication, and coil design and development. Generators represent a large established worldwide market with growth projections forecasting that over 1000 GW of new generation capacity will be needed in the next 10 years, with 173 GW needed in the U.S.
- 2. Fault Current Limiter In FY 94, the fault-current limiter project undertook conceptual studies of various device designs, provided a market survey for current limiter applications, completed an energy benefit assessment, conduct a network interface assessment, determined conductor requirements, and analyzed the economic potential of fault current limiters. Fault current limiters can be used on transmission and distribution systems to improve system flexibility, reliability and performance.
- 3. Motor Electrical and mechanical design and thermal analysis was completed. In addition, the construction of the components for a motor prototype will be nearly completed, with assembly and testing to follow in FY 95. Superconducting motors can have a large impact on electrical energy utilization through reduced losses and size compared to conventional iron core motors. Reduced losses and smaller size will be the driving force for the commercial introduction of superconducting motors in industrial applications.
- 4. High Temperature Superconducting Power Cable The first phase of the contract calls for the development and fabrication of a 30-meter prototype 115KV HTS underground power transmission cable which will be tested at a utility site. Additionally, the project will conclude with design of a 3-phase, 100 meter cable system.

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

Thermal Energy Storage Program

Materials Properties, Behavior, Characterization or Testing

150. High Temperature Composite Phase Change Material	FY 1994
PNL Contact: W. Kevin Winegardner, (509) 375-3839	\$40,000
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). A high temperature test facility was designed, constructed, and used in experiments to validate the model subsequently used for parametric studies to identify key variables and parameters influencing thermodynamic efficiencies. Use of the test facility to evaluate the performance of CPCM pellets revealed poor stability of the material.

Keywords: Heat Storage, Phase Change Materials, Composites

151.	Geochemistry Dynamics Associated with Ground Water Heating	<u>FY 1994</u>
		\$100,000

PNL Contact: 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. Software includes a package, H_{20} treat, specifically developed to aid engineers in the design and siting of aquifer heat storage systems.

Keywords: Minerals, Permeability, Aquifer
Device or Component Fabrication, Behavior or Testing

152. Phase Change Thermal Storage for Domestic Water Heating

FY 1994 \$59,000

PNL Contact: 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 but occupy the same volume. Prototypes based on two concepts are being performance tested. One prototype uses a bed of high density polyethylene pellets whose internal structure has undergone crosslinking. The crosslinking step allows the pellets to store significant amounts of energy in a phase transition and maintain the structural integrity of the pellet. The second design uses a sensible heat concept and stores the required amount of energy via large temperature changes in the storage medium.

Keywords: Phase Change Materials, Encapsulation, Corrosion

153.	Complex	x Compour	nd Thermal	Energy Storage	System			<u>FY 1994</u> \$255.000
PNL	Contact:	W. Kevin	Winegardne	r, (509) 375-383	9	• •	·	, \$233,000

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 various applications will be identified and the performance of the media, in terms of amount and rate of adsorption and desorption characterized. A prototype unit is being designed and fabricated.

Keywords: Adsorption Refrigeration, Adsorbing Materials, Complex Compound

OFFICE OF ENERGY RESEARCH

	<u>FY 1994</u>
Office of Energy Research - Grand Total	\$348,260,033
Office of Basic Energy Sciences	\$297,371,424
Division of Materials Sciences	\$277,125,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	\$ 32,680,000
Materials Structure and Composition	\$ 34,230,000
Properties, Behavior, Characterization or Testing	\$101,810,000
Facilities and Equipment	\$108,405,000
Division of Chemical Sciences	\$ 5,300,000
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

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OFFICE OF ENERGY RESEARCH (Continued)

	<u>FY 1993</u>
Office of Basic Energy Sciences (continued)	
Division of Chemical Sciences (continued)	``.
Materials Precursor Chemistry	\$ 1,730,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	\$ 990,000
Materials Structure and Composition	\$ 740,000
Division of Engineering and Geosciences	\$ 7,406,424
Engineering Sciences Research	\$ 4,836,821
Materials Properties, Behavior, Characterization or Testing	\$ 4,836,821
Bounds on Dynamic Plastic Deformation	126,000
Continuous Damage Mechanics - Critical States	50,441
An Investigation of the Effects of History Dependent	02 125
Micromechanical Viscoplastic Stress-Strain Model	95,125
with Grain Boundary Sliding	50,440
Micromechanical Viscoplastic Stress-Strain Model	,
with Grain Boundary Sliding	51,332
An Analytical-Numerical Alternating Method for 3-D	
Inelastic Fracture and Integrity Analysis of	(0.710
Pressure-vessels and Piping at Elevated Temperatures	60,718
High Velocity Particles	485 000
Intelligent Control of Thermal Processes	530,000
Elastic-Plastic Fracture Analysis Emphasis on	000,000
Surface Flaws	430,000
Modeling of Thermal Plasma Processes	233,000

<u>FY 1994</u>

Office of Basic Energy Sciences (continued)

Division of Engineering and Geosciences (continued)

Engineering Sciences Research (continued)

Materials Properties, Behavior, Characterization or Testing (continued)

Nondestructive Evaluation of Superconductors	200,000
Stress Induced Phase Transformations	66,751
Pulse Propagation in Inhomogeneous Optical Waveguides	84,272
Multivariable Control of the Gas-Metal/Arc Welding	
Process	165,870
Metal Transfer in Gas-Metal Arc Welding	128,622
Modeling and Analysis of Surface Cracks	205,640
Thermal Plasma Processing of Materials	279,602
Development of Measurement Capabilities for the	
Thermophysical Properties of Energy-Related Fluids	573,000
Low Resistivity Ohmic Contacts Between Semiconductors	
and High-T. Superconductors	108,000
Thin Film Characterization and Flaw Detection	90,452
The Evolution of a Hele-Shaw Interface and Related	-
Problems in Dendritic Crystal Growth	66,118
Experiments on the Gas Dynamics of the	
High Velocity Oxy-Fuel (HVOF) Thermal Spray Process	94,142
Transport Properties of Disordered Porous Media	
from the Microstructure	0
Effect of Forced and Natural Convection on Solidification	
of Binary Mixtures	93,664
Inelastic Deformation and Damage at High Temperature	0
Flux Flow, Pinning and Resistive Behavior in	
Superconducting Networks	70,519
Application of Magnetomechanical Hysteresis	
Modelling to Magnetic Techniques for Monitoring	
Neutron Embrittlement and Biaxial Stress	0
Stability and Stress Analysis of Surface Morphology	
of Elastic and Piezoelectric Materials	0

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Office of Basic Energy Sciences (continued)		
Division of Engineering and Geosciences (continued)		
Engineering Sciences Research (continued)		
Materials Properties, Behavior, Characterization or <u>Testing</u> (continued)		
Energy Changes in Transforming Solids Optical Techniques for Superconductor Characterization Degenerate Four Wave Mixing as a Diagnostic of		174,600 0
Plasma Chemistry Effective Elastic Properties and Constitutive Equations for		195,907
Brittle Solids Under Compression 3-D Experimental Fracture Analysis at High Temperature		60,324 69,282
Geosciences Research	\$ 2	2,569,603
Materials Preparation, Synthesis, Deposition, Growth or Forming	\$	275,000
An Investigation of Organic Anion-Mineral Surface Interactions During Diagenesis Transition Matel Catalysis in the Constantion of Patroleum		178,000
and Natural Gas		97,000
Materials Structure and Composition	\$	153,000
Infrared Spectroscopy and Hydrogen Isotope Geochemistry of Hydrous Silicate Glasses		153,000
Materials Properties, Behavior, Characterization or Testing	\$ 2	2,141,603
Cation Diffusion Rates in Selected Silicate Minerals Shear Strain Localization and Fracture Evolution in Rocks Poroelasticity of Rock		85,000 72,000 59,833

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<u>FY 1994</u>

Office of Basic Energy Sciences (continued)

Division of Engineering and Geosciences (continued)

Materials Properties, Behavior, Characterization or Testing (continued)

Oxygen and Cation Diffusion in Oxide Materials	238,270
Grain Boundary Transport and Related Processes in	
Natural Fine-Grained Aggregates	302,000
New Method for Determining Thermodynamic Properties	
of Carbonate Solid-Solution Minerals	78,000
Investigation of Ultrasonic Wave Interactions with	
Fluid-Saturated Porous Rocks	161,000
Three-Dimensional Imaging of Drill Core Samples Using	
Synchrotron-Computed Microtomography	150,000
Thermodynamics of Minerals Stable Near the Earth's Surface	145,000
Theoretical Studies of the Adsorption of Gold Complexes	
and Flotation Collectors onto Sulfide Mineral Surfaces	35,000
Transport Phenomena in Fluid-Bearing Rocks	144,000
Structure and Reactivity of Ferric Oxide and Oxyhydroxide	
Surfaces: Quantum Chemistry and Molecular Dynamics	127,500
Micromechanics of Failure in Brittle Geomaterials	171,000
Energetics of Silicate Melts from Thermal-Diffusion Studies	169,000
Cation Chemisorption at Oxide Surfaces and Oxide-Water	
Interfaces: X-Ray Spectroscopic Studies and Modeling	204,000
Division of Advanced Energy Projects	\$ 7,540,000
Materials Preparation, Synthesis, Deposition, Growth	
or Forming	\$ 4,466,000
	• •,•••,•••
Combustion Synthesis and Engineering of Nanoparticles for	
Electronic. Structural and Superconductor Applications	186.000
Creation and Destruction of C_{co} and Other Fullerene Solids	301.000
Synthesis and Properties of High Strength Nanolavered	,
Composites	315,000
Optimally Controlled Interior Manipulation of Solids	349,000
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<u>FY 1994</u>

Office of Basic Energy Sciences (continued)

Division of Advanced Energy Projects (continued)

Materials Preparation, Synthesis, Deposition, Growth or Forming (continued)

Design of Materials with Photonic Band Gaps	297,000
High-Flux, Large-Area Carbon-Cluster Beams for Thin Film	
Deposition and Surface Modification	355,000
Novel Composite Coatings for High Temperature Friction and	
Wear Control	260,000
Synthesis of Advanced Composite Ceramic Precursor Powders	
by the Electric Dispersion Reactor	325,000
Development of an Ion Replacement Electrorefining Method	450,000
Evaporation Through Tungsten to Achieve High-Rate Vapor	
Phase Processing of Intermetallics	291,000
Ultrasonic and Dielectric Noninvasive Diagnostics for	
Sintering of Ceramic Composites	358,000
Compact MeV Ion Implantation	294,000
Thermoelectric Quantum Wells	350,000
Porous Carbons: Controlling Structure, Composition and	•
Performance	335,000
Materials Properties Rehavior Characterization or Testing	¢1 019 000
materials rioperties, benavior, Characterization of Testing	\$1,010,000
Nonlinear Optics in Doped Fibers	366.000
Feasibility of a Novel Approach for Fast, Economical	,
Determination of Radiation Damage in Nuclear Reactor	
Cores	145.000
Hot Carrier Solar Cells	330,000
Atomic and Nanoscale Engineering of Thermophotovoltaic Semi-	,
conductor Using Scanning Probe Microscopy Techniques	177,000
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	<u>FY 1994</u>
Division of Advanced Energy Projects (continued)	
Device or Component Fabrication, Behavior or Testing	\$ 2,056,000
Ultrafast Molecular Electronic Devices Photo-Induced Electron Transfer From a Conducting Polymer to Buckminsterfullerene: A Molecular	405,000
Approach to High Efficiency Photovoltaic Cells	283.000
Superconducting Bitter Magnets	300.000
Blue-Emitting Devices Based on Gallium Nitride	319.000
Solid State Multi-Lavered Batteries	419.000
PV-Powered, Electrochromic Windows	330,000
Office of Fusion Energy	\$14,488,000
Materials Properties, Behavior, Characterization or Testing	\$14,488,000
Structural Materials Development	389,000
Repair Welding of Fusion Reactor Components	90,000
Insulating Ceramics for Fusion	290,000
Modeling Irradiation Effects in Solids	60,000
Fusion Systems Materials	2,355,000
Structural Materials for Fusion Systems	1,791,000
Development of Radiation-Hardened Ceramic Composites for	
Fusion Applications	49,000
Radiation Effects and Micromechanics of SiC/SiC Composites	97,000
Damage Analysis and Fundamental Studies for	
Fusion Reactor Materials Development	180,000
Development of Lithium-Bearing Ceramic Materials	,
for Tritium Breeding in Fusion Reactors	250,000
Post-Irradiation Examination of Lithium-Bearing Ceramic	,
Materials for Tritium Breeding in Fusion Reactors	500,000
ITER Materials Development for Plasma Facing Components	3,000,000
ITER Structural Materials Development	630,000
ITER Ceramic Materials	358.000
Radiation Hardened Fiber Optics for ITER Fusion Diagnostic	, - , - , - , - , - , - , - , - , -
Systems	50,000

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FY 1994

Office of Fusion Energy (continued)

Materials Properties, Behavior, Characterization or Testing (continued)

ITER Materials Evaluation ITER Structural Materials Evaluation	1,459,000 840,000
Development of Nb ₃ Sn Superconducting Wire for the ITER Magnet Program Structural Materials Development for the Conduit of ITEP	1,000,000
Cable-in-Conduit-Conductors	1,100,000
Small Business Innovation Research Program	\$35,030,124*
Materials Preparation, Synthesis, Deposition, Growth	
or Forming	\$16,358,332
Phase I Projects:	\$ 2,465,397
Low Cost, High Purity Silicon by Alkaline Glycolic	
Digestion of Silica	75,000
High Speed Sheet Growth of Thin Silicon Films	75,000
An Innovative Approach for Large Area Photovoltaic	,
Material Processing	74,940
Low Cost Solar Cell Leads for Use in Photovoltaic Modules Very Low-Cost/High-Efficiency Thin-Film Silicon Photovoltaic	75,000
Technology	74,992
Improved Activated Carbon for Hydrogen Storage A Superplastic Oxide Dispersion Strengthened Magnesium	73,821
Allov for Automotive Applications	74.350
Low Cost Synthesis of Nanocrystalline Silicon Carbide Starting	,
with Fullerene Precursors	75,000
A Ceramic Material and Process for Use in Monolithic Ceramic	,
Cross-Flow Filters	74,937

Includes 84 new Phase I and 31 new Phase II projects initiated in FY 1994 and 22 Phase II projects initiated in FY 1993. The funding shown for each Phase II project is the total allocated for the duration of the project (up to two years).

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<u>FY 1994</u>

Small Business Innovation Research Program (continued)	
Materials Preparation, Synthesis, Deposition, Growth	
or Forming (continued)	
Phase I Projects: (continued)	
High Temperature Brazing of Silicon Carbide	74,492
Molecular Composite Plastics for Lightweight Green Cars	74,749
Irradiation	74,769
A Novel Method for Manufacture of High Temperature	,
Superconducting Coils for High Temperature Operation	75,000
Design and Applications of Close-Spaced Thermionic	74 242
Converters with Novel Isothermal Electrodes	74,342
Coefficient of Performance Heat Pumps	74 999
Growth of Lutetium Phosphate Scintillator Crystals	7 1,999
for Positron Emission Tomography	75,000
Top-Seeded Solution Growth of Lutecium Phosphate	,
from Potassium Pyrophosphate Flux	74,159
Production of Carbon-11-Labeled Compounds for Positron	
Emission Tomography with a Low Energy Accelerator	74,981
Sapphire-Metal Joining for Low-Loss Gyrotron Windows	74,983
Economical and Reliable Niobium-Tin Conductors via	75 000
An Innovative Technique to Bond One Dimensional Carbon-	75,000
Carbon Composites to Dispersion Strengthened Copper	75 000
Advanced Low-Stress Brazing of Plasma-Facing Fusion	75,000
Components with High Energy Electron Beams	73,994
Joining of Aluminum to Carbon-Carbon Composites for	-
Fusion Reactor Applications	75,000
Ductile Joining of Beryllium to Copper	75,000
A Multilayer Silicon Carbide Fiber Coating for Toughened,	
Neutron Kadiation-Kesistant Silicon Carbide/Silicon	70.057
Carolice Composites	12,051

<u>FY 1994</u>

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Small Business Innovation Research Program (continued	<u>Small</u>	Business	Innovation	Research	Program	(continued)
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Materials Preparation, Synthesis, Deposition, Growth, or Forming (continued)

Phase I Projects: (continued)

Niobium Titanium Multifilamentary Materials with Silicon	
in the Matrix 75	.000
A Novel Approach to Fabrication of Niobium-Tin Conductor	,
with Artificial Pinning Centers 75	.000
High Quality Chemically Vapor Deposited Niobium Coatings	,
for Superconducting Radio Frequency Cavities 75	.000
Niobium-Titanide Tin/Copper Multifilamentary Superconducting	,
Wire with Niobiuim/Titanium Composite Filaments 74	.995
Development of Niobium-Titanium-Tantalum Artificial Pinning	
Center Superconductors for Very High Field Applications 74	.954
Jet Vapor Deposition of Thick Films for the Production of	,
Radioactive Beams of Chemically Active Elements 75	.000
Microchannel Plates Fabricated by Track Etch Lithography 74	.981
Radiation-Hard and Solar Blind Ultraviolet X-ray Chemically	,
Vapor Deposited-Diamond Photoiode Detectors 73	,902
Phase II Projects: (First Year) \$ 8,393	,382
Multi Layer, Quantum Well Layer Film Thermoelectrics 595	,070
Production of Carbon Materials from Biomass 599	988
Oxide Dispersion Strengthened Silver for Use in High-	,
Temperature Superconductor Composite Wires 600	.000
Low Temperature Deposition of Titanium Nitride 599	677
Coated Micrograin Carbides for Wear Resistance 599	577
Comparis Diama Dahara Manlaran	
Composite Plasma-Polymer Memoranes 599.	,916
Improved Coated-Metal Hydrogen Extraction Membranes 599	,916 ,314
Composite Plasma-Polymer Membranes599Improved Coated-Metal Hydrogen Extraction Membranes599Methods of Improving Internal-Tin Niobium-Tin for599	,916 ,314
Composite Plasma-Polymer Memoranes599Improved Coated-Metal Hydrogen Extraction Membranes599Methods of Improving Internal-Tin Niobium-Tin for Fusion Applications600	,916 ,314 ,000
Composite Plasma-Polymer Memoranes599Improved Coated-Metal Hydrogen Extraction Membranes599Methods of Improving Internal-Tin Niobium-Tin for Fusion Applications600,Advanced Nondestructive Evaluation for Quality Assurance600,	,916 ,314 ,000

OFFICE OF ENERGY RESEARCH (Continued)

	<u>FY 1994</u>
Small Business Innovation Research Program (continued)	
Materials Preparation, Synthesis, Deposition, Growth, or Forming (continued)	
Phase II Projects: (First Year) (continued)	
Dense, High Conductivity, Copper/Aluminum/Beryllium Functionally Gradient, Plasma Facing Components	599,995
Flexible Electrochromic Window Materials Based on Poly (Diphenyl Amine) and Related Conducting Polymers Advanced Window Materials Based on Conducting Polymer/	599,893
Sol-Gel Ceramic Composites An Innovative Approach for the Formation of Silicon	600,000
Carbide/Silicon Carbide Composites	599,952
to Enhance Thermal Conductivity	600,000
Phase II Projects: (Second Year)	\$5,499,553
Development of a Novel Reverse-Osmosis Membrane with High	400.011
Rejections for Organic Compounds Development of a Process to Synthesize Tubular Fullerenes	499,911
Continuous Production of Fullerenes from Hydrocarbon	500,000
Precursors	500,000
Preparation of Low-Density Microcellular Matearials from	
Fullerenes	500,000
New Gadolinium-Boron Compounds for Neutron Capture Therapy Refractory Metal Coatings on Carbon/Carbon Composites for	500,000
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 Rediction Demose Resistant Silican for Particle Physics	500,000
Radiation Damage Resistant Silicon for Particle Physics	500.000
Detectors	200,000

	<u>FY 1994</u>
Small Business Innovation Research Program (continued)	
Materials Properties, Behavior, Characterization or Testing	\$ 2,223,643
Phase I Projects:	\$ 1,124,040
A Long Life Zinc-Oxide-Titanium-Oxide Sorbent High Temperature Thermally Stable Multi-Layer Quantum	75,000
Well Films	75.000
Hydrogen Permeation Barriers for Bimodal Reactors	74,987
Fracture Toughness Testing with Minimal Material	74.811
A Novel High Strength Ceria-Zirconia Toughened Alumina Ceramic with Superior High Temperature Corrosion and Erosion	,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,
Resistance	75.000
Rare Earth Endohedral Fullerenes as New Nonlinear Optical Materia	uls 75,000
X-ray Absorption Spectroscopy for Trace Analysis of Chemical	,
Phase and Composition	74,674
An Apparatus for Structural Analysis of High Temperature	
Materials Using Synchrotron Radiation	74,978
A Novel Detector for Neutron Diffraction Studies	75,000
An Analytical Research Materials Characterization	
Facility Based on Synchrotron Radiation	74,710
Application of the Meandering Winding Magnetometer	
to an In-Situ Determination of Age Related Degradation	75,000
Improvement in the Loss and Critical Current Density	
Properties of Internal-Tin Niobium-Tin	75,000
A Feasibility Study to Correlate Vanadium (Chromium,	
Titanium) Alloy Weld Strength with Weld Chemistry	74,910
Improvement in the Characteristics of Ternary Niobium	
Titanium Tantalum Alloys	75,000
Activated Optical Ceramics: A New Class of Materials	
for Environmental Monitoring	74,970

	•	<u>FY 1994</u>
Small Business Innovation Research Program (continued)		
Materials Properties, Behavior, Characterization or Testing (continued)		
Phase II Projects: (First Year)	\$	599,672
A Testing Process to Define Electrode Current Wear Mechanisms and Develop Improved Electrodes		599,672
Phase II Projects: (Second Year)	\$	499,931
A Novel Energy-Efficient Membrane System for the Recovery of Volatile Organic Contaminants from Industrial Process Gases		499,931
Device or Components Fabrication, Behavior or Testing	\$16	5,448,149
Phase I Projects:	\$ 2	2,621,134
Monolithic Integration of Thin Film Photovoltaics on Insulated Metal Substrates		74,924
Development of a Low Cost High Concentration Photovoltaic Dense Array Module for Use with Reflective Concentrators Non-Precious Metal Catalysts for Proton Exchange Membrane		74,314
Fuel Cells by Ion Beam Synthesis		75,000
Membrane Fuel Cells Contamination Tolerate Anodes for Proton Exchange Membrane		75,000
Fuel Cells Metal Carbide Nanoclusters for Polymer Electrolyte Membrane		75,000
Fuel Cells		75,000
A New Semiconductor Radiation Sensor for Expedited Waste Site Characterization		74,922
An Acoustic Plate Mode Aqueous Mercury Sensor		74.600
An Off-Line-Locked Laser Diode Sensor (OLDS)		75.000
High Energy Resolution Cadmium-Zinc-Telluride Semiconductor		,
Radiation Detectors		74,955

FY 1994

Small Business Innovation Research Program (continued) Materials Properties, Behavior, Characterization or Testing (continued) Device or Components Fabrication, Behavior or Testing (continued) Phase I Projects: (continued) Gas Separation Membranes Based on Permselective Films of Buckminsterfullerenes 75.000 Fullerene Based Catalysts for Heavy Oil Upgrading 75.000 Coal Ash Tiles by Microwave Processing 75,000 Development of Expansive Cements Using Dry Flue Gas **Desulfurization Solid Wastes** 74,992 Metal Monoliths for Conversion of Natural Gas to Liquid Fuel 74,826 Oxygen-Evolving Anodes for the Electrolysis of Calcium Oxide 75,000 A Long Life Perovskite Oxygen Electrode for Calcium Oxide 74,997 Processing in Nuclear Fuel Cycles A Low Emission Alkali Metal Thermal to Electric Converter Automotive Power System 74,558 Advanced Catalysts for Ultra-Low Emission Control in Natural Gas Fueled Vehicles 75,000 A Membrane Reactor for the Production of Hydrogen Fuel from Hydrocarbon Liquids 75,000 Economical Photochromic Films for Solar Thermal Control 75,000 Thermophotovoltaic Generator Efficiency Improvement 74,500 High-Performance Membranes for Gas, Vapor, and Liquid **Separations** 75,000 Organic-Inorganic Composite Membranes for Gas Separation and Vapor Permeation 75,000 Electrode Materials for Rechargeable Lithium Batteries 75,000 Novel High Performance Glassy Polymer Composite Membranes for Gas Separation 75,000 Highly Selective Membranes for the Separation of Organic Vapors Using Super-Glassy Polymers 75.000

	<u>FY 1994</u>
Small Business Innovation Research Program (continued)	
Device or Components Fabrication, Behavior or Testing (continued)	
Phase I Projects: (continued)	
A Continuous Cryopump/Pellet-Fabrication Apparatus for	
Fusion	74,649
Innovative Electrochemical Sensors for In-Situ Real-Time	
Monitoring of Lead in Aqueous Media	75,000
Fluoroionophores for Use in a Fiber Optic Sensor for	
Mercuric Ions	75,000
Potentiometric Sensors for Lead and Mercury	75,000
A Compressed Xenon Gamma Sensor for Environmental	
Measurements	74,955
Fiber Optic Sensors for Heavy Metal Cations	74,941
Innovative Sorbents for the Selective Removal of Heavy	
Metals from Groundwater	74,985
An Ultra-Compact Cesium Iodide/Mercuric Iodide Gamma-Ray	
Scintillation Spectrometer	74,016
Phase II Projects: (First Year)	\$ 8,859,634
Glass-Ceramic Construction Tiles from Coal-Fired Boiler	
Flyash	599,861
A High Repetition-Rate, High Power, All-Solid-State	
Pulsed Driver for Electrodeless Inductive Thrusters	599,937
Demonstration of an Integrated Carbon Dioxide/Thermal	
Management System for Carbonate Fuel Cells	599,968
Porous Aluminum Nitride Part Fabrication to Support	
Advanced Battery Development	599,703
Capacitive Energy Storage Using High Surface Area Transition	
Metal Compounds	600,000
Advanced Ceramic Fibers for a Carbonate Fuel Cell Matrix	599,950
An <i>in-Situ</i> Particle Sensor for Metal Forming Processes	595,070
Development of a High Spatial Resolution Neutron Detector	472,688
A High Resolution Scintillator-Based Neutron Detector	600.000

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Small Business Innovation Research Program (continued)	
Device or Components Fabrication, Behavior or Testing (continued)	
Phase II Projects: (First Year) (continued)	
On-Chip Infrared-Spectral Sensors by Superconducting	
Detector Arrays	592,568
for Euclon Applications	600.000
Helium-Cooled Divertors with Low-Activation Materials and	000,000
Simple Fabrication Techniques	599,918
Niobium-Tin Superconducting Wire with Built-in Niobium Surface	
Coating to Limit Inter-Strand Eddy Currents in Cables	599,978
Ceramic Filters for Ultrafine Particulate Separation in	
Combustion Gas Environments	600,000
A Carbonate Fuel Cell Monolith for Low-Cost and High	
Power Density Operation	599,993
Phase II Projects: (Second Year)	\$ 4,967,381
Digital Processing Electronics for X-Ray Detector Arrays A Cold/Thermal Beam Bender Using Capillary Optics to	500,000
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	100.000
Superconductors for High Field Applications	499,988
Fabrication of Nioblum-Aluminum Superconducting Strands	400.062
Durable Low Cost Ceramic Materials for Use in Hot Cas	499,902
Filtration Equipment	403 071
I madon Equipment	773,071

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Small Business Innovation Research Program (continued)		
Device or Components Fabrication, Behavior or Testing (continued)		
Phase II Projects: (First Year) (continued)		
High Cation Mobility Lithium Polymer Batteris A Real-Time X-ray Detector		499,968 500,000
Small Business Technology Transfer Program	\$ 1	1,370,485
Materials Preparation, Synthesis, Deposition, Growth or Forming	\$ 1	1,074,725
Phase I Projects:	\$1	1,074,725
Preparation of Monolithic Porous Carbon Materials Using Controlled Functionalization of Fullerenes A Continuous Chemical Manufacturing Process for Direct		100,000
Production of Titanium Powder with a Reagent Recycle		974,725
Device or Component Fabrication, Behavior or Testing	\$	295,760
Phase I Projects:	\$	295,760
Feasibility of Nitride Phosphors for Thin Film Electroluminescent Displays An Integrated X-ray Sensor Improved Mineral Insulated Cables for Fusion Reactor Diagnostics		100,000 97,829 97,931

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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 50 research projects in FY 1994, at the Frederick Seitz Materials Research Laboratory at the University of Illinois. The Laboratory is also funded by 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, 143 CRADAs involving about 110 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 1994, among the 3,467 scientists who conducted X-ray and neutron beam experiments at Basic Energy Sciences-supported user facilities, there were 434 industrial scientists from 92 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 212 Phase I projects in FY 1994.

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 1994 for the Division of Materials Sciences were \$277,125,000. These funds were allocated to 458 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 124 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 (229 in FY 1994) 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 multiinstitutional 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 highpayoff, 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 14 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 science programs of the Division of Materials Sciences are grouped into three subprograms:

- <u>Metallurgy and Ceramics</u> seeks to understand the synergistic relationship between synthesis, processing, structure, properties, and behavioral parameters of materials.
- <u>Solid State Physics</u> is concerned with understanding the interactions of electrons, atoms, and defects and their role in determining the structure and properties of condensed matter.
- <u>Materials Chemistry</u> 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 contact listed in the accompanying table may be contacted by calling (301) 903-3427. The reader also is referred to DOE publication <u>Materials Sciences Programs Fiscal Year 1994</u> (DOE/ER-0648 dated April 1995). This publication contains summaries of all funded programs, summaries of all 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		
DIVISIO	DIVISION OF MATERIALS SCIENCES		
Robert J. Gottschall	Acting 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		
Alan L. Dragoo	Ceramics		
Otto Buck	Mechanical Behavior, NDE		
John N. Mundy	Physical Behavior, Irradiation Effects		

NAME	PROGRAM AREA	
Yok Chen	Physical Behavior, Irradiation Effects	
Michael E. Kassner	Mechanical Behavior	
Helen M. Kerch	Microstructure, Processing	
Arthur B. Denison	Magnetic Materials, Condensed Matter Physics	
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	
Dale Koelling	Solid State Theory, Magnetism, Advanced Computational Methods	

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 1994 for materials-related programs was \$5,300,000 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 3dimensional 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) 903-5804. The reader also is referred to DOE publication <u>Summaries of FY 1994 Research in the Chemical Sciences</u> (DOE/ER-0144/12 dated September 1994) 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
Env	ronmental Safety and Health
Sat Goel	
Ted Tomczak	
1	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
Stephen A. Butter	Chemical Energy
Robert L. Beyerlein	Chemical Energy
Steven G. Barnhart	Advanced Battery Program
William S. Millman	Chemical Energy
Harry J. Dewey	Separations and Analysis

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 geosciencesrelated 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

154. Bounds on Dynamic Plastic Deformation

<u>FY 1994</u> \$126,000

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

155.	Continuous Damage Mechanics - Critical States	<u>FY 1994</u>
		\$50,441
DOE	Contact: Oscar P. Manley, (301) 903-5822	
Arizo	na State University Contact: D. Krajcinovic, (602) 965-8656	

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

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

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

Keywords: Metals: Ferrous, Fracture, Fatigue, Creep

156. <u>An Investigation of the Effects of History Dependent</u> Damage in Time Dependent Fracture Mechanics

FY 1994 \$93,125

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

157. <u>Micromechanical Viscoplastic Stress-Strain Model with</u> <u>Grain Boundary Sliding</u>

<u>FY 1994</u> \$50,440

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, Hig Temperature, Experiments	1
158. <u>Mic</u> <u>Grai</u>	romechanical Viscoplastic Stress-Strain Model with in Boundary Sliding FY 199 \$51.33	<u>1</u> 2
DOE Conta Engineering	act: Oscar P. Manley, (301) 903-5822 g Science Software, Inc., Contact: K. P. Walker, (401) 231-3182	-
This the previou	project is joint with the University of Connecticut project described above. See s paragraph for a description.	2
Keywords:	Micromechanical, Viscoplasticity, Grain Boundary, Crystallographic Slip, High Temperature, Constitutive Model	1
159. <u>An A</u> <u>Frac</u> at E	Analytical-Numerical Alternating Method for 3-D Inelastic ture and Integrity Analysis of Pressure-Vessels and Piping levated Temperatures FY 199	<u>1</u>

<u>FY 1994</u> \$60,718

DOE Contact: Oscar P. Manley, (301) 9903-5822 Georgia Institute of Technology Contact: S. Atluri, (404) 894-2758

This research effort involves the application of highly efficient and accurate analytical- numerical alternating methods for the non-linear analysis of surface-flawed pressure vessels and piping under (1) elastic-plastic fracture, (2) high-temperature creep and viscoplastic fracture, and (3) pressurized thermal shock conditions. These procedures are highly efficient because only the uncracked structure is modeled numerically (finite element and boundary element approaches) and the severity of the stress state due to the presence of the 3-dimensional flaw is accounted for entirely analytically. This procedure is a novel application of the Schwartz-Neumann alternating method, which is a superposition method for linear problems, being extended to the nonlinear problems of elastoplasticity and creep through the generalized mid-point radial return mapping procedures which return the elastic estimates of stress in the cracked body to the appropriate yield surface. This effort is being conducted in collaboration with researchers at the University of Washington (see Number 33) where some seminal experimental work is being conducted to verify and validate the analytical work done at Georgia Tech. Keywords: Fracture, Failure Analysis

160. <u>In-Flight Measurement of the Temperature of Small, High Velocity</u> Particles

<u>FY 1994</u> \$485,000

DOE Contact: Oscar P. Manley, (301) 903-5822 Idaho National Engineering Laboratory Contact: J. R. Fincke, (208) 526-2031

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

Keywords: Plasma Processing, Particle/Plasma Interaction

161. Intelligent Control of Thermal Processes

<u>FY 1994</u> \$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

162. <u>Elastic-Plastic Fracture Analysis Emphasis on</u> <u>Surface Flaws</u>

<u>FY 1994</u> \$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

163. Modeling of Thermal Plasma Processes

<u>FY 1994</u> \$233,000

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 threedimensional 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 submodels for the various plasma-particle and particle-particle interaction processes, including melting, evaporation, condensation, nucleation, agglomeration, and coalescence.

Keywords: Plasma Processing, Optimization, Computational Model

164.Nondestructive Evaluation of SuperconductorsFY 1994\$200,000\$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

165. Stress Induced Phase Transformations

<u>FY 1994</u> \$66,751

DOE Contact: Oscar P. Manley, (301) 903-5822 University of Illinois Contact: H. Schitoglu, (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 nonmetallic materials.

Keywords: Phase Transformation, Stress, Strain

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Pulse Propagation in Inhomogeneous Optical Waveguides	<u>Fy 1994</u>
	\$84,272
	Pulse Propagation in Inhomogeneous Optical Waveguides

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 modeholding 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

167.	Multivariable Control of the Gas-Metal/Arc Welding Process	<u>FY 1994</u>
		\$165,870
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 realtime 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

168. Metal Transfer in Gas-Metal Arc Welding

DOE Contact: Oscar P. Manley, (301) 903-5822 MIT Contacts: T. W. Eagar and J. Lang, (617) 253-3229

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

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

Keywords: Welding, Control

<u>FY 1994</u> \$128,622

169. Modeling and Analysis of Surface Cracks

<u>FY 1994</u> \$205,640

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

170. Thermal Plasma Processing of Materials	<u>FY 1994</u>
	\$279,602
DOE Contact: Oscar P. Manley, (301) 903-5822	
University of Minnesota Contact: E. Pfender, (612) 625	5-6012

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

171. Development of Measurement Capabilities for the Thermophysical Properties of Energy-Related Fluids FY 1994

<u>FY 1994</u> \$573,000

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

National Institute of Standards and Technology Contacts: R. Kayser, (301) 975-2483 and J. M. H. Sengers, (301) 975-2463

The major objective of this project is to develop state-of-the-art experimental apparatus that can be used to measure the thermophysical properties of a wide range of fluids and fluid mixtures important to the energy, chemical, and energy-related industries and to carry out carefully selected benchmark measurements on key systems. The research is being done jointly by two groups within the Thermophysics Division of the NIST Chemical Science and Technology Laboratory; one group is located in the Gaithersburg, MD, laboratories and the other at the Boulder laboratories. The specific measurement capabilities to be developed in this project include new apparatus for transport properties (thermal conductivity and viscosity), for thermodynamic properties (pressure-volumetemperature 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

172. Low Resistivity Ohmic Contacts Between Semiconductors and High-T. Superconductors

<u>FY 1994</u> \$108,000

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

National Institute of Standards and Technology Contacts: J. Moreland, (303) 497-3641 and J. W. Ekin, (303) 497-5448

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

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

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

173.	Thin Film Characterization and Flaw Detection	<u>FY 1994</u>
		\$90,452
DOE	Contact: Oscar P. Manley, (301) 903-5822	
North	western 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 neartip 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

174. <u>The Evolution of a Hele-Shaw Interface and Related Problems in</u> <u>Dendritic Crystal Growth</u>

<u>FY 1994</u> \$66,118

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 socalled 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

175. <u>Experiments on the Gas Dynamics of the High Velocity</u> Oxy-Fuel (HVOF) Thermal Spray Process

<u>FY 1994</u> \$94,142

DOE Contact: Oscar P. Manley, (301) 903-5822 Pennsylvania State University Contact: G. Settles, (814) 863-1504

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

Keywords: Surface Coatings, HVOF Sprays

176. <u>Transport Properties of Disordered Porous Media from the</u> <u>Microstructure</u>

<u>FY 1994</u> \$0

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 energyrelated 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

177. Effect of Forced and Natural Convection on Solidification of Binary Mixtures

FY 1994 \$93,664

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 (NH₄ Cl-H₂O) systems.

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

178. Inelastic Deformation and Damage at High Temperature

<u>FY 1994</u> \$0

DOE Contact: Oscar P. Manley, (301) 903-5822 Rensselaer Polytechnic Institute Contact: Erhard Krempl, (518) 266-6432

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

Keywords: Fracture, Damage

179. Flux Flow, Pinning and Resistive Behavior in Superconducting Networks FY 1994 \$70,519

DOE Contact: Oscar P. Manley, (301) 903-5822 University of Rochester Contact: S. Teitel, (716) 275-4039

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

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

Keywords: Flux Flow, Pinning, Vortex Motion, Superconductors

180. <u>Application of Magnetomechanical Hysteresis Modelling to Magnetic</u> <u>Techniques for Monitoring Neutron Embrittlement and Biaxial Stress</u>

<u>FY 1994</u> \$0

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

181. Stability and Stress Analysis of Surface Morphology of Elastic and Piezoelectric Materials FY

<u>FY 1994</u> \$0

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

182. Energy Changes in Transforming SolidsFY 1994
\$174,600DOE Contact: Oscar P. Manley, (301) 903-5822\$174,600Stanford 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

183.	<u>Optical</u>	Techniques for	Superconductor	Characterization	<u>FY 1994</u>
			-		\$0
DOF	Contact	Ocean P. Man	av (201) 002 502	17	

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

184.Degenerate Four-Wave Mixing as a Diagnostic of Plasma ChemistryFY 1994
\$195,907DOE Contact:Oscar P. Manley, (301) 903-5822\$195,907Stanford University Contact:R. Zare, (415) 723-3062\$195,907

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-inducivelycoupled plasma and the target radicals include CH, CH₂, C₂, C₂H, and CH₃ 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

185. <u>Effective Elastic Properties and Constitutive Equations for</u> Brittle Solids Under Compression

FY 1994 \$60,324

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

186. <u>3-D Experimental Fracture Analysis at High Te</u>	mperature FY 1994
	\$69,282
DOE Contact: Oscar P. Manley, (301) 903-5822	
University of Washington Contact: Albert Kobayashi,	(206) 543-5488

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

Keywords: Fracture, Failure Analysis

Geosciences Research

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

Materials Preparation, Synthesis, Deposition, Growth or Forming

187. <u>An Investigation of Organic Anion-Mineral Surface Interactions</u> <u>During Diagenesis</u>

<u>FY 1994</u> \$178,000

DOE Contact: W. C. Luth, (301) 903-5822 SNL Contacts: Patrick Brady and Randall Cygan, (505) 844-7216

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

Keywords: Surface reactions, Aluminosilicate Minerals, Adsorption Mechanisms

188. <u>Transition Metal Catalysis in the Generation of Petroleum and</u> Natural Gas

<u>FY 1994</u> \$97,000

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 progresssive thermal breakdown of kerogen and oil. Alternatively, transition metals, activated under the reducing conditions of diagenesis, can be proposed as catalysts in the generation of light hydrocarbons. Transition metal-rich kerogeneous sedimentary rocks were reacted under reducing conditions at temperatures for which the

substrates alone, N-octadecene + hydrogen, are stable indefinitely. Catalytic activity was measured to be on the order of 10^{-7} g CH₄/d/g kerogen, suggesting robust catalytic activity over geologic time at moderate sedimentary temperatures.

Keywords: Transition Metals, Catalysis, Petroleum

Materials Structure and Composition

189. Infrared Spectroscopy and Hydrogen Isotope Geochemistry of Hydrous Silicate Glasses FY 1994 \$153,000

DOE Contact: W. C. Luth, (301) 903-5822 Caltech Contacts: S. Epstein, (818) 356-6100 and E. Stolper, (818) 356-6504

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

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

Materials Properties, Behavior, Characterization or Testing

190.	Cation Diffusion Rates in Selected Silicate Minerals	<u>FY 1994</u>
		\$85,000

DOE Contact: W. C. Luth, (301) 903-5822 Sandia National Laboratory Contacts: Randall T. Cygan, H. R. Westrich 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 ordere to measure the relativel slow diffusion of Mg^{2+} , Mn^{2+} , and Ca^{2+} in garnets and pyroxenes. Depth profiles of tracer isotopes are then evaluated using an ion microprobe. Comparison of the diffusion coefficients determined under various oxygen fugacities provides information about the diffusion mechanism and the defect structure of the mineral sample. Results suggest a slower mechanism for magnesium diffusion in pyrope for relatively reducing conditions.

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

191. Shear Strain Localization and Fracture Evolution in Rocks	<u>FY 1994</u>
	\$72,000
DOE Contact: W. C. Luth, (301) 903-5822	
Northwestern University Contact: J. W. Rudnicki, (708) 491-3411	

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

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

192. Poroelasticity of Rock

<u>FY 1994</u> \$59,833

DOE Contact: W. C. Luth, (301) 903-5822 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

193.	Oxygen and Cation Diffusion in Oxide Materials	FY 1994
		\$238,270
DOE	Contact: W. C. Luth, (301) 903-5822	·
LLNI	Contact: F. J. Ryerson, (510) 422-6170	
Unive	rsity of California at Los Angeles Contact: K. D. McKeegan, (310) 825-277	79

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

194.	Grain Boundary Transport and Related Processes in Natural	
	Fine-Grained Aggregates	<u>FY 1994</u>
		\$302,000

DOE Contact: W. C. Luth, (301) 903-5822 Brown University Contacts: R. A. Yund, (401) 863-1931 and J. R. Farver, (401) 868-193x

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 monominerallic 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

195. <u>New Method for Determining Thermodynamic Properties of</u> Carbonate Solid-Solution Minerals

FY 1994 \$78,000

DOE Contact: W. C. Luth, (301) 903-5822 UC Davis Contacts: 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 establishe; (2) models of solute speciation are not required; (3) the measurements do not perturb the chemistry significantly.

Keywords: Carbonate Minerals, Solubility, Electrochemical Cell

196.	Investigation of Ultrasonic Wave Interactions with		
	Fluid-Saturated Porous Rocks		<u>FY 1994</u>
			\$161,000
DOE	Contact: W. C. Luth, (301) 903-5822		
01.			((1)) 000 0(55

Ohio State University Contacts: L. Adler, (614) 292-1266 and P.B. Nagy, (614) 292-3655

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

197. <u>Three-Dimensional Imaging of Drill Core Samples Using</u> Synchrotron-Computed Microtomography

<u>FY 1994</u> \$150,000

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

198.	Thermoo	<u>dynamics</u>	of Minera	ls Stable	Near the	Earth's S	Surface	<u>FY 199</u>	4
		•						\$145,00	0
DOE	Contact:	WCL	uth. (301) (013-5822					

Princeton University Contact: A. Navrotsky, (609) 258-4674

The purpose of this work is to expand our data base and understanding of the thermochemistry of minerals and related materials through a program of high temperature solution calorimetric studies. The technique of oxide melt calorimetry (in molten $2PbOB_2O_3$) 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

199. Theoretical Studies of the Adsorption of Gold Complexes and Flotation Collectors onto Sulfide Mineral Surfaces

FY 1994 \$35.000

DOE Contact: W. C. Luth, (301) 903-5822 University of Maryland Contact: John Tossell, (301) 314-1868

The project involves quantum mechanical (Hartree Fock) calculations of relative stabilities of species participating in dissolution and precipitation of gold on sulfide minerals. Although the solubility and surface adsorption of aqueous Au species on sulfide minerals are important agents of ore deposition, current understanding is limited by lack of information on surface complexation sites and speciation. Calculated site geometries and stabilities will be used to evaluate reactivity of various As and Sb sulfide mineral surfaces, addressing questions such as how structural differences among amorphous and crystalline forms of As_2S_3 influence interactions with surface water and Au complexes. Flotation processes to concentrate Au from ore rely on selective adsorption of oxysulfide collector molecules on Au-bearing sulfide minerals. Calculations of relative energies of molecular orbitals of various C-containing sulfide collectors (xanthates and/or carbamates) and P(OH)₃ complexes with Au+, Au₂, and Au(SH) will help to identify candidate collector molecules with improved efficiency.

Keywords: Surface Complexation, Gold Sulfides, Metal Transport

200. Transport Phenomena in Fluid-B	earing Rocks FY 1994
	\$144,000
DOE Contact: W. C. Luth, (301) 903-58	322

Renssalaer Polytechnic Institute Contact: E. B. Watson, (518) 276-6475

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

measurements and bulk fluid (air) diffusion through the samples. Direct imaging of the pore structure will also be attempted with Scanning Electron Microscopy and synchrotron X-ray tomography.

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

201.	Structure and Reactivity of Ferric Oxide and Oxyhydroxide Surfaces:	
	Quantum Chemistry and Molecular Dynamics	<u>FY 1994</u>
		\$127,500

DOE Contact: W. C. Luth, (301) 903-5822 PNL Contacts: Jim Rustad, David Sherman and Andrew Felmy, (509) 376-1134

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

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

202.	Micromechanics of Failure in Brittle Geomaterials	<u>FY 1994</u>
		\$171,000
DOF	Contact: W.C. Luth (201) 002 5822	-

DOE Contact: W. C. Luth, (301) 903-5822 SUNY - Stony Brook Contact: Teng-Fong Wong, (516) 632-8240 SNL Contact: Joanne Fredrich, (505) 846-0965

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

Keywords:	Brittle	Failure,	Plastic	Deformation,	Experimental	Rock	Deformation,
•	Cement	tation					

203.	Energetics of Silicate Melts from Thermal-Diffusion Studies	<u>FY 1994</u>
		\$169,000

DOE Contact: W. C. Luth, (301) 903-5822 Columbia University Contacts: David Walker, (914) 359-2900 and Marie Johnson, (914) 365-8712 University of California at Davis Contact: C. Lesher, (916) 752-9779

The research is to measure thermodynamic and kinetic properties of multicomponent fluid silicate systems that form the basis for predictive models of chemical diffusion, mineral dissolution, and complexation. Measurements of self and chemical diffusion of Sr and Nd in aluminosilicate melts have been obtained. Quantitative predictions of ion mobility based on Darken's theory have been extended to Pb and Hf. Measurements of thermal, self and chemical diffusion in the system CaO-MgO-SiO₂ are underway as the basis for extending the experimental data base to other major components in silicate melts.

Keywords: Multicomponent Diffusion, Silicate Melts, Thermal Diffusion

204.	Cation Chemisorption at Oxide Surfaces and Oxide-Water Interfaces:	
	X-Ray Spectroscopic Studies and Modeling	FY 1994
		\$204.000

DOE Contact: W. C. Luth, (301) 903-5822 Stanford University Contacts: G. E. Brown and G. A. Parks, (415) 723-9168

The research focuses on reactions and reaction mechanisms between aqueous metal ions and oxide surfaces representative of those found in the earth's crust as an aid to developing large-scale models of contaminant transport. Objectives are to (1) characterize reactions by direct sorption measurements, *in-situ* synchrotron-based x-ray absorption spectroscopy (XAS) of atomic environments at solid-water interfaces, and UV/Vis/IR spectroscopy; (2) investigate how these properties are affected by the solid surface and fluid composition; and (3) develop molecular-scale and macroscopic models for the sorption process. The reactions involve aqueous Co(II) and Pb(II) with Al₂O₃ (corundum), Fe₂O₃, and TiO₂, and the effect of organic liquids. New measurements of Pb(II) sorption on powdered corundum indicate sorption of polymeric species, suggesting that substrate structure is influencing the surface Pb(II) complexation. Comparative studies of the role of organic complexation on the sorption of Cu(II) on the surface of amorphous SiO_2 and on powdered corundum are aimed at specifying surface complexation mechanisms.

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

Division of Advanced Energy Projects

The Division of Advanced Energy Projects (AEP) provides support to explore the feasibility of novel, energy-related concepts that evolve from advances in basic research. These concepts are typically at an early stage of scientific 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

205. <u>Combustion Synthesis and Engineering of Nanoparticles for</u> Electronic, Structural and Superconductor Applications

FY 1994 \$186,000

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 BaTiO₃, 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.

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

206.	<u>Creation</u>	and Destruction of C ₆₀ and Other Fullerene Solids	FY 1994
DOE	Contact:	Dr. Walter M. Polansky, (301) 903-5995	\$301,000

University of Arizona Contact: Donald R. Huffman, (602) 621-4804

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

Keywords: Fullerenes, Diamond Powders, Buckyballs

207. Synthesis and Properties of High Strength Nanolayered CompositesFY 1994
\$315,000DOE Contact: Walter M. Polansky, (301) 903-5995\$315,000

Los Alamos National Laboratory Contact: Michael Nastasi, (505) 667-7007

The objective of this project is to synthesize and evaluate ultra high strength vapordeposited 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

208.	Optimally Controlled Interior Manipulation of Solids	<u>FY 1994</u> \$349,000
DOE Prince	Contact: Walter M. Polansky, (301) 903-5995 ton 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

209.	Design of Materials with Photonic Band Gaps	<u>FY 1994</u>
• •	•	\$297,000
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

210. <u>High Flux, Large-Area Carbon-Cluster Beams for Thin Film Deposition</u> and Surface Modification FY 1994 \$355,000

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 carbonimplanted 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

211. <u>Novel Composite Coatings for High Temperature Friction and</u> <u>Wear Control</u>

<u>FY 1994</u> \$260,000

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

212. <u>Synthesis of Advanced Composite Ceramic Precursor Powders by the</u> <u>Electric Dispersion Reactor</u>

<u>FY 1994</u> \$325,000

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 liquidliquid system while achieving intraparticle stoichiometric consistency. This leads to the production of high-quality precursor powders which, in turn, yields dense, consistent greenbody 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

213. <u>Development of an Ion Replacement Electrorefining Method</u>	<u>FY 1994</u>
	\$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

214.	Evaporation Through Tungsten to Achieve High-Rate Vapor Phase	
	Processing of Intermetallics	<u>FY 1994</u>
		\$291,000
		\$ 291,

DOE Contact: Walter M. Polansky, (301) 903-5995 General Electric Company Contact: David W. Skelly, (518) 387-6534

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

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

215. <u>Ultrasonic and Dielectric Noninvasive Diagnostics for</u> <u>Sintering of Ceramic Composites</u>

<u>FY 1994</u> \$358,000

DOE Contact: Walter M. Polansky, (301) 903-5995 Johns Hopkins University Contact: Moshe Rosen, (410) 516-8678

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

Keywords: Microwave Sintering, Ceramics, Noninvasive Diagnostics

216. <u>Compact MeV Ion Implanter</u>

<u>FY 1994</u> \$294,000

DOE Contact: Walter M. Polansky, (301) 903-5995 Lawrence Berkeley Laboratory Contact: Simone Anders, (510) 486-6745

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

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

217. <u>Thermoelectric Ouantum Wells</u>

<u>FY 1994</u> \$350,000

DOE Contact: Walter M. Polansky, (301) 903-5995 Lawrence Livermore National Laboratory Contact: Joseph C. Farmer, (510) 423-6574

Solid state thermoelectric devices have no moving parts and can be used to convert heat directly into electricity. Such devices can also be used as chlorofluorocarbon (CFC)-free refrigerators, provided that an external voltage is applied. Unfortunately, thermoelectric devices are not as efficient as their mechanical counterparts. However, theoretical physicists at the Massachusetts Institute of Technology have recently used quantum mechanics to design a new class of thermoelectric materials that may improve the efficiency (figure of merit) of thermoelectric devices to a point where they are competitive with conventional internal combustion engines and CFC-based refrigerators. Process technology developed at Lawrence Livermore National Laboratory for the fabrication of Xray optics is now being used to synthesize these new multilayer thermoelectric thin films. Multilayers are being made by alternately sputtering quantum well and barrier layers onto a moving substrate from dual magnetrons. A number of multilayer films, including hightemperature Si_{0.8}Geo_{.2}/Si and low-temperature Bi_{0.9}Sb_{0.1}/PbTe_{0.8}Se_{0.2}, are being synthesized and evaluated. This research can lead to new materials and devices.

Keywords: Quantum Wells, Thermoelectric Devices

218. Porous Carbons: Controlling Structure, Composition and Performance

<u>FY 1994</u> \$335,000

DOE Contact: Walter M. Polansky, (301) 903-5995 Lawrence Livermore National Laboratory Contact: Richard W. Pekala, (510) 422-0152

This research examines the synthesis and processing conditions necessary to tailor the local structure and composition of porous carbons for potential applications in energy storage devices. Carbon aerogels are being formed from resorcinol-formaldehyde and phenolic-furfural precursors. These porous carbons have low electrical resistivity, an ultrafine pore size distribution, high surface area (400 to 1100 square meters per gram, roughly the size of one or two basketball courts), and a solid matrix composed of interconnected particles or fibers. Preliminary data show that these materials are attractive electrodes for double layer capacitors. The project investigates sol-gel polymerization of multifunctional organic monomers, the phase separation of polymer/solvent mixtures, the

formation of porous composites, intrinsic chemical doping, and pyrolysis in controlled atmospheres. A variety of characterization tools are being used to study the structure and properties of porous carbons. The overall objective is to develop a fundamental understanding of how morphology, chemical composition, and local order affect the electrochemical performance of porous carbons. The potential payoff from this research is the development of new energy storage devices with superior performance.

Keywords: Porous Carbons, Energy Storage Devices

Materials Properties, Behavior, Characterization or Testing

219. Nonlinear Optics in Doped Fibers

<u>FY 1994</u> \$366,000

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

220. <u>Feasibility of a Novel Approach for Fast, Economical</u> Determination of Radiation Damage in Nuclear Reactor Cores

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

221. Hot Carrier Solar Cells

<u>FY 1994</u> \$330,000

<u>FY 1994</u> \$145,000

DOE Contact: Walter M. Polansky, (301) 903-5995 National Renewable Energy Laboratory Contact: Mark C. Hanna, (303) 384-6620

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

Keywords: Hot Carrier Solar Cells, High Efficiency Energy Conversion

222.	Atomic and Nanoscale Engineering of Thermophotovoltaic	
	Semiconductors Using Scanning Probe Microscopy Techniques	<u>FY 1994</u>
		\$177,000

DOE Contact: Walter M. Polansky, (301) 903-5995 National Renewable Energy Laboratory Contact: Lawrence L. Kazmerski, (303) 275-3711

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

Keywords: Thermophotovoltaics, Atomic Force Microscopy

Device or Component Fabrication, Behavior or Testing

223.	Ultrafast Molecular Electronic Devices	<u>FY 1994</u>
		\$405,000
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 photoinitiated 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

Office of Energy Research

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

224. <u>Photo-Induced Electron Transfer From a Conducting Polymer to</u> <u>Buckminsterfullerene: A Molecular Approach to High Efficiency</u> <u>Photovoltaic Cells</u>

FY 1994 \$283,000

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

225. Superconducting Bitter Magnets

<u>FY 1994</u> \$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

226.	Blue-Emitting Devices Based on Gallium Nitride	<u>FY 1994</u>
		\$319,000
DOE	Contact: Walter M. Polansky, (301) 903-5995	
Lawre	nce Berkeley Laboratory Contact: Michael D. Rubin, (510) 486-7124	

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

Keywords: Gallium Nitride, Blue-Emitting Devices

227. Solid State Multi-Layered Batteries

<u>FY 1994</u> \$419,000

DOE Contact: Walter M. Polansky, (301) 903-5995 Lawrence Livermore National Laboratory Contact: Richard M. Bionta, (510) 423-4846

The purpose of this project is to develop thin film solid-electrolyte batteries fabricated by the advanced multilayer sputtering techniques developed for X-ray optics. This technique allows the battery to be constructed *in situ* by depositing the anode, electrolyte, and cathode as distinct layers. Solid-electrolyte batteries have long been attractive because of their shelf-life and compatibility with severe environments. Recently,

rechargeable lithium cells that operate at ambient temperature have been developed based on ionically conducting solid polymer electrolytes. This project will concentrate on the development of thin-film solid-electrolyte cells constructed of lithium based inorganic materials fabricated by multilayer sputtering. The ability of this fabrication technique to discretely layer or compositionally grade thin films provides a unique opportunity to investigate the effect of electrode-electrolyte interface structure on cell performance. Finally, the computer control associated with this fabrication technique will allow the deposition of multiple cells in a bipolar configuration with either series or parallel connection. It is anticipated that this research will directly lead to power sources for modern electronic circuits (i.e., microsensors, memory elements, displays, and timers).

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

228. PV-Powered, Electrochromic Windows

FY 1994 \$330,000

DOE Contact: Walter M. Polansky, (301) 903-5995 National Renewable Energy Laboratory Contact: David K. Benson, (303) 384-6462

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

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

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 F	Properties.	Behavior,	Characterization	or Testing
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229.	Structural Materials Development	<u>FY 1994</u>
		\$389,000
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

230. <u>Repair Welding of Fusion Reactor Components</u>	<u>FY 1994</u>
	\$90,000
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 transmutationproduced 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

231. Insulating Ceramics for Fusion

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

232. Modeling Irradiation Effects in Solids

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

<u>FY 1994</u> \$290,000

<u>FY 1994</u> \$60,000 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

233. Fusion Systems Materials

<u>FY 1994</u> \$2,355,000

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 ferritic/ martensitic steels, vanadium alloys and SiC/SiC composites. Investigations focus on the most critical questions or limiting properties in each of these systems: ferritic/martensitic steels - DBTT transition shifts and fracture toughness, vanadium alloys - 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.

234. Structural Materials for Fusion Systems

<u>FY 1994</u> \$1,791,000

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

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

235. <u>Development of Radiation-Hardened Ceramic Composites for</u> <u>Fusion Applications</u>

FY 1994 \$49,000

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

236. <u>Radiation Effects and Micromechanics of SiC/SiC Composites</u>

FY 1994 \$97,000

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

237.	Damage Analysis and Fundamental Studies for Fusion	
	Reactor Materials Development	<u>FY 1994</u>
		\$180,000
DOE	Contact: F. W. Wiffen, (301) 903-4963	,
UCSB	Contacts: G. R. Odette, (805) 893-3525 and G. E. Lucas, (805) 893-4069	1

This research is directed at developing a fundamental understanding of both the basic damage process and microstructural evolution that take place in a material during neutron

irradiation. This understanding is used with empirical data to develop physically-based models of irradiation effects. The focus is on the fracture properties of vanadium alloys, austenitic and ferritic stainless steels, including helium effects, to (a) develop an integrated approach to integrity assessment, (b) develop advanced methods of measuring fracture properties, and (c) analyze the degradation of the mechanical properties of austenitic stainless steels. The program contributes to the assessment of the feasibility of using these alloys in ITER and other fusion systems.

Keywords: Vanadium, Steels, Irradiation Effects, Fracture

238. <u>Development of Lithium-Bearing Ceramic Materials for</u> <u>Tritium Breeding in Fusion Reactors</u>

<u>FY 1994</u> \$250,000

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

239. <u>Post-Irradiation Examination of Lithium-Bearing Ceramic Materials</u> for Tritium Breeding in Fusion Reactors

FY 1994 \$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) is nearing completion.

Keywords: Ceramics, Lithium Ceramics, Tritium Release

240. International Thermonuclear Experimental Reactor (ITER) Materials Development for Plasma Facing Components

<u>FY 1994</u> \$3,000,000

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

241.	ITER	Structural	Materials	Development

<u>FY 1994</u> \$630,000

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

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

Keywords: Vanadium, Irradiation Effects, Compatibility

242. ITER Ceramic Materials

<u>FY 1994</u> \$358,000

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

243. Radiation Hardened Fiber Optics for ITER Fusion Diagnostic Systems

FY 1994 \$50,000

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

244. <u>ITER Materials Evaluation</u>

<u>FY 1994</u> \$1,459,000

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 of the database needed for the use of these materials. Irradiation effects, compatibility and weldability of these materials are under study. The insulating ceramics work is focused on the electrical properties under irradiation, and the in situ measurement techniques to determine this response are being developed. The work at ORNL emphasizes the use of the HFIR to perform the irradiations in support of the ITER materials development and evaluation.

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

245. ITER Structural Materials Evaluation

<u>FY 1994</u> \$840,000

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

246. <u>Development of Nb₃Sn Superconducting Wire for the</u> <u>ITER Magnet Program</u>

<u>FY 1994</u> \$1,000,000

DOE Contact: M. M. Cohen, (301) 903-4253 MIT Contact: J. Minervini, (617) 253-5503

Activities include development of Nb₃Sn 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, Nb₃Sn

247. <u>Structural Materials Development for the Conduit of ITER</u> <u>Cable-in-Conduit-Conductors</u>

<u>FY 1994</u> \$1,100,000

DOE Contact: M. M. Cohen, (301) 903-4253 MIT Contact: J. Minervini, (617) 253-5503

Activities include fabrication of conduit for the conductors of the central solenoid and toroidal field model coils for ITER. The conduit material, Incoloy alloy 908, was developed via collaboration of INCO Alloys International and MIT. Work is proceeding on development of the database for this material. Alloy 908 has a low coefficient of expansion and minimizes the compressive strain in the Nb₃Sn 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 and FY 1994, the award size was increased to \$75,000. Phase II is the principal research or research and development effort and is performed in a period of up to two years. Phase II awards were limited to \$500,000 until FY 1994, when the maximum was increased to \$600,000. Under Phase III, commercial applications of the research or research and development are to be pursued by small businesses with non-Federal capital or, alternatively, Phase III may involve follow-on non-SBIR Federal contracts for products or processes desired by the Government.

The materials-related projects, like all other projects in the DOE SBIR program, were selected using the specific evaluation criteria listed in the program solicitation. 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: <u>Abstracts of Phase I Awards, 1994</u> (DOE/ER-0630 and -0606), <u>Abstracts of Phase II</u> <u>Awards, 1994</u> (DOE/ER-0628), and <u>Abstracts of Phase II Awards, 1993</u> (DOE/ER-0600). Copies of these publications may be obtained by calling Mrs. Kay Etzler on (301) 903-5867.

Materials Preparation, Synthesis, Deposition, Growth or Forming

Phase I Projects:

Low Cost, High Purity Silicon by Alkaline Glycolic Digestion of Silica - DOE Contact Alec Bulawka, (202) 586-5633; AstroPower, Inc. Contact Mr. Thomas J. Stiner, (302) 366-0400

High Speed Sheet Growth of Thin Silicon Films - DOE Contact Alec Bulawka, (202) 586-5633; AstroPower, Inc. Contact Mr. Thomas J. Stiner, (302) 366-0400

An Innovative Approach for Large Area Photovoltaic Material Processing - DOE Contact Alec Bulawka, (202) 586-5633; International Solar Electric Technology, Inc. Contact Dr. Bulent Basol, (310) 216-4427

Low Cost Solar Cell Leads for Use in Photovoltaic Modules - DOE Contact Alec Bulawka, (202) 586-5633; Solar Engineering Applications Corporation Contact Mr. Neil Kaminar, (408) 986-9231

<u>Very Low-Cost/High-Efficiency Thin-Film Silicon Photovoltaic Technology</u> - DOE Contact Alec Bulawka, (202) 586-5633; Spire Corporation Contact Mr. Patrick N. McDonnell, (617) 275-6000

Improved Activated Carbon for Hydrogen Storage - DOE Contact JoAnn Milliken, (202) 586-2480; Arcanum Corporation Contact Mr. Helmut F. Stern, (313) 665-4421

<u>A Superplastic Oxide Dispersion Strengthened Magnesium Alloy for Automotive</u> <u>Applications</u> - DOE Contact Sidney Diamond, (202) 586-8032; Chesapeake Composites Corporation Contact Dr. Alexander Brown, (302) 324-9110

Low Cost Synthesis of Nanocrystalline Silicon Carbide Starting with Fullerene Precursors - DOE Contact Clifford Smith, (412) 892-4518; Materials and Electrochemical Research Corporation Contact Dr. R. O. Loutfy, (602) 574-1980

<u>A Ceramic Material and Process for Use in Monolithic Ceramic Cross-Flow Filters</u> -DOE Contact Thedore J. McMahon, (304) 291-4865; Blasch Precision Ceramics, Inc. Contact Mr. David W. Bobrek, (518) 372-9416 High Temperature Brazing of Silicon Carbide - DOE Contact Charles Thomas, (412) 892-5731; Busek Company, Inc. Contact Mrs. J. Budny, (617) 449-3929

<u>Molecular Composite Plastics for Lightweight Green Cars</u> - DOE Contact Robert Astheimer, (301) 903-4410; Maxdem, Inc. Contact Dr. Matthew Marrocco, (909) 394-0644

<u>Surface Hardening of Polymeric Composites by High Energy Ion Irradiation</u> - DOE Contact Robert Astheimer, (301) 903-4410; UES, Inc. Contact Mr. Robert W. Vukusich, (513) 426-6900

<u>A Novel Method for Manufacture of High Temperature Superconducting Coils for</u> <u>High Temperature Operation</u> - DOE Contact Cynthia Carter, (301) 903-5997; IGC Advanced Superconductors, Inc. Contact Mr. B. A. Zeitlin, (203) 753-5215

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

<u>Development of Metal Hydride Materials for High Coefficient of Performance Heat</u> <u>Pumps</u> - DOE Contact Cynthia Carter, (301) 903-5997; Thermal Electric Devices, Inc. Contact Dr. Charles Stein, (505) 272-7505

<u>Growth of Lutetium Phosphate Scintillator Crystals for Positron Emission</u> <u>Tomography</u> - DOE Contact Gerald Goldstein, (301) 903-5348; ALEM Associates/ Radiation Monitoring Devices Contact Dr. Alexander Lempicki, (617) 353-9581

<u>Top-Seeded Solution Growth of Lutecium Phosphate from Potassium Pyrophosphate</u> <u>Flux</u> - DOE Contact Gerald Goldstein, (301) 903-5348; Deltronic Crystal Industries, Inc. Contact Mr. Stuart Samuelson, (201) 361-2222

<u>Production of Carbon-11-Labeled Compounds for Positron Emission Tomography</u> with a Low Energy Accelerator - DOE Contact Gerald Goldstein, (301) 903-5348; Science Research Laboratory, Inc. Contact Dr. Jonah Jacob, (617) 547-1122

<u>Sapphire-Metal Joining for Low-Loss Gyrotron Windows</u> - DOE Contact T. V. George, (301) 903-4957; FM Technologies, Inc. Contact Dr. Frederick M. Mako, (703) 425-5111

Economical and Reliable Niobium-Tin Conductors via Innovations in Stabilizers -DOE Contact T. V. George, (301) 903-4957; IGC Advanced Superconductors, Inc. Contact Mr. B. A. Zeitlin, (203) 753-5215 An Innovative Technique to Bond One Dimensional Carbon-Carbon Composites to Dispersion Strengthened Copper - DOE Contact T. V. George, (301) 903-4957; Materials and Electrochemical Research Corporation Contact Dr. R. O. Loutfy, (602) 574-1980

Advanced Low-Stress Brazing of Plasma-Facing Fusion Components with High Energy Electron Beams - DOE Contact T. V. George, (301) 903-4957; Science Research Laboratory, Inc. Contact Dr. Jonah Jacob, (617) 547-1122

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

Ductile Joining of Beryllium to Copper - DOE Contact T.V. George, (301) 903-4957; Surmet Corporation Contact Dr. Suri A. Sastri, (617) 272-3250

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

Niobium Titanium Multifilamentary Materials with Silicon in the Matrix - DOE Contact Jerry Peters, (301) 903-5228; IGC Advanced Superconductors, Inc. Contact Mr. B. A. Zeitlin, (203) 753-5215

<u>A Novel Approach to Fabrication of Niobium-Tin Conductor with Artificial Pinning</u> <u>Centers</u> - DOE Contact Jerry Peters, (301) 903-5228; IGC Advanced Superconductors, Inc. Contact Mr. B. A. Zeitlin, (203) 753-5215

High Quality Chemically Vapor Deposited Niobium Coatings for Superconducting Radio Frequency Cavities - DOE Contact Jerry Peters, (301) 903-5228; Sumi Tech, Inc. Contact Mrs. Mallika D. Ilindra, (703) 552-8334

<u>Niobium-Titanide Tin/Copper Multifilamentary Superconducting Wire with</u> <u>Niobium/Titanium Composite Filaments</u> - DOE Contact Jerry Peters, (301) 903-5228; Supercon, Inc. Contact Ms. Elaine Drew, (508) 842-0174

Development of Niobium-Titanium-Tantalum Artificial Pinning Center Superconductors for Very High Field Applications - DOE Contact Jerry Peters, (301) 903-5228; Supercon, Inc. Contact Ms. Elaine Drew, (508) 842-0174 Jet Vapor Deposition of Thick Films for the Production of Radioactive Beams of Chemically Active Elements - DOE Contact Richard Rinkenberger, (301) 903-3613; Jet Process Corporation Contact Mr. Jerome J. Schmitt, (203) 786-5130

<u>Microchannel Plates Fabricated by Track Etch Lithography</u> - DOE Contact Richard Rinkenberger, (301) 903-3613; Spire Corporation Contact Mr. Patrick N. McDonnell, (617) 275-6000

Radiation-Hard and Solar Blind Ultraviolet X-Ray Chemically Vapor Deposited-Diamond Photodiode Detectors - DOE Contact Richard Rinkenberger, (301) 903-3613; Vactronic Laboratory Equipment, Inc. Contact Mr. Robert Salat, (516) 567-0520

Phase II Projects: (First Year)

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

<u>Production of Carbon Materials from Biomass</u> - 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 <u>Composite Wires</u> - DOE Contact Cynthia Carter, (301) 903-5997; American Superconductor Corporation Contact Mr. Edward P. Hamilton, (617) 923-1122

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

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

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

Improved Coated-Metal Hydrogen Extraction Membranes - DOE Contact Robert Marianelli, (301) 903-5804; REB Research and Consulting Contact Dr. Robert E. Buxbaum, (517) 332-0243 <u>Methods of Improving Internal-Tin Niobium-Tin for Fusion Applications</u> - DOE Contact Warren Marton, (301) 903-4965; IGC Advanced Superconductors, Inc. Contact Mr. B. A. Zeitlin, (203) 753-5215

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

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

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

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

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

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

<u>Phase II Projects:</u> (Second 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

<u>Development of a Process to Synthesize Tubular Fullerenes</u> - DOE Contact Robert Marianelli, (301) 903-5804; Materials and Electrochemical Research Corporation Contact Dr. J. C. Withers, (602) 574-1980

<u>Continuous Production of Fullerenes from Hydrocarbon Precursors</u> - DOE Contact Robert Marianelli, (301) 903-5804; TDA Research, Inc. Contact Mr. John D. Wright, (303) 422-7918

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<u>Preparation of Low-Density Microcellular Materials from Fullerenes</u> - DOE Contact Robert Marianelli, (301) 903-5804; TDA Research, Inc. Contact Dr. William L. Bell, (303) 420-4329

<u>New Gadolinium-Boron Compounds for Neutron Capture Therapy</u> - DOE Contact Gerald Goldstein, (301) 903-3213; Boron Biologicals, Inc. Contact Dr. Bernard F. Spielvogel, (919) 832-2044

<u>Refractory Metal Coatings on Carbon/Carbon Composites for First Wall</u> <u>Applications</u> -DOE Contact Marvin Cohen, (301) 903-4253; Applied Sciences, Inc. Contact Mr. Jyh-Ming Ting, (513) 766-2020

<u>A Thermal Composite Plasma Facing Material</u> - DOE Contact Marvin Cohen, (301) 903-4253; Energy Science Laboratories, Inc. Contact Dr. Timothy R. Knowles, (619) 552-2034

<u>A Niobium-Tin Multifilamentary Composite Superconductor with Artificial Copper</u> (Bronze) Inclusions - DOE Contact Marvin Cohen, (301) 903-4253; Supercon, Inc. Contact Dr. Dingan Yu, (508) 842-0174

<u>A Porous Metal Heat Exchanger Cooled Microwave Cavity</u> - DOE Contact T. V. George, (301) 903-4957; Thermacore, Inc. Contact Mr. John H. Rosenfeld, (717) 569-6551

<u>Development of Silicon Carbide Ceramic Composites for Fusion Reactor</u> <u>Applications</u> - 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

Materials Properties, Behavior, Characterization or Testing

Phase I Projects:

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

High Temperature Thermally Stable Multi-Layer Ouantum Well Films - DOE Contact Bill Barnett, (301) 903-3097; Hi-Z Technology, Inc. Contact Mr. Norbert B. Elsner, (619) 535-9343 <u>Hydrogen Permeation Barriers for Bimodal Reactors</u> - DOE Contact John Warren, (301) 903-6491; Thermacore, Inc. Contact Mr. Richard W. Longsderff, (717) 569-6551

<u>Fracture Toughness Testing with Minimal Material</u> - DOE Contact Dennis Harrison, (301) 903-2884; Packer Engineering, Inc. Contact Dr. James A. Begley, (412) 921-6441

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

<u>Rare Earth Endohedral Fullerenes as New Nonlinear Optical Materials</u> - DOE Contact Cynthia Carter, (301) 903-5997; TDA Research, Inc. Contact Mr. Michael E. Karpuk, (303) 940-2301

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

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

<u>A Novel Detector for Neutron Diffraction Studies</u> - DOE Contact Manfred Leiser, (301) 903-3426; Radiation Monitoring Devices, Inc. Contact Dr. Gerald Entine, (617) 926-1167

An Analytical Research Materials Characterization Facility Based on Synchrotron Radiation - DOE Contact Manfred Leiser, (301) 903-3426; X-Ray Analytics, Ltd. Contact Dr. Kevin L. D'Amico, (708) 887-9941

Application of the Meandering Winding Magnetometer to an *In-Situ* Determination of Age Related Degradation - DOE Contact Oscar Manley, (301) 903-5822; Jentek Sensors, Inc. Contact Dr. Neil J. Goldfine, (617) 254-5552

Improvement in the Loss and Critical Current Density Properties of Internal-Tin Niobium-Tin - DOE Contact T.V. George, (301) 903-4957; IGC Advanced Superconductors, Inc. Contact Mr. B. A. Zeitlin, (203) 753-5215 <u>A Feasibility Study to Correlate Vanadium (Chromium, Titanium) Alloy Weld</u> <u>Strength with Weld Chemistry</u> - DOE Contact F. W. Wiffen, (301) 903-4963; Charles Evans and Associates Contact Mr. James E. Plank, (415) 369-4567

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

Activated Optical Ceramics: A New Class of Materials for Environmental Monitoring - DOE Contact Caroline Purdy (301) 903-7672; ALEM Associates Contact Dr. Alexander Lempicki, (617) 236-1025

Phase II Projects: (First Year)

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: (Second Year)

<u>A Novel Energy-Efficient Membrane System for the Recovery of Volatile Organic</u> <u>Contaminants from Industrial Process Gases</u> - DOE Contact Dan Kung, (708) 252-2023; Bend Research, Inc. Contact Dr. Scott B. McCray, (503) 382-4100

Device or Component Fabrication, Behavior or Testing

Phase I Projects:

<u>Monolithic Integration of Thin Film Photovoltaics on Insulated Metal Substrates</u> -DOE Contact Alec Bulawka, (202) 586-5633; Energy Photovoltaics, Inc. Contact Mr. David A. Jackson, (609) 587-3000

Development of a Low Cost High Concentration Photovoltaic Dense Array Module for Use with Reflective Concentrators - DOE Contact Alec Bulawka, (202) 586-5633; SunPower Corporation Contact Dr. Richard Swanson, (408) 991-0908

<u>Non-Precious Metal Catalysts for Proton Exchange Membrane Fuel Cells by Ion</u> <u>Beam Synthesis</u> - DOE Contact JoAnn Milliken, (202) 586-2480; Electrochem, Inc. Contact Dr. Radha Jalan, (617) 932-3383 <u>Contamination Tolerant Anodes for Polymer Electrolyte Membrane Fuel Cells</u> -DOE Contact JoAnn Milliken, (202) 586-2480; ICET, Inc. Contact Mr. Srinivasan Sarangapani, (617) 769-6064

<u>Contamination Tolerant Anodes for Proton Exchange Membrane Fuel Cells</u> - DOE Contact JoAnn Milliken, (202) 586-2480; Lynntech, Inc. Contact Dr. G. Duncan Hitchens, (409) 693-0017

Metal Carbide Nanoclusters for Polymer Electrolyte Membrane Fuel Cells - DOE Contact JoAnn Milliken, (202) 586-2480; TDA Research, Inc. Contact Mr. Michael E. Karpuk, (303) 940-2301

<u>A New Semiconductor Radiation Sensor for Expedited Waste Site Characteriza-</u> <u>tion</u> - DOE Contact Caroline Purdy, (301) 903-7672; Aurora Technologies Corporation Contact Dr. J. F. Butler, (619) 549-4645

An Acoustic Plate Mode Aqueous Mercury Sensor - DOE Contact Paul Hart, (301) 903-7456; BIODE, Inc. Contact Dr. Douglas McAllister, (207) 883-1492

An Off-Line-Locked Laser Diode Sensor (OLDS) - DOE Contact Paul Hart, (301) 903-7456; Spectral Sciences, Inc. Contact Dr. Fritz Bien, (617) 273-4770

High Energy Resolution Cadmium-Zinc-Telluride Semiconductor Radiation Detectors - DOE Contact Ken Sheely, (202) 586-1620; Opire Corporation Contact Mr. Patrick N. McDonnell, (617) 275-6000

Gas Separation Membranes Based on Permselective Films of Buckminsterfullerenes - DOE Contact Charles Thomas, (412) 892-5731; CeraMem Corporation Contact Dr. Robert L. Goldsmith, (617) 899-0467

Fullerene Based Catalysts for Heavy Oil Upgrading - DOE Contact Udaya Rao, (412) 892-4743; TDA Research, Inc. Contact Mr. Michael E. Karpuk, (303) 940-2301

<u>Coal Ash Tiles by Microwave Processing</u> - DOE Contact Mary Ashbaugh, (304) 291-4966; Chemat Technology, Inc. Contact Mr. Patrick Lin, (818) 727-9786

Development of Expansive Cements Using Dry Flue Gas Desulfurization Solid Wastes - DOE Contact Mary Ashbaugh, (304) 291-4966; Praxis Engineers, Inc. Contact Ms. Suzanne C. Shea, (408) 945-4282 <u>Metal Monoliths for Conversion of Natural Gas to Liquid Fuel</u> - DOE Contact Rodney D. Malone, (304) 291-4723; Alabama Cryogenic Engineering, Inc. Contact Ms. Mary T. Hendricks, (205) 536-8629

Oxygen-Evolving Anodes for the Electrolysis of Calcium Oxide - DOE Contact Eli Goodman, (301) 903-2966; EMEC Consultants Contact Dr. Rudolf Keller, (412) 325-3260

<u>A Long Life Perovskite Oxygen Electrode for Calcium Oxide Processing in Nuclear</u> <u>Fuel Cycles</u> - DOE Contact Eli Goodman, (301) 903-2966; Eltron Research, Inc. Contact Ms. Eileen E. Sammells, (303) 440-8008

<u>A Low Emission Alkali Metal Thermal to Electric Converter Automotive Power</u> <u>System</u> - DOE Contact Robert Astheimer, (301) 903-4410; Advanced Modular Power Systems, Inc. Contact Dr. Thomas K. Hunt, (313) 677-4260

Advanced Catalysts for Ultra-Low Emission Control in Natural Gas Fueled <u>Vehicles</u> - DOE Contact Robert Astheimer, (301) 903-4410; Goremotive Industries, Inc. Contact Mr. Arthur D. Sweet, (818) 884-0015

<u>A Membrane Reactor for the Production of Hydrogen Fuel from Hydrocarbon</u> <u>Liquids</u> - DOE Contact Robert Astheimer, (301) 903-4410; Membrane Technology and Research, Inc. Contact Ms. E. G. Weiss, (415) 328-2228

Economical Photochromic Films for Solar Thermal Control - DOE Contact Cynthia Carter, (301) 903-5997; EIC Laboratories, Inc. Contact Dr. A.C. Makrides, (617) 769-9450

<u>Thermophotovoltaic Generator Efficiency Improvement</u> - DOE Contact Cynthia Carter, (301) 903-5997; Quantum Group, Inc. Contact Dr. Mark Goldstein, (619) 457-3048

High-Performance Membranes for Gas, Vapor, and Liquid Separations - DOE Contact Robert Marianelli, (301) 903-5804; Bend Research, Inc. Contact Dr. Rod Ray, (503) 382-4100

<u>Organic-Inorganic Composite Membranes for Gas Separation and Vapor</u> <u>Permeation</u> - DOE Contact Robert Marianelli, (301) 903-5804; CeraMem Corporation Contact Dr. Robert L. Goldsmith, (617) 899-0467

189

<u>Electrode Materials for Rechargeable Lithium Batteries</u> - DOE Contact Robert Marianelli, (301) 903-5804; Materials and Electrochemical Research Corporation Contact Dr. J. C. Withers, (602) 574-1980

<u>Novel High Performance Glassy Polymer Composite Membranes for Gas</u> <u>Separation</u> - DOE Contact Robert Marianelli, (301) 903-5804; Membrane Technology and Research, Inc. Contact Ms. E. G. Weiss, (415) 328-2228

<u>Highly Selective Membranes for the Separation of Organic Vapors Using</u> <u>Super-Glassy Polymers</u> - DOE Contact Robert Marianelli, (301) 903-5804; Membrane Technology and Research, Inc. Contact Ms. E. G. Weiss, (415) 328-2228

<u>A Continuous Cryopump/Pellet-Fabrication Apparatus for Fusion</u> - DOE Contact T. V. George, (301) 903-4957; Cryogenic Applications F, Inc. Contact Dr. Christopher A. Foster, (615) 435-5433

Innovative Electrochemical Sensors for *In-Situ* Real-Time Monitoring of Lead in Aqueous Media - DOE Contact Caroline Purdy, (301) 903-7672; ANDCARE, Inc. Contact Mrs. Carolyn J. Henkens, (919) 544-8220

<u>Fluoroionophores for Use in a Fiber Optic Sensor for Mercuric Ions</u> - DOE Contact Caroline Purdy, (301) 903-7672; Covalent Associates, Inc. Contact Dr. Victor R. Koch, (617) 938-1140

Potentiometric Sensors for Lead and Mercury - DOE Contact Caroline Purdy, (301) 903-7672; ICET, Inc. Contact Dr. S. Sarangapani, (617) 769-6064

<u>A Compressed Xenon Gamma Sensor for Environmental Measurements</u> - DOE Contact Caroline Purdy, (301) 903-7672; Contact Dr. John Kevin Markey, (203) 230-0894

<u>Fiber Optic Sensors for Heavy Metal Cations</u> - DOE Contact Caroline Purdy, (301) 903-7672; Research International, Inc. Contact Ms. Joyce M. Brien, (206) 486-7831

Innovative Sorbents for the Selective Removal of Heavy Metals from Groundwater -DOE Contact Jeffrey Walker, (301) 903-7966; Foster-Miller, Inc. Contact Mr. Adi R. Guzdar, (617) 890-3200

An Ultra-Compact Cesium Iodide/Mercuric Iodide Gamma-Ray Scintillation Spectrometer - DOE Contact Michael O'Connell (202) 586-9311; Xsirius, Inc. Contact Dr. Jan S. Iwanczyk (805) 484-8300 Phase II Projects: (First Year)

<u>Glass-Ceramic Construction Tiles from Coal-Fired Boiler Flyash</u> - DOE Contact Mary B. Ashbaugh, (304) 291-4966; Vortec Corporation Contact Dr. James G. Hnat, (215) 489-2255

<u>A High Repetition-Rate, High Power, All-Solid-State Pulsed Driver for</u> <u>Electrodeless Inductive Thrusters</u> - DOE Contact John Warren, (301) 903-6491; Science Research Laboratory, Inc. Contact Dr. Jonah Jacob, (617) 547-1122

Demonstration of an Integrated Carbon Dioxide/Thermal Management System for Carbonate Fuel Cells - DOE Contact Clifford Carpenter, (304) 291-4041; Energy Research Corporation Contact Dr. Hans Maru, (203) 792-1460

Porous Aluminum Nitride Part Fabrication to Support Advanced Battery Development - DOE Contact Cynthia Carter, (301) 903-5997; Advanced Refractory Technologies, Inc. Contact Mr. Keith A. Blakely, (716) 875-4091

<u>Capacitive Energy Storage Using High Surface Area Transition Metal Compounds</u> -DOE Contact Cynthia Carter, (301) 903-5997; Chemat Technology, Inc. Contact Ms. Xin Qin, (818) 727-9786

Advanced Ceramic Fibers for a Carbonate Fuel Cell Matrix - DOE Contact Bruce Harrington, (304) 291-5427; Energy Research Corporation Contact Dr. Hans Maru, (203) 792-1460

<u>An In-Situ Particle Sensor for Metal Forming Processes</u> - DOE Contact Manfred Leiser, (301) 903-3426; Advanced Fuel Research, Inc. Contact Dr. David G. Hamblen, (203) 528-9806

Development of a High Spatial Resolution Neutron Detector - DOE Contact Manfred Leiser, (301) 903-3426; BioTraces, Inc. Contact Dr. A. K. Drukier, (301) 864-0816

<u>A High Resolution Scintillator-Based Neutron Detector</u> - DOE Contact Manfred Leiser, (301) 903-3426; Nanoptics, Inc. Contact Dr. James K. Walker, (904) 378-6620

<u>On-Chip Infrared-Spectral Sensors by Superconducting Detector Arrays</u> - DOE Contact Robert Marianelli, (301) 903-5804; Advanced Fuel Research, Inc. Contact Dr. David G. Hamblen, (203) 528-9806 Radiation Resistant Radio Frequency Feedthrough Insulators for Fusion Applications - DOE Contact Warren Marton, (301) 903-4965; Composite Technology Development, Inc. Contact Dr. Naseem A. Munshi, (303) 447-2226

<u>Helium-Cooled Divertors with Low-Activation Materials and Simple Fabrication</u> <u>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</u> <u>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>Ceramic Filters for Ultrafine Particulate Separation in Combustion Gas</u> <u>Environments</u> - DOE Contact Richard Tischer, (412) 892-4891; Materials and Electrochemical Research Corporation Contact Dr. J. C. Withers, (602) 574-1980

A Carbonate Fuel Cell Monolith for Low-Cost and High Power Density Operation -DOE Contact Venkat Venkataraman, (304) 291-4105; Energy Research Corporation Contact Dr. Hans Maru, (203) 792-1460

Phase II Projects: (Second Year)

<u>Digital Processing Electronics for X-Ray Detector Arrays</u> - DOE Contact Manfred Leiser, (301) 903-3426; X-Ray Instrumentation Associates Contact Dr. William K. Warburton, (415) 903-9980

<u>A Cold/Thermal Beam Bender Using Capillary Optics to Increase the Number of</u> <u>End-Guide Instrument Positions</u> - 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 <u>Concept Testing</u> - 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

<u>Low-Cost Microstrip Detectors on Conductivity-Modified Polyimide</u> - 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

<u>Fabrication of Niobium-Aluminum Superconducting Strands Using Mechanical</u> <u>Alloying and Other Techniques</u> - DOE Contact Gerald Peters, (301) 903-5228; IGC Advanced Superconductors, Inc. Contact Mr. G. M. Ozeryansky, (203) 753-5215

<u>Durable, Low Cost Ceramic Materials for Use in Hot Gas Filtration Equipment</u> -DOE Contact Norman Holcombe, (304) 291-4829; Industrial Filter and Pump Manufacturing Company Contact Mr. Paul Eggerstedt, (708) 656-7800

<u>High Cation Mobility Lithium Polymer Batteries</u> - DOE Contact Al Landgrebe, (202) 586-1483; Covalent Associates, Inc. Contact Dr. Larry A. Dominey, (617) 938-1140

<u>A Real-Time X-ray Detector</u> - DOE Contact Stan Sobczynski, (202) 586-1878; Advanced Technology Materials, Inc. Contact Mr. David Kurtz, (203) 794-1100

Small Business Technology Transfer Program

The Small Business Technology Transfer (STTR) program, now completing its first year, was established as a three-year pilot program in compliance with the Small Business Research and Development Enhancement Act of 1992, Public Law 102-564. Grant applications are solicited from small science- and technology-based U.S. firms (with 500 employees or less) in collaboration with a non-profit research institution (e.g. National laboratories and universities). Awards are made competitively to the small business with the collaborating research institution serving as a subcontractor. STTR supports innovative R&D and encourages conversion of that R&D into commercial applications of economic benefit to the Nation. The STTR program is designed for implementation in three phases, with Phase I determining, insofar as possible, the scientific or technical merit and feasibility of ideas proposed for investigation. The period of performance in this initial phase is about nine months, and awards are limited to \$100,000. Phase II is the principal research or R&D effort, and only Phase I awardees can compete for Phase II awards of up to \$500,000 in FY 1995 for work to be performed in a period of up to two years. In Phase III, commercial application of the research or R&D is pursued using non-Federal funding or, alternatively, it may involve follow-on non-STTR Federal contracts for products or services desired by the Government.

The materials-related projects, like all other projects in the STTR program and the SBIR program, were selected on the basis of scientific and technical merit, as judged against the specific criteria listed in the solicitation. Conclusions were reached on the basis of

reviews performed by personnel in DOE laboratories, universities, private industry, and government.

As in the SBIR program, these projects represent high-risk research, but the potential benefits are also high if the objectives are met. Brief descriptions of all DOE STTR projects, not only those of interest in materials research, are given in <u>Abstracts of Phase I Awards 1994</u> (DOE/ER-0623).

Materials Preparation, Synthesis, Deposition, Growth or Forming

Phase I Projects:

<u>Preparation of Monolithic Porous Carbon Materials Using Controlled</u> <u>Functionalization of Fullerenes</u> - DOE Contact Rick Peavy, (202) 586-7907; TDA Research, Inc. Contact Mr. Michael E. Karpuk, (303) 940-2301; Research Institute: Sandia National Laboratory

<u>A Continuous Chemical Manufacturing Process for Direct Production of Titanium</u> <u>Powder with a Reagent Recycle</u> - DOE Contact Robert Astheimer, (301) 903-4410; Kroftt-Brakston International, Inc. Contact Dr. Donn R. Armstrong, (708) 655-3065; Research Institute: Argonne National Laboratory

Device or Component Fabrication, Behavior or Testing

Phase I Projects:

Feasibility of Nitride Phosphors for Thin Film Electroluminescent Displays - DOE Contact Charles Fowler, (202) 586-5834; Planar Systems, Inc. Contact Dr. Christopher N. King, (503) 690-1100; Research Institute: Los Alamos National Laboratory

<u>An Integrated X-ray Sensor</u> - DOE Contact Richard Rinkenberger, (301) 903-3613; ARACOR Contact Mr. Ed LeBaker, (408) 733-7780; Research Institute: Lawrence Berkeley Laboratory

Improved Mineral Insulated Cables for Fusion Reactor Diagnostics - DOE Contact T. V. George, (301) 903-4957; DELTA M Corporation Contact Mr. A. D. White, (615) 483-1569; Research Institute: Oak Ridge National Laboratory

OFFICE OF ENVIRONMENTAL MANAGEMENT

	<u>FY 1994</u>
Office of Environmental Management - Grand Total	\$37,914,500
Office of Waste Management	\$14,766,500
High Level Waste Division	\$14,766,500
Materials Preparation, Synthesis, Deposition, Growth or Forming	\$ 8,036,000
Technical Support to West Valley Demonstration Project	2,071,000
Sulfur Polymer Cement	342,000
Ceramic Final Forms	300,000
Microencapsulation in Final Forms	67,000
Final Waste Form Program	2,800,000
CIF Blowdown and Ash Stabilization	70,000
Macroencapsulation	15,000
Glass Formulation	2,371,000
Materials Properties, Behavior, Characterization or Testing	\$ 6,730,500
Materials Characterization Center Testing of West Valley	
Formulation Glass	384,500
Development of Test Methods and Testing of West Valley	,
Reference Formulation Glass	564,000
Process and Product Quality Optimization for the	
West Valley Waste Form	422.000
Waste Form Qualification	5.000.000
Iron-Enriched Basalt Testing	360,000
Office of Environmental Restoration	\$ 2,874,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	\$ 2,874,000
Minimum Additive Waste Stabilization (MAWS)	2,874,000

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OFFICE OF ENVIRONMENTAL MANAGEMENT

<u>FY 1994</u>

Office of Technology Development	\$20,274,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	\$13,376,000
Polymer Solidification	2,450,000
Microwave Solidification	2,197,000
Polymer Solidification National Effort	485,000
Expedited Development-Polymer Macroencapsulation	237,000
Fixed Hearth Plasma Treatment Process	2,075,000
Fixed Hearth Plasma Radioactive Waste Test	1,200,000
PHP Slag Chemistry and Slag/Metal Processing (ANL-W)	400,000
Phosphate-Bonded Ceramic Waste Forms	300,000
Mixed Waste Treatability - Thermoplastic Final Forms	600,000
High Temperature Melter Systems Evaluation	1,335,000
MAWS Plasma Testing and Support	2,097,000
Materials Properties, Behavior, Characterization or Testing	\$ 6,898,000
Vitrify to Delist to Dispose	1,798,000
Vitrification of Rocky Flats Waste	750,000
Plasma Hearth Process Radioactive Waste Test - Idaho	1,800,000
Waste Form Performance Criteria	180,000
Vitreous Ceramic Compositional Envelope Study	500,000
Arc Melter Vitrification	900,000
Graphite DC Plasma Arc Melter	970,000

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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:

- 1. Office of Waste Management The Office of Waste Management uses current technologies to minimize production of DOE-generated waste, alters current processes to reduce waste generation, and works with the Office of Technology Development to develop innovative technologies for the treatment and disposal of present and future waste streams. The mission of the Office is to minimize, treat, store, and dispose of DOE waste to protect human health, safety, and the environment.
- 2. Office of Environmental Restoration The Office of Environmental Restoration directs the cleanup of inactive facilities and sites contaminated by waste generated from past nuclear operations. The mission of the Office is to ensure that risks to the environment and to human health and safety posed by inactive and surplus facilities and sites are either eliminated or reduced to prescribed, acceptable levels.
- 3. Office of Technology Development The Office of Technology Development is responsible for managing the national program of environmental applied research and technology development. The Office manages and directs research, development, demonstration, testing, and evaluation programs and activities that are designed to provide complete innovative technologies and technology systems to address the major problems facing the Office of Environmental Management.
- 4. Office of Facility Transition and Management One of the Office of Environmental Management (EM) goals is to ensure that the risks to human health and safety and to the environment posed by inactive and surplus facilities are either eliminated or reduced to prescribed, acceptable levels. The Office of Facility Transition and Management was established within EM to develop and institutionalize a Departmental process for the timely and effective transfer of surplus facilities and to implement that process in transitioning surplus facilities to EM for final disposition.

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Five Focus Areas were formed to focus the EM-wide technology development activities on DOE's most pressing environmental management problems and are co-led by all EM offices:

- Contaminated Plume Containment and Remediation
- Landfill Stabilization
- High-Level Waste Tank Remediation
- Mixed Waste Characterization, Treatment, and Disposal
- Facility Transition

Materials development work may be performed in any of these five Focus Areas. Funding levels are reported for the total project, which includes materials development and demonstration. For most projects, materials development accounts for less than 25% of the funds.

Office of Waste Management

High Level Waste Division

The objective of the High Level Waste Division is to conduct waste management activities for ending interim storage of high-level waste and achieving permanent disposal of high-level waste at the Savannah River Site in South Carolina. Additionally, Congress directed the Department in 1980 to demonstrate the solidification of liquid high-level waste at West Valley (New York) which originated at the nation's only commercial plant to reprocess spent nuclear fuel. At both of these sites a program is in place to immobilize the high-level waste in preparation for geologic disposal.

At Savannah River and West Valley, high-level waste will be immobilized in a borosilicate glass prepared in a liquid-fed ceramic joule-heated melter. The Defense Waste Processing Facility at Savannah River is beginning 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.

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Materials Preparation. Synthesis. Deposition. Growth or Forming

248. <u>Technical Support to West Valley Demonstration Project</u>

<u>FY 1994</u> \$2,071,000

> <u>FY 1994</u> \$342,000

DOE Contact: W. S. Ketola, (716) 942-4314 PNL Contact: W. F. Bonner, (509) 376-3340

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; fabrication of a radioactive glass sample made from actual West Valley high-level wastes; 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

249. <u>Sulfur Polymer Cement</u>

DOE Contact: Jamie Johnson, (301) 903-7114

The work consists of demonstrating the technical feasibility of sulfur polymer cement (SPC) as an immobilization technique for producing a final waste form for alpha low level stored waste. Major areas of focus include determining the longevity of SPC encapsulated waste forms and determining waste types that may be compatible with SPC encapsulation. The workscope also includes obtaining resolution to technical issues to aid in developing conceptual design direction for SPC process and equipment requirements, providing support for a full-scale equipment demonstration of SPC encapsulation techniques, and providing support for attendance at ASTM Subcommittee 34.07 (Mixed Radioactive Hazardous Waste).

Keywords: Polymer, Cement, Final Waste Form, Sulfur

250. <u>Ceramic Final Forms</u>

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DOE Contact: Ronald D. Streit, (510) 422-7045 LLNL Contact: Robert Hoppert, (510) 423-2420

Operations of the Mixed Waste Management Facility (MWMF) will yield ash-like residues (oxides, nitrates, etc. containing RCRA metals and radioactive elements) from the organic components of low-level mixed waste. These residues will be stabilized as a durable

FY 1994 \$300.000 and leach-resistant ceramic waste form produced by traditional high-temperature powder technologies. Formulations for various input waste streams are being optimized.

Keywords: Ceramic, Final Waste Form, Ash

251. <u>Microencapsulation in Final Forms</u>

DOE Contact: Ronald D. Streit, (510) 422-7045 LLNL Contact: Robert Hoppert, (510) 423-2420

Operations of the Mixed Waste Management Facility (MWMF) will yield residues from the destruction of organic components of low-level mixed waste. Salts containing RCRA metals and radioactive elements will be stabilized by microencapsulation in polyethylene or in a thermosetting polymer. Volatile inorganic solids will be microencapsulated in sulfur polymer cement. These technologies are being optimized for MWMF operations.

Keywords: Final Waste Form, Encapsulation, Polymer

252. <u>Final Waste Form Program</u>

DOE Contact: Michael Torbert, (301) 903-7109

In support of the Oak Ridge Reservation (ORR) LDR Federal Facility Compliance Agreement as well as the Federal Facility Compliance Act, a program is underway to demonstrate, at the bench-scale level, applicable final waste forms for sludges, soils, other treatment residues, and secondary wastes. The primary focus of this activity is to demonstrate appropriate grout waste forms as a first alternative, glass waste forms as a second alternative, and thermoplastic waste forms as a third alternative. This work is being done on actual ORR wastes and supports the LDR FFCA, and the design of the ORR Mixed Waste Treatment Facility. It will provide technology support to ORR privatization activities. This activity will support a joint CRADA with Savannah River Technical Center and SEG.

Keywords: Final Waste Form, Grout, Glass, Thermoplastic, Bench-Scale

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<u>FY 1994</u> \$2.800.000

<u>FY 1994</u> \$67,000

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Office of Environmental Management

253. CIF Blowdown and Ash Stabilization

DOE Contact: Kurt Fisher, (301) 903-7412

This activity will develop stabilization technology for the Consolidated Incineration Facility (CIF) blowdown and ash waste streams. The current focus of this activity is developing a cementitious waste form.

Keywords: Stabilization, Cement

254. <u>Macroencapsulation</u>

DOE Contact: Hannibal Joma, (510) 423-8394

This study is designed to stabilize radioactive and hazardous constituents by "grouting" or amalgamating in order to limit the leachability of these constituents. This study uses the LDR BDAT for lead pieces and elemental mercury to affect treatment.

Keywords: Macroencapsulation, Lead, Stabilization

255. Glass Formulation

DOE Contact: Denny Wynne, (301) 903-4967

This activity includes evaluation of alternatives within glass formulation, structure and chemistry studies, and durability studies. This activity supports design of the low-level waste Vitrification Facility at Hanford.

Keywords: Glass, Vitrification, Low-Level Waste

Materials Properties, Behavior, Characterization or Testing

256. <u>Materials Characterization Center Testing of West Valley Formulation</u> <u>Glass</u>

<u>FY 1994</u> \$384,500

DOE Contact: W. S. Ketola, (716) 942-4314 PNL Contact: G. L. Smith, (509) 372-1957

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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

<u>FY 1994</u> \$70,000

<u>FY 1994</u> \$15,000

<u>FY 1994</u> \$2,371,000 radionuclides. The MCC also began testing of a small sample of glass containing actual West Valley high-level waste.

Keywords: Radioactive Waste Host

257. Development of Test Methods and Testing of West Valley Reference Formulation Glass FY 1994

DOE Contact: W. S. Ketola, (716) 942-3414 PNL Contact: P. B. Macedo, (202) 319-5329

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

258.	Process and Product Quality Optimization for the	
	West Valley Waste Form	<u>FY 1994</u>
		\$422,000

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

259. <u>Waste Form Qualification</u>

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<u>FY 1994</u> \$5,000,000

\$564,000

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

260. <u>Iron-Enriched Basalt Testing</u>

<u>FY 1994</u> \$360,000

DOE Contact: Jamie Johnson, (301) 903-7114

The work consists of continuing development of a final waste form (Iron-Enriched Basalt) for the Idaho Waste Processing Facility (IWPF). Activities include:

- Modeling slag and offgas process chemistry for several waste streams using a computer model to simulate the process chemistry and mass flow balance;
- Conducting studies and tests to determine methods to retain High Vapor Pressure Metals (HVPM) in an Iron-Enriched Basalt (IEB) waste form and;
- Reviewing the development needs for IEB as a waste form for the IWPF including IEB development work being planned/performed by other projects (e.g., Buried Waste Integrated Demonstration, Pit 9 Project).

Keywords: Final Waste Form, Basalt

Office of Environmental Restoration

The Office of Environmental Restoration directs the assessment and cleanup of inactive facilities and sites contaminated by waste generated from past nuclear operations. The Environmental Restoration program assessment and cleanup activities include remedial actions and decontamination and decommissioning. Remedial actions are concerned with all aspects of the assessment and cleanup of inactive release sites. The tasks associated with remedial actions encompass (1) site discovery, preliminary assessment, and site inspection; (2) site characterization, analysis of cleanup alternatives, and selection of remedy; (3) cleanup and site closure; and (4) site compliance monitoring. Most remedial action activities are concerned with contaminated soil and groundwater.

Materials Preparation, Synthesis, Deposition, Growth or Forming

261. <u>Minimum Additive Waste Stabilization (MAWS)</u>

<u>FY 1994</u> \$2,874,000

DOE Field Office Contact: Rod Warner, (513) 648-3156 DOE HQ Program Manager: David Kozlowski, (301) 427-1858 ANL Contact: Nick Beskid, (708) 252-6677

This project demonstrated soil washing in combination with vitrification of Fernald OU-1 sludges and soils. Work included the testing of the 0.25 cu.yd./hr soil wash unit and 300 kg/day joule heated melter. This project was completed after producing several

thousand kg of glass from OU-1 high fluoride sludges and soils contaminated with uranium and thorium.

Keywords: Vitrification, Soil Washing, Glass

Office of Technology Development

The Office of Technology Development (TD) has the mission to facilitate EM's 30year goal by developing and implementing new technologies to assist DOE in achieving compliance with all applicable statutes 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 and ceramics are being pursued to better understand high-temperature technologies, useful for containment of contaminated soils. Vitrification and plasma technologies are being developed for treating specific mixed waste streams. 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

262. Polymer Solidification

<u>FY 1994</u> \$2,450,000

DOE Field Office Contact: Sherri Rudolph, (303) 966-5788 DOE HQ Program Manager: Alison Johnson, (301) 903-7923 EG&G Rocky Flats Contact: Andrea Faucette, (303) 966-6420

Polymer encapsulation of mixed wastes encloses waste products in thermoplastic materials using commercially available processing technologies. The configuration under development at the Rocky Flats Environmental Technology Site uses a twin-screw extruder to microencapsulate waste. The process aims at meeting applicable disposal site, EPA, and DOT acceptance criteria for various wastes. Microencapsulation involves combining thermoplastic polymers (i.e. polyethylene) with dried waste; melting, mixing, and extruding the combination in a commercially-available extruder; and allowing the molten plastic to cool and solidify. Hazardous constituents are immobilized in the plastic matrix. Nitrate salts, bypass sludge, incinerator ash, and secondary wastes are the target streams. Microencapsu-

FY 1994

\$2,197,000

lation tests of a variety of waste streams have been performed with the extruded waste forms meeting TCLP leach test performance limits. Waste loadings from 40 percent to 60 percent were successfully demonstrated for surrogate bypass sludge, spray dried nitrate salts (saltcrete stream), DETOX solution, and analytical lab solutions (nitrate, chloride salts).

Keywords: Alternative Final Waste Form, Polymer Solidification, Hydroxide Sludge, Polyethylene

263. Microwave Solidification

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DOE Field Office Contact: Sherri Rudolph, (303) 966-5788 DOE HQ Program Manager: Alison Johnson, (301) 903-7923 EG&G Rocky Flats Contact: Greg Sprenger, (303) 966-3159

The microwave solidification project is developing a method to immobilize wastes for compliance with EPA disposal regulations and to minimize the volume of wastes for storage and disposal. Microwave solidification uses 915 MHz microwave energy to vitrify waste solids. Dried waste and glass formers are fed into drums and melted "in the drum" from applied microwave heating. This technology is being evaluated as a potential method to treat several mixed wastes, including process sludges, incinerator ash, and miscellaneous wastes, such as crucibles and foundry materials. Four tests on samples of actual transuranic precipitation sludge from the Rocky Flats Plant were vitrified in a bench scale (6 kW) system. A 60 percent to 70 percent volume reduction and 60 percent to 70 percent waste loading were achieved. Simulated waste was vitrified in a 20 Kw-915 Mhz pilot scale system with 75 percent volume reduction achieved. Such large size reductions result in significant disposal cost savings compared to baseline technologies.

- Keywords: Alternative Final Waste Form, Microwave Solidification, Vitrification, In Drum Melting
- 264. <u>Polymer Solidification National Effort</u> DOF Field Office Contact: Steve Webster (708) 252-2093

DOE Field Office Contact: Steve Webster, (708) 252-2093 DOE HQ Program Manager: Alison Johnson, (301) 903-7923 Brookhaven NL Contact: Paul Kalb, (516) 282-7644

The objective of this project was to demonstrate a pilot scale system for the polymer microencapsulation of surrogate wastes such as Rocky Flats nitrate salts using a single screw extruder. The demonstration incorporated many aspects of the process including the drying of the salts, the encapsulation of the salts, and the testing of the waste forms for compliance with disposal criteria. This process is applicable for forming final waste forms for several waste streams including precipitated hydroxide sludge, soils, ground glass, beryllium dust,

<u>FY 1994</u> \$485,000 and others. This process produces a highly durable, leach resistant waste form that produces a much smaller volume of waste for final disposal compared to cementation. The smaller volume saves money in storage, transport and disposal. By using an off-the-shelf extruder with minor modifications, equipment costs were reduced for small waste streams.

Keywords: Alternative Final Waste Form, Polymer Microencapsulation, Solidification, Nitrate Salts, Polymer Extrusion

265. Expedited Development-Polymer MacroencapsulationFY 1994\$237,000

DOE Field Office Contact: Sherri Rudolph, (303) 966-5788 DOE HQ Program Manager: Alison Johnson, (301) 903-7923 EG&G Rocky Flats Contact: Joseph Lucerna, (303) 966-7229

This project developed macroencapsulation of debris and lead waste and produced an expedited radioactive demonstration of the technology. Macroencapsulation involves suspending bulk mixed waste (i.e., waste contaminated with both radioactive and hazardous constituents) materials, debris, or lead in a drum and filling in around the waste with molten polyethylene or with thermoset plastics, such as epoxy. Upon cooling, the polymer hardens, surrounding and immobilizing the hazardous constituents. This will allow wastes stored at Rocky Flats and other sites to meet land disposal restrictions. Macroencapsulation tests of bulk debris surrogates for U and Be-fines contaminated solids have been successfully completed. The task is a continuation of FY93 work and included in FY94 the complete cold testing with surrogate waste, and the purchase of a full scale extruder for use during hot testing of actual waste. Work also included the preparation of test and safety plans for conducting the hot demonstration of real waste in accordance with all internal and external policies and procedures, and the performance of a hot demonstration and documentation of the results.

266. Fixed Hearth Plasma Treatment Process

<u>FY 1994</u> \$2,075,000

DOE Field Office Contact: Thomas Williams, (208) 526-2460 DOE HQ Program Manager: Paul Hart, (301) 903-7456 EG&G Idaho Contact: Steve Bates, (208) 526-6970

This technology, the Plasma Hearth Process (PHP), converts entire drums of lowlevel mixed waste (LLMW) directly into an enhanced waste form without extensive pretreatment or characterization. Organics are destroyed while metals and inorganics are melted, creating a vitrified slag and molten metal. The process is characterized by high-

Keywords: Polymer Macroencapsulation, Alternative Final Waste Form, Debris, Lead, Thermoset Plastic

FY 1994

\$1,200,000

efficiency destruction of organics, encapsulation of heavy metals and radionuclides in the vitrified final waste form, large volume reduction of waste to be disposed, possible recycling of metals, low off-gas flow rates, and the capability of processing many waste types in a single-step process. The non-radioactive proof-of-principle concept demonstration has been completed. The remaining work in this task focuses on design, fabrication, and demonstration of a near full-scale pilot system for non-radioactive operation.

Keywords: Plasma, Final Form, Low-Level Mixed Waste, Full-Scale

267. Fixed Hearth Plasma Radioactive Waste Test

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DOE Field Office Contact: Steve Webster, (708)-252-2822 DOE HQ Program Manager: Paul Hart, (301) 903-7456 ANL-W Field Contact: Grant McClellan, (208) 533-7257

This project involves the design and construction of the facility modifications to house the bench-scale Plasma Hearth Process to be tested in the Plasma Hearth Process Radioactive Waste Test - Idaho. It also includes tasks to develop the mechanisms by which actual waste can be repackaged for testing in the bench-scale system, the radioactive waste forms produced by the process can be sampled and analyzed, and the pertinent analysis to be made to ensure safe operation of the plasma system in the ANL-W TREAT facility. Waste operations and sampling and analysis during the bench-scale demonstration are covered in the task.

Keywords: Plasma, Final Form, Low-Level Mixed Waste, Bench-Scale

268.	Plasma Hearth Process (PHP) Slag Chemistry and Slag/Metal	
	Processing (ANL-W)	<u>FY 1994</u>
		\$400,000
DOE	Field Office Contact: Steve Webster, (708)-252-2822	
DOE	HQ Program Manager: Paul Hart, (301) 903-7456	
Argon	ne National Laboratory Contact: Ankur Purohit, (708) 252-6670	

The purpose of this task is to define the design basis and validate the final design of the slag and metal removal and handling system to be built for the field-scale radioactive plasma hearth process (PHP) system by SAIC and Retech, Inc. Initial slag/metal separation tests have been completed at the STAR Center for design validation. This task will ensure that the design will meet DOE nuclear facility design and safety requirements for plutonium service, will allow an actual facility to operate in a production mode making acceptable slag and metal products, and will reflect the best applicable practices from the primary metal production industries with particular emphasis being in the electric steel making processes. Keywords: Plasma, Final Form, Low-Level Mixed Waste, Field-Scale

269. Phosphate-Bonded Ceramic Waste Forms

<u>FY 1994</u> \$300,000

DOE Field Office Contact: Steve Webster (708) 252-2822 DOE HQ Program Manager: Paul Hart, (301) 903-7456 Argonne National Laboratory Contact: A. Wagh, (708) 252-4295,

Chemically-bonded ceramics (CBCs) are being investigated as an alternative final waste form for streams that cannot be handled by other established methods. Phosphate bonded ceramics are a subclass of CBCs and have several advantages over other systems for stabilization and encapsulation of LLMW. These include insolubility in water, high-temperature stability, and the ability to cure at room temperatures. Studies are underway to stabilize waste streams containing liquid mercury, mercury-contaminated aqueous liquids, toxic and heavy metal containing materials, salt cakes, beryllium wastes, and pyrophorics by encapsulating them in phosphate-bonded ceramics. Feasibility tests on ash and salt wastes were completed at Argonne National Laboratory in FY94.

Keywords: Alternate Final Waste Form, Ceramics, Phosphate

270. Mixed Waste Treatability - Thermoplastic Final Forms

<u>FY 1994</u> \$600,000

DOE Field Office Contact: Steve Webster (708) 252-2822 DOE HQ Program Manager: Paul Hart, (301) 903-7456 Brookhaven National Laboratory Contact: P. Kalb, (516) 282-7644

The focus of this project will be on the evaluation and demonstration of polyethylene and modified sulfur cement encapsulation of mixed wastes, which contains high chloride, mercury, and tritium. Brookhaven National Laboratory has developed several polymer solidification final waste form processes for the treatment of DOE waste. Treatability studies using the encapsulation agents on the surrogate wastes were completed in FY94. A field-scale demonstration of polyethylene encapsulation of high-nitrate surrogate mixed waste was accomplished in FY94 using a fully integrated single-screw process.

Keywords: Thermoplastic, Alternate Final Waste Form, Polyethylene, Solidification

271. <u>High Temperature Melter Systems Evaluation</u>

<u>FY 1994</u> \$1,335,000

DOE Field Office Contact: Tom Williams (208) 526-2460 DOE HQ Program Manager: Grace Ordaz, (301) 903-7440 Catholic University Contact: Ian Pegg, (202) 319-6700 This project investigated innovative methods of vitrification that provide higher temperature processing capabilities. High temperature processing is desirable where there is insufficient fluxing agents available within the wastes. Higher temperatures, however, can also increase volatilization which is undesirable. Vitrification methods under consideration include microwave, plasma, and high-temperature joule heating which will allow a cold cap of unmelted materials to minimize volatilization. The project tested each of these methods at bench-scale. Those showing the most promise will be scaled up.

Keywords: Vitrification, High Temperature

272. MAWS Plasma Testing and Support

<u>FY 1994</u> \$2,097,000

<u>FY 1994</u> \$1,798,000

DOE Field Office Contact: Gary Staats (412) 892-6741 DOE HQ Program Manager: Grace Ordaz, (301) 903-7440 Catholic University Contact: Jeff Ruffner, (406) 494-7412

This project included the testing of several high-metals content feeds in the Plasma Centrifugal Furnace and general engineering/technical support in high temperature processing areas for a future MAWS demonstration. A small-scale plasma unit was purchased for expedited testing on a variety of wastes in support of slag waste form compositional envelope development. This was required before full-scale testing in the larger PACT 6 plasma unit.

Keywords: Plasma, Centrifugal Furnace, MAWS

Materials Properties, Behavior, Characterization or Testing

273. <u>Vitrify to Delist to Dispose</u>

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DOE Field Office Contact: M. O'Rear, (803) 725-5541 DOE HQ Program Manager: Paul Hart, (301) 903-7456 Savannah River Site Contact: Denny Bickford, (803) 725-3737

Vitrification involves converting wastes, which are primarily inorganic in nature, into a durable, leach-resistant glass. Emphasis has been placed on broadening the number of waste streams applicable to vitrification by establishing the processing envelopes for specific representative waste streams. Surrogates of radioactive waste streams have been vitrified in pilot-scale demonstrations conducted at Clemson University in FY94. In addition, a pilotscale radioactive demonstration on actual Savannah River Site M-area sludge was conducted at Catholic University. A major effort was initiated in FY94 to identify an actual mixed waste stream and procure the equipment to assemble a transportable field-scale vitrification unit. The waste stream, Oak Ridge WETF (an inorganic wastewater treatment residue)

209
sludge, was successfully vitrified at the bench-scale at Oak Ridge. A field-scale radioactive demonstration using the transportable vitrification system will commence in September, 1995 at the Oak Ridge K-25 Site.

Keywords: Vitrification, Low-Level Mixed Waste, Joule Heated Glass Melter

274. Vitrification of Rocky Flats Waste

DOE Field Office Contact: Deborah Trader, (509) 376-1831 DOE HQ Program Manager: Paul Hart, (301) 903-7456 Pacific Northwest Laboratory: Richard Peters, (509) 376-3903

This project determined the vitrification process envelop for three actual waste streams. The process envelopes were defined in terms of waste stream compositional variability, glass forming additives, and the limits of incorporation of troublesome species. The process envelopes were determined by a combination of crucible tests, pilot-scale melter runs and vitrification processing modeling. Leaching tests show that the mixed waste glasses are generally as durable or more durable than high-level waste glasses.

Keywords: Vitrification, Low-Level Mixed Waste, Joule Heated Glass Melter

275. Plasma Hearth Process (PHP) Radioactive Waste Test - Idaho	<u>FY 1994</u>
	\$1,800,000
DOE Field Office Contact: Thomas Williams, (208) 526-2460	
DOE HQ Program Manager: Paul Hart, (301) 903-7456	

DOE HQ Program Manager: Paul Hart, (301) 903-7456 EG&G Idaho Contact: Steve Bates, (208) 526-6970

This project involved the design, construction, testing, and evaluation of a bench-scale Plasma Hearth Process. The primary goal of this work was to assess the performance of the PHP on actual radioactive wastes and to determine the fate of the radionuclides contaminating the waste upon treatment. The successful conclusion of this project will ensure that the PHP can be employed in radioactive service. In addition data collected in this work will improve the simulation of radionuclides in full-scale systems by surrogates.

Keywords: Plasma, Final Form, Low-Level Mixed Waste, Bench-Scale

<u>FY 1994</u> \$750,000

276. <u>Waste Form Performance Criteria</u>

DOE Field Office Contact: Steve Webster, (708) 252-2822 DOE HQ Program Manager: Paul Hart, (301) 903-7456 Brookhaven National Laboratory Contact: Eena-Mai Franz, (516) 282-7103

This project involved the completion of the Waste Form Performance Criteria and Testing/Evaluation Methods that could be used as guidance in judging viability of a waste form as a physical-chemical barrier to releases of radionuclides and RCRA regulated hazardous components. This report was published in August 1994 and is available through NTIS as document DOE/MWIP-30.

Keywords: Waste Form, Performance Criteria

277. Vitreous Ceramic Compositional Envelope Stud	ly <u>FY 1994</u>
	\$500,000
DOE Field Office Contact: Steve Webster, (708) 252-2	2822
DOE HQ Program Manager: Grace Ordaz, (310) 903	-7440
ANL Contact: Dave Wronkiewicz, (708) 252-7263	

This project is part of a larger effort to develop acceptable glass and ceramic waste forms. By better understanding the compositional effects on glass performance and identifying compositional areas where good performance is assured the MAWS program can rapidly screen potential combinations of waste that might be good candidates for vitrification. This project specifically looks at vitrified waste forms where there is a tendency to form stable crystals upon slow cooling.

so, words. Composition, Characterization, Min My	Keywords:	Composition,	Characterization,	MAW
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278. Arc Melter Vitrification	<u>FY 1994</u>
	\$900,000
DOE HQ Program Manager: Jaffer Mohiuddin, (301) 903-7965	-
EG&G Idaho Contact: Kevin Kostelnik, (208) 526-9642	

The objective of this project was to demonstrate the applicability of Arc Melter Vitrification for the treatment of mixed wastes and contaminated soils and in 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.

<u>FY 1994</u> \$180,000 University, industry, in addition to other laboratory participants, are being solicited to accelerate the potential for technology transfer.

Keywords: Arc, Melter, Vitrification

279. Graphite DC Plasma Arc Melter

FY 1994 \$970,000

DOE HQ Program Manager: Jaffer Mohiuddin, (301) 903-7965 EG&G Idaho Contact: Kevin Kostelnik, (208) 526-9642

The objective of this project was to demonstrate the applicability of the Graphite DC Plasma Arc Melter for treating mixed wastes and contaminated soils and for providing an extremely durable waste form for disposal. This pilot-scale unit is expected to process a nominal 0.5 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.

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Keywords: Graphite, DC, Plasma, Arc, Melter

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OFFICE OF NUCLEAR ENERGY

	<u>FY 1994</u>
Office of Nuclear Energy - Grand Total	\$55,265,000
Office of Space and Defense Power Systems	\$12,265,000
Radioisotope Power Systems Division	\$ 2,425,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	\$ 2,055,000
Development of Improved Thermoelectric Materials for Space Nuclear Power Systems Development of an Improved Process for the Manufacture	360,000
of DOP-26 Iridium Alloy Blanks, Product Characterization and Exploratory Alloy Improvement Studies Carbon-Bonded Carbon Fiber Insulation Production	1,135,000
Maintenance, Manufacturing Process Development and Product Characterization	560,000
Materials Properties, Behavior, Characterization or Testing	\$ 370,000
Development of an Improved Carbon-Carbon Composite Graphite Impact Shell Replacement Material	370,000
Space Reactor Power Systems Division	\$9,840,000
Thermoelectric Space Nuclear Power Systems Technology	\$3,205,000
SP-100 Ground Engineering System Project	3,205,000

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OFFICE OF NUCLEAR ENERGY (Continued)

	<u>FY 1994</u>
Space Reactor Power Systems Division (continued)	
Thermionic Space Nuclear Power System Technology	\$ 6,635,000
Thermionic Fuel Element (TFE) Verification Program (DOE) Thermionic Space Nuclear Reactor Design and	4,300,000
Technology Demonstration Plan (DOD)	1,800,000
Space Power and Propulsion Application Studies	535,000

Office of Naval Reactors

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\$43,000,000^{*}

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[•]This excludes \$54 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.

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 gaseous diffusion plants are now being operated by the USEC under a lease arrangement with DOE.

Materials R&D activities in FY 1994 within the Office of Uranium Programs were varied and, for the most part, classified Restricted Data. The DOE contact is William VanDyke, (301) 903-4201.

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

280. <u>Development of Improved Thermoelectric Materials for</u> <u>Space Nuclear Power Systems</u>

<u>FY 1994</u> \$360,000

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 silicongermanium (Si-Ge) type thermoelectric materials. The goal or target properties are average Figure of Merits, Z of 0.8 and 1.2×10^{-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 1994, emphasis continued to be placed on the optimization of the mechanical alloying process and associated consolidation parameters for the production of low oxygen improved performance Si-Ge thermoelectric materials. A cooperative program was initiated with Martin Marietta Astro Space for the demonstration of improved Si-Ge thermoelectrics in a Unicouple device, an 18 couple module. Scale-up of the hot isostatic pressing consolidation process yielded product suitable for Unicouple manufacture. Thermoelectric properties of production material was fully characterized. Exploration of techniques for the addition of nano-size second phase particulates was continued.

Keywords: Mechanical Alloying, Consolidation of Powder, Powder Synthesis, Semiconductors, Thermoelectrics

281. <u>Development of an Improved Process for the Manufacture of DOP-26</u> <u>Iridium Alloy Blanks, Product Characterization, and Exploratory</u> <u>Alloy Improvement Studies</u>

<u>FY 1994</u> \$1,135,000

DOE Contact: W. Barnett, (301) 903-3097 RNL Contacts: E. P. George, (615) 574-5085 and E. K. Ohriner, (615), 574-8519

An iridium alloy, DOP-26 (i.e., Ir-0.3 wt.% W with Th and Al dopant additions), serves as the fuel clad or capsule material for isotope heat sources employed in recent and contemporary space power systems for NASA deep space missions. This program is aimed at the optimization of the new improved process route previously selected for the production of DOP-26 iridium alloy sheet, namely a consumable vacuum arc cast/extrusion/"warm" rolling route. The effectiveness of this production process was further demonstrated in the FY 1994 production of DOP-26 alloy blanks, foil and clad vent sets for the Cassini Mission. Production yields have continued to exceed our goals.

Studies of bare rolling, of blank stock and bare forming of cups was initiated.

Continued product characterization studies, particularly for simulated service conditions, continued to show behaviors equivalent or superior to the prior process product.

Studies of alternate iridium alloy doping agents were continued. The objective is to maintain or exceed the properties of the DOP-26 alloy at a significantly lower thorium dopant level. An iridium alloy containing 0.3 wt.%W with dopant additions of 40 appm cerium and 15 appm thorium was selected for scale-up to a nominal six kilogram consumable arc melted ingot.

Keywords: Consumable Arc Melt, Extrusion, Noble Metal

282. <u>Carbon-Bonded Carbon Fiber Insulation Production Maintenance</u>, <u>Manufacturing Process Development and Product Characterization</u> <u>FY 1994</u>

\$560,000

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 1994 program encompassed (1) maintenance of capability for both tube and plate billet production through the year, and (2) characterization of Cassini CBCF insulation thermal conductivity. Evaluation of three available data analysis algorithms has led to the selection of the Clark and Taylor algorithm for current use in processing thermal diffusivity data. During FY 1994 characterization efforts have been focused on experimental evaluation of short term (i.e., 5 to 760 seconds) high temperature (2200 to 3000°C) exposures on the degree of graphitization and its influence on thermal conductivity. A review of analytical methods for extrapolating thermal conductivity measurements in the ambient to 2000°C range to temperatures circa 4000°C was initiated.

Keywords: Insulators/Thermal, High Temperature Service, Fibers

Materials Properties, Behavior, Characterization or Testing

283.	Development of an Improved Carbon-Carbon Composite Graphite Impact	
	Shell Replacement Material	<u>FY 1994</u>
		\$370,000
DOF	E Contact: W. Barnett. (301) 903-3097	

Oak Ridge National Laboratory Contact: G. R. Romanowski, (616) 574-4838

The Graphite Impact Shell (GIS), a component of the General Purpose Heat Source isotopic heat source module is a closed end/capped tubular shape machined from AVCO 3D-CC fine weave pierced fabric material. It is anticipated that a change in the fiber reinforcement architecture from the current orthogonal structure to a cylindrical type structure will enhance energy absorption in high velocity impact. The current program is a feasibility study of commercially available and experimental materials.

During FY 1994 impact tests were conducted on 23 of 38 candidate materials representing at least two levels of densification for each architectural variant. Impact testing was performed at 55 m/s using a copper mass simulant to match the typical mass of a GPHS fueled clad. Force versus time was measured at the impact face. Testing and data analysis is continuing.

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 and assessment; 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 method development and application; and ground and flight system safety analysis.

Thermoelectric Space Nuclear Power System Technology

284. SP-100 Ground Engineering System Project	<u>FY 1994</u>
	\$3,205,000
DOE Contact: Lyle Rutger, (301) 903-6470	
Martin Marietta Astro Space Contact: Richard H. Hemler, (610) 354-3045	

The objective of this program was to develop space reactor power system components for use in future civil, commercial, and defense applications. Included in this comprehensive program were numerous activities related to materials development, fabrication, and testing. This project was discontinued in FY 1994. The work described below was accomplished in closing out the program:

Principal materials activities are:

Thermoelectric Cell Materials Development (\$860,000) - Silicon-germanium multicell 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 were tested.

Reactor Materials (\$155,000) - Stress tests of niobium zirconium alloys were conducted.

Heat Transport Materials (\$510,000) - Assembly of a thermoelectric electromagnetic pump consisting of niobium alloy ducts, thermoelectric cells, permanent magnets and niobium clad copper bus-bars was demonstrated.

Reactor Control Drive Materials (\$1,680,000) - Reactor control drive motor components were tested. These components incorporated a variety of technologies including wear resistant surfaces, bearings, and lubricants for use in a high temperature-radiation vacuum environment.

Keywords: Thermoelectric Cells, Refractory Metals, Tribology, 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. The MOU is still in effect, though funding shortfalls have curtailed several aspects of the agreement.

285. Thermionic Fuel Element (TFE) Verification Program	<u>FY 1994</u>
	\$4,300,000 - DOE
	\$0 - DOD

DOE Contact: J. Warren, (301) 903-6491 Hanford Contact: J. Hales, (509) 376-4069

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 was 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. This project was also terminated in FY 1994, with the principal effort during FY 1994 focused on program closeout activities. Some closeout tasks, including post irradiation examinations (PIEs) of TFE test articles, will be completed during FY 1995. TFE materials tested during the program included uranium dioxide fueled tungsten emitters, niobium collectors, alumina and yttria ceramic insulators and seals, and radiation resistant graphite cesium storage reservoirs.

Keywords: Thermionic, Uranium Dioxide, Ceramics, Graphite, Tungsten, Niobium, Alumina, Yttria, Space Reactors

286. <u>Thermionic Space Nuclear Reactor Design and Technology</u> <u>Demonstration Plan</u>

<u>FY 1994</u> \$0 - DOE \$1,800,000 - DOD

DOE Contact: D. Culp, (301) 903-3667 Rocketdyne Contact: R. Harty, (818) 586-3140 Space Power, Inc. Contact: K. Koester, (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. A 40 kWe end-of-life point design will be developed as a baseline using technology that is applicable over a 5 to 40 kWe power range. Two separate contract teams began work in 1992, Rocketdyne Division of Rockwell International and Space Power, Inc., with both pursuing in-core thermionic power conversion systems and utilizing Russian subcontractors. Significant accomplishments include one and two dimensional creep testing of single crystal molybdenum-niobium thermionic emitter materials in Russia; fabrication of an advanced 320-watt single cell thermionic fuel element in Russia with preparations for testing in the U.S.; testing of an advanced beryllium-yttrium hydride neutron moderator design in both the U.S. and Russia to assess lifetime and performance under irradiation as well as hydrogen retention at prototypic temperature conditions; and completion of preparations for lifetime testing of alumina sheath insulator specimens in Russia under prototypic thermal, applied voltage and fluence conditions.

Keywords: Thermionic, Molybdenum-Niobium, Beryllium-Yttrium Hydride, Alumina, Emitters, Moderators, Space Reactors

287.	Space Power and Propulsion Application Studies	<u>FY 1994</u>
		\$535,000

DOE Contact: Don Culp, (301) 903-3667

Assistance grants have been awarded to U.S. industry in response to a DOE Notice of Program Interest entitled, *Invitation for Proposals Designed to Support Federal Agencies and Commercial Interests in Meeting Special Power and Propulsion Needs for Future Space Missions*. Materials-related work to be accomplished includes compatibility tests of Russian binary uranium carbide fuel pellets with tungsten emitter sheaths for high temperature thermionic converter applications; investigating oxygen-ion-implanted niobium electrodes for higher thermionic power conversion efficiencies at lower temperatures; and evaluating design concepts for venting hydrogen from liquid-metal heat pipes in bimodal reactor applications. A few of the grant awardees have subcontracts with Russian entities which may provide technology transfer of Russian expertise or manufacturing capability to U.S. industry.

Keywords: Thermionics, Uranium Carbide, Tungsten, Niobium, Heat Pipes, Space Reactors

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 \$97 million in FY 1994 including approximately \$54 million as the cost for irradiation testing in the Advanced Test Reactor. The Naval Reactors contact is David I. Curtis, (703) 603-5565.

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OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT

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	<u>FY 1994</u>
Office of Civilian Radioactive Waste Management - Grand Total	\$2,200,000
Materials Properties. Behavior, Characterization or Testing	\$2,100,000
Waste Packages	\$2,100,000
Device or Component Fabrication, Behavior or Testing	\$100,000
Alternate Defense Waste Processing Facility (DWPF) Canister Fabrication Methods	\$100,000

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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

288. Waste Packages

<u>FY 1994</u> \$2,100,000

DOE Contact: Dean Stucker, (702) 794-7275 B&W Fuel Company Contact: Hugh Benton, (702) 794-1891

The waste package and waste form materials effort continued. Waste form studies include oxidation of spent fuel and dissolution of waste glasses, uranium oxides, spent fuel, and oxidized spent fuel. Degradation modes for corrosion-allowance materials were surveyed. The potential use of nonmetallic barriers was studied. Development of a qualityassured database of materials properties was begun. More realistic thermal and criticality models were developed, and the effects of rock fall were analyzed. Methods for fabricating waste containers were studied. Models for degradation of container materials were developed.

Keywords: Waste Packages, Ferrous Metals, Geologic Repository

Device or Component Fabrication, Behavior or Testing

289.	Alternate Defense	Waste	Processing	Facility	(DWPF)
	Canister Fabricatio	n Met	hods	-	

<u>FY 1994</u> \$100,000

DOE Contact: Timothy C. Gunter, (803) 557-2524 Westinghouse Contact: John Harbour, (803) 725-8725

Savannah River Technology Center (SRTC) has initiated a program to develop second generation canisters for capture and isolation of high-level radioactive waste glass produced at the Defense Waste Processing Facility (DWPF). Currently DWPF uses conventional rolland-welded fabrication for production of the cylindrical portion of the canister. The top and bottom heads are hot formed and then welded onto the ends of the cylinder. A machined nozzle is then welded onto the top head to complete the canister. All components are made of 304L stainless steel. The initial phase of this work began by ordering two developmental deep-drawn canisters from Norris, a Division of NI Industries, Inc. In the first prototype, one central girth weld at half-height and one nozzle-to-top head weld were required. The two developmental deep-drawn canisters, produced by Norris Industries, arrived on site in April 1993.

Glass filling of one of the canisters at DWPF was completed on August 20, 1994. This canister has been decontaminated but not yet final welded. It is still located within the vitrification building. The second deep-drawn canister was scheduled to be glass-filled in December 1994. It is anticipated that one of the canisters will be drop tested and the other sectioned in order to obtain coupons for metallographic examination and corrosion testing. Dimensional measurements and surface analysis will be carried out prior to these tests. Estimated completion for this testing is mid-1995.

Canister fabrication by spin forming is also being investigated. In this process, the metal is flow-formed through the application of forming rolls. In this process a forged cup is placed on a mandrel and the piece is then spun into a cylinder. What results is an integral unit ~ 9 feet in length having an internal diameter equal to the diameter of the mandrel. A preformed integral head and nozzle unit is then electron beam welded onto the spun cylinder. Final machining is performed in order to meet the dimensional specification.

An order was placed with Spin Forge International for two developmental canisters. The two canisters were estimated to have a delivery date of November 1994.

Keywords: Waste Canisters, Glass Waste, Testing

	<u>FY 1994</u>
Office of Defense Programs - Grand Total	\$78,279,848
The Weapons Research, Development and Test Program	\$78,279,848
Sandia National Laboratories	\$32,222,000
Device or Component Fabrication, Behavior or Testing	\$ 5,682,000
Analysis	\$ 1,540,000
Wavelength Selective Devices on a Chip for a	
Miniature Spectrometer	300,000
Advanced Materials for Electrostatic Chucks	150,000
Alternate Modules	340,000
Porous Silicon Humidity Sensor	100,000
Protected Volumes Liner	200,000
Thin-Film Capacitors for Advanced Packaging	450,000
Metals	\$ 3,193,000
Advanced Welded Turbine Engine Alloys	300,000
Intelligent Systems for Induction Hardening Processes	277,000
Low-Residue Flux, Lead-Free Solder Project	1,100,000
Materials Engineering for the Press/CM	301,000
Materials Replacement Engineering for the Stockpile	1,084,000
SMARTWELD	131,000
Organics	\$ 949,000
Advanced Gas Transfer Materials Studies	474,000
Inertial Confinement Fusion Target Fabrication	475,000

226

^{*}Budget summary numbers do not include funding for projects that were not reported because of CRADA proprietary, patent, or classification restrictions.

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The Weapons Research, Development and Test Program (continued)		
Sandia National Laboratories (continued)		
Instrumentation and Facilities	\$	885,000
Analysis	\$	735,000
Noninvasive Blood Alcohol Monitor Noninvasive Blood Glucose Monitor		135,000 600,000
Metals	\$	150,000
Laser Welding Diagnostics		150,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	\$15	5,016,000
Ceramics	\$ 2	2,145,000
Advanced Materials for Biomedical and Aerospace Applications Biomimetic Processing of Oriented Crystalline Ceramic		350,000
Films		300,000
Diamond Films		200,000
Diamond Films		415,000
Surface, Interface, and Bulk Properties of Advanced Ceramics		179,000
Synthesis and Microstructural Development of Oxide Thin Films Synthesis Of Ceramics Using Supercritical Fluids		345,000 356,000
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<u>FY 1994</u>

The Weapons Research, Development and Test Program (continued)

Sandia National Laboratories (continued)

Materials Preparation. Synthesis. Deposition. Growth or Forming (continued)

Metals	\$ 7,127,000
Advanced Brazing Technology Development	200,000
Advanced Laser Processing Technology	150,000
Advanced Welding Technology	500,000
Development of Novel Laser Coating and	
Joining Technology	180,000
Electro-Slag Remelting - Fundamentals and	
Controller Development	1,175,000
FASTCAST Rapid Prototyping Development	250,000
FASTCAST Software Development And Experiments	750,000
Lightweight Materials For Automotive Applications	560,000
Materials Projects In The Former Soviet Union	660,000
Materials Projects In The Ukraine And Russia	870,000
Solidification Studies	114,000
Titanium Facecoat Development	250,000
Titanium Nitride Dissolution In Molten Titanium	200,000
Vacuum Arc Remelting Process Control	1,068,000
Welding and Processing of an Advanced Titanium Alloy	200,000
Organics	\$ 5,744,000
Advanced Materials Synthesis	300,000
Development of Sticky Foams Without Chlorofluorocarbons	200,000
Engineered Monodisperse Porous Materials	320,000
Environmental Conscience Manufacturing Technology	672,000
Fullerene-Based Materials	420,000
Low-Dielectric Insulating Films for Microelectronics	175,000
Microengineered Materials	350,000
Microporous and Composite Materials	1,774,000

FY 1994

The Weapons Research. Development and Test Program (continued)

Sandia National Laboratories (continued)

Materials Preparation, Synthesis, Deposition, Growth or Forming (continued)

Organics (continued)

New Adhesive Systems Based on Functionalized Block		
Copolymers		228,000
Organic Electronic and Optical Materials		400,000
Polymeric Nonlinear Optical Materials and Devices		
Development		355,000
Polyphosphaacetylenes: New Organic-Inorganic		
Electrical Conductors		300,000
Polysilane Photoresist Technology		250,000
Materials Structure and Composition	\$ 2	2,229,000
Analysis		\$984,000
Phase Identification in a Scanning Electron Microscope		304,000
Pyrolytically Derived Carbon		200,000
Thin Film X-Ray Diffraction Development		180,000
X-Ray Micro-Tomography		300,000
Ceramics	\$	136,000
Defect Studies of ZnO Phosphors		136,000
Metals	\$	409,000
Containment Materials for Transferable Explosives		409,000

	<u>FY 1994</u>
The Weapons Research, Development and Test Program (continued)	. • . •
Sandia National Laboratories (continued)	
Materials Structure and Composition (continued)	
Organics	\$ 700,000
Polymer Blends and Interfaces Polymer Degradation and Lifetime	350,000 350,000
Materials, Properties, Behavior, Characterization or Testing	\$ 8,410,000
Analysis	\$ 2,006,000
Chemometric Development Dismantled Weapon Hardware - Characterization and	300,000
Analysis Materials Characterization Using Ultrafast Optical	180,000
Techniques	250,000
Materials Identification for Weapon Dismantlement	229,000
Metal Deposition On Semiconductor Surfaces	150,000
Non-Nuclear Laboratory Operation Reconfiguration Support	230,000
Process Applications	667,000
Ceramics	\$ 1,190,000
A Mechanical Test for Qualifying Ceramic Granules	92,000
Analysis of Glass Properties for Stockpile Components Electrical and Optical Properties of Ferroelectric	118,000
Thin Films	325,000
Ferroelectric Read/Write Optical Disc	550,000
Lead Magnesium Niobate-Lead Titanate Granules	105,000

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<u>FY 1994</u>

The Weapons Research, Development and Test Program (continued)

Sandia National Laboratories (continued)

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Materials, Properties, Behavior, Characterization or Testing (continued)

Metals	\$ 2,155,000
A Novel Technique for the Mechanical Characterization	
of Thin Films	307,000
Development of Alternatives for Lead Based Solders	278,000
NCMS Printed Wiring Board Surface Finishes Program	650,000
Specialty Metals Product Characterization and Quality	695,000
Welding of AerMet 100	225,000
Organics	\$ 3,059,000
Carbons For Electrochemical Energy Storage	298,000
Catalytic Carbon Foam Filters	338,000
Chlorinated Polyethylene	358,000
High Density Electronic Interconnects	890,000
Materials For Improved Tire Technology	1,000,000
Semiconductor Application of IRIS to Semiconductor	
Processing	175,000
Lawrence Livermore National Laboratory	\$19,030,848
Materials Preparation, Synthesis, Deposition, Growth	
or Forming	\$ 3,403,000
Engineered Nanostructure Laminates	1,300,000
Sol Gel Coatings	325,000
KDP Growth Development	900,000
Advanced Finishing Development	300,000
Doped Polymers for ICF	50,000
ICF Capsule Ablators via Plasma Polymerization	428,000
Excimer Laser Micromachining	100,000

	<u>FY 1994</u>
The Weapons Research. Development and Test Program (continued)	
Lawrence Livermore National Laboratories (continued)	
Materials Properties, Behavior, Characterization or	
Testing	\$ 3,618,000
Advanced Synchrotron Radiation Study of Materials	200,000
Structural Transformation and Precursor Phenomena	169,000
Very High Energy Density Materials	1,060,000
Interfaces, Adhesion, and Bonding	300,000
Laser Damage: Modeling and Characterization	400,000
KDP Characterization	400,000
Damage Testing	800,000
Energy Transfer Dynamics in Energetic Materials	120,000
Processing-Structure-Property Correlation in Laminated	
Metal Composites	169,000
Instrumentation and Facilities	\$12,009,848
Scanning Tunneling Microscopy (STM) and Atomic Force	
Microscopy (AFM)	390,000
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)	425,000
Lithium Cell Development	200,000
Environmentally Safe Disposal of Explosive Wastes:	
SERDP Project	800,000
Laminated Metal Composites for Aerospace Applications	700,000
Fatigue of Metal Matrix Composites	450,000
Molecular Dynamics Simulation Studies of Radiation Effects	
in Solids	60,000
Fundamental Studies of Particle-Solid Interactions	176,000
Radiation Effects in Materials for Inertial Confinement	
Fusion	50,000
Novel Materials for Optoelectronics and Photonics	500,000
Uranium Manufacturing Lead Lab Program	3,000,000

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<u>FY 1994</u>

The Weapons Research, Development and Test Program (continued)

Lawrence Livermore National Laboratory (continued)

Instrumentation and Facilities (continued)

Plutonium Manufacturing Lead Lab Program	3,000,000
Novel Materials Studies at High Pressures and Temperatures	
by Using In-Situ X-ray Laser Heating Experiments in	
a DAC	400,000
Advanced Molecular Dynamics Simulations of Molecular-Beam	
Induced Surface Processes	607,000
High-Speed Tribology of the Head Disk Interface by	
Computer Simulation	300,000
Massively Parallel Simulation of Large Molecular Systems	
with Long-Range Interactions	200,000
Advanced Atomic-Level Materials Design for Massively	
Parallel Environment (High Performance Parallel	
Processor Computing Initiative: H4P)	175,000
Growth and Formation of Advanced Heterointerfaces	500,000
Materials Produced with Dynamic High Pressure	500,000
Properties of Hydrogen at High Shock Pressures and	
Temperatures	250,000
Low Density Foam Shells for Cryogenic ICF Experiments	700,000
Molecular Hydrodynamics	500,000
Metastable Solid-Phase High Energy Density Materials	207,000
Sub-Picosecond Laser Induced Damage	100,000
Novel High Energy Density Materials: Synthesis by	
Megabar Hot Pressing	328,000
AFM Investigations of Crystal Growth	210,000
Plutonium Process Technology Development	6,000,000

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OFFICE OF DEFENSE PROGRAMS (Continued)

	<u>FY 1994</u>
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
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

OFFICE OF DEFENSE PROGRAMS (Continued)

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	<u>FY 1994</u>
Los Alamos National Laboratory (continued)	
Device or Component Fabrication, Behavior or Testing	\$ 3,900,000
Target Fabrication	1,500,000
Filament Winder	100,000
High Energy Density Welding in Hazardous Environments	800,000
Uranium Scrap Conversion and Recovery	1,500,000
Laboratory Directed Research and Development	\$10,802,000
Electronically Correlated Materials at Ambient and	
Extreme Conditions	328,000
Organometallic Chemical Vapor Deposition	248,000
Polymer Sorbents for Hazardous Metal Uptake	164,000
Microscopic Materials Modeling: Textures and Dynamics	109,000
Surface Modification of Materials	315,000
Integration of Fundamental Knowledge in Plasticity and Textures to Provide Technical Tools for Microscopic	
Applications	290.000
High Resolution Electron Microscopy of Materials	350.000
Nano-Fabrication	255.000
Thin Film Micro-Electrochemical Sensor Development	210.000
Liquid Crystal Thermosets	200.000
Neutron and Resonant X-ray Scattering by Materials	350.000
Structural and Electronic Competitions in Low-	,
Dimensional Materials	360.000
Fundamental Aspects of Photoelectron Spectroscopy in	· · · , · · · ·
Highly Correlated Electronic Systems	300.000
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

OFFICE OF DEFENSE PROGRAMS (Continued)

	<u>FY 1994</u>
Los Alamos National Laboratory (continued)	
Laboratory Directed Research and Development (continued)	
Pressure Dependency of the Structure of High Explosives:	
Nitromethane	192,000
Neutron Reflection Studies of Thin Film and Multilayer	2 00 000
Structures	300,000
Neutron Reflectivity Studies of In Situ Corrosion of	145.000
Metal Surfaces	145,000
The Dynamics of Amorphous Materials	330,000
Advanced Material Science Algorithms for Supercomputer	55 000
Architectures	/5,000
Metal vapor Synthesis in Organometallic Chemistry	235,000
Separation Chemistry of Toxic Metals	250,000
Polymers for Integrated Optical Interconnects	200,000
High Temperature Materials Synthesis Without Heat:	
Oxide Layer Growth on Electronic Materials Using	164.000
High Kinetic Energy Atomic Species	164,000
Dynamic Deformation of Advanced Materials	855,000
Strain Measurements in Individual Phases of Multi-	120.000
Phase Materials	: 130,000
Artificially Structured Nonlinear Optic and Electro-	465.000
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

<u>FY 1994</u>

OFFICE OF DEFENSE PROGRAMS (Continued)

Los Alamos National Laboratory (continued)	
Laboratory Directed Research and Development (continued)	
Neutron Scattering as a Probe of the Structure of	
Liquid Crystal Polymer-Reinforced Composite	190.000
Materials Strain Measurements in Individual Phases of Multi-	180,000
Phased Materials During Thermomechanical Loading:	
LANSCE Neutron Scattering Experiment Support	318,000
A New Approach to Texture Measurements: ODF	
Determination by Rietveld Refinement	73,000
Applications of Fullerenes in Nuclear Technology	360,000
Ceramic Oxide Foams for Separation	400,000
Materials Modeling Project	125,000
Synthesis and Optical Characterization of Novel	
Fullerene-Based Composites	50,000
Technology Transfer Initiative	\$ 3,533,000
A Pilot Program: Chemical Vapor Deposition of	
Diamond in a Fluidized-Bed for Cutting Tool and	
Tribological Applications	250,000
Advanced Beryllium Processing	632,000
Automated Pulsed Laser Deposition System	130,000
Plasma Source Ion Implantation for the Automotive	
Industry	1,326,000
Processing Modeling and Control for U.S. Steel	1 105 000
maustry	1,195,000

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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 FY94 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

Device or Component Fabrication, Behavior or Testing

290. <u>Wavelength Selective Devices on a Chip for a</u> <u>Miniature Spectrometer</u>

FY 1994 \$300,000

DOE Contact: Maurice Katz, (202) 586-5799 SNL Contact: Brian R. Stallard, (505) 844-2631

Miniature, rugged, low cost sensors for industrial process and for environmental monitoring are needed for a variety of applications. Infrared and optical spectrometers can be used as monitors, but size, cost and a lack of robustness limit their use for many applications. We are pursuing the design, fabrication and characterization of one element of such a spectrometer, the wavelength selective device on a semiconductor surface. We have demonstrated the feasibility of one design using it to measure diethanol amine in ethanol and are investigating two other designs.

Keywords: Analysis, Spectroscopy

291. Advanced Materials for Electrostatic Chucks

<u>FY 1994</u> \$150,000

DOE Contact: J. L. VanFleet, (202) 586-5782 SNL Contact: Michael J. Hurst, (505) 845-0809

In collaboration with Sematech companies and Oak Ridge, Sandia has begun to synthesize and screen candidate dielectrics and conductors for high temperature electrostatic chuck (ESC) components. The goal is to design a chuck appropriate for advanced tungsten deposition and aluminum etching processes of the type that will be found in future processing equipment. ESCs have distinct advantages over mechanical chucks: no lost real estate, no moving parts, thermal uniformity, and minimal particle generation. ESCs work by columbic attraction between a wafer (maintained at a potential by the processing plasma) and the chuck. The trick is to find materials that work at elevated temperatures. Our most promising attempt, tested at Sematech, has been a combination of plasma-sprayed and solgel ceramics, although a darkhorse ESC etched from a single Si wafer is showing promise as well.

Keywords: Ceramics, Coating, Plasma, Plasma-Sprayed, Silicon

292. <u>Alternate Modules</u>

<u>FY 1994</u> \$340,000

DOE Contact: G. J. D'Alessio, (301) 903-6688 SNL Contact: Michael J. Hurst, (505) 845-0809

Secure containers are used for the protection of important assets such as critical information, circuitry, or money. Potential threats are not just deliberate theft and entry, but also damage by fire or vibration. The ideal container should be scalable from the size of a Brinks truck down to the package around an integrated circuit. A scheme for the design of such scalable modules was investigated through the development of materials and processes to fabricate fault-tolerant devices whose proclivity toward failure is independent of enclosed volume. Most of the work is classified at this time.

Keywords: Ceramics, Packaging, Protected Volumes, Secure Containers, Surety

293. <u>Porous Silicon Humidity Sensor</u>

<u>FY 1994</u> \$100,000

DOE Contact: J. L. VanFleet, (202) 586-5782 SNL Contact: Alan J. Hurd, (505) 845-8629

The purpose of this CRADA project is to compare the performance of porous silicon humidity sensors with that of commercially available aluminum oxide humidity sensors with an intent to commercialize the porous silicon sensor. In our approach, we seek to define the morphological differences between these two sensors and examine their electrical response. Performance comparisons are performed using a prototype test cell made at Sandia. We calibrated the sensors in both "wetting up" (increasing humidity) and "drying down" (decreasing humidity) modes and analyzed the sensor impedance as a function of humidity. In modeling, we are using RC circuit analysis and permitivity mixing rule to gain insight into the mechanism of capacitance change with humidity; our goal is a predictive model of sensor behavior that can be used for further sensor refinement in future device generations. We are supplementing our modeling effort with examinations of the comparative microstructures of our porous silicon prototype sensors and the commercial alumina sensors manufactured by Thunder Scientific to understand how differences in pore geometry and size affect sensor response.

Keywords: Ceramics, Microporous, Silicon

294. Protected Volumes Liner

DOE Contact: G. J. D'Alessio, (301) 903-6688 SNL Contact: Alan J. Hurd, (505) 845-8629

Protected volumes (PVs) are needed for the surety of weapons components against undetected or unmitigated entry by an adversary. Basically a burglar alarm, PVs in weapons should be immune to cold, heat, corrosion, shock, and vibration while remaining exquisitely sensitive to penetration. Our research focused on materials and process development for a new generation of PV protection that promises to supplant existing technology in the stockpile. In addition to laboratory-level work, we teamed with the Sandia manufacturing groups to develop a scalable manufacturing process for future commercialization. Much of the work is classified.

Keywords: Ceramics, Surety

295. <u>Thin-Film Capacitors for Advanced Packaging</u>

DOE Contact: G. J. D'Alessio, (301) 903-6688 SNL Contact: Duane B. Dimos, (505) 844-6385

To improve the performance and decrease the size and weight of next-generation multichip module (MCM) systems, it is necessary to develop decoupling and filter capacitors that can be more fully integrated into electronic packages than current multi-layer ceramic capacitors. To address this need, we have been developing thin-film capacitors using high dielectric constant, lead zirconate titanate sol-gel films. Two approaches are being investigated for integrating these capacitors into MCMs. The first is to develop a solder bump bonded, flip-chip compatible format. This approach requires the development of an

<u>FY 1994</u> \$200,000

<u>FY 1994</u> \$450,000 appropriate wetting/nonwetting materials combination for solder deposition and reflow. The second is to incorporate free-standing, thin-film capacitors directly onto integrated circuits and connect them together as part of a standard repattering process. This approach requires development of a technique for preparing free-standing thin films (< 25 μ m). Studies to improve process reproducibility, capacitor yield, and metallization are also being carried out. Capacitor performance will be assessed by characterizing the properties of individual capacitors and the performance of systems with integrated capacitors.

Keywords: Ceramics, Dielectric, Ferroelectric, Film, Packaging, Sol Gel

296. <u>Advanced Welded Turbine Engine Alloys</u>

<u>FY 1994</u> \$300,000

DOE Contact: J. L. VanFleet, (202) 586-5782 SNL Contact: Gerald A. Knorovsky, (505) 844-1129

The goal of this project (a CRADA with GE Aircraft Engines) is to enhance the commercial and defense application of selected advanced alloys. The approach is to increase understanding of their metallurgy and mechanical properties, particularly as affected by welding and associated processing (including welds to dissimilar materials). The materials of interest include: a high-strength controlled thermal expansion alloy, Thermospan, a high strength Ni-base superalloy with enhanced properties and weldability beyond that of Alloy 718, GTD-222, a high performance cast g-Titanium Aluminide, and a high strength orthorhombic Ti-Al-Nb alloy. In addition to an initial literature survey, the project includes differential thermal analysis, weldability testing, kinetic investigations of phase transformation behavior, and mechanical testing. Analytic Electron Microscopy will also be an important feature.

Keywords: Metals, Alloy, Joining, Melting, Microstructure, Weld

297.	Intelligent Systems for Induction Hardening Processes	<u>FY 1994</u>
	• •	\$277,000
DOE	Contact: J. L. VanFleet, (202) 586-5782	·

SNL Contact: J. Bruce Kelley, (505) 845-3105 Induction heat treating is widely used to produce high strength automotive and industrial components. Current technology requires that process development be

accomplished by trial and error and that the process be run with open loop process controllers. As part of a CRADA with the Saginaw Division of GM, research is being conducted in four areas: experimental process characterization, materials characterization to evaluate dominant process parameters, computational modeling, and neural net controller development. Aspects of these efforts will be incorporated into process controllers which allow the hardened case depth to be selected and then achieved via closed loop control. Intelligent process controllers have the potential to save millions of dollars per year in scrap, waste, and inefficiency. This project requires development of advanced sensor technologies, process diagnostics and controls, complex computational models, and advanced computer architectures for handling very high speed data acquisition and analysis.

Keywords:	Metals, Induction Heat Treating, Intelligent Neural Net Controllers, Materials
-	Characterization, Modeling, Process Characterization

298. Low-Residue Flux, Lead-Free Solder Project	<u>FY 1994</u>
•	\$1,100,000
DOE Contact: G. J. D'Alessio, (301) 903-6688	
SNL Contact: Floyd M. Hosking, (505) 845-8401	

Ozone depleting chemicals and lead-containing solders have been identified as significant hazards to the environment. Since both types of materials have been routinely used for assembling microelectronic circuits, their proposed phase out presents significant problems to the DOE DP sector. New materials and processes must be developed to replace the current list of offending technologies, while still yielding the same level of product reliability. Low-residue soldering technologies are presently being validated for fabricating commercial and military electronic devices. Most of this work has focused on printed wiring assembly (PA) technology. Activities related to hybrid microcircuit (HMC) assembly are less mature. The principal objectives of this project are to develop and demonstrate a low-residue, lead-free soldering technology for manufacturing reliable HMCs for radars. The wetting, aging, and mechanical behavior of prototype solder joints are under investigation. Results are intended for DP and other commercial/military use.

Keywords: Metals, Solder, Alloy, Cleaning, Joining, Joint, Packaging

299. <u>Materials Eng</u>	gineering for the Press/CM	<u>FY 1994</u> \$301.000
DOE Contact: G. J.	D'Alessio, (301) 903-6688	+,
SNL Contact: John	E. Smugeresky, (510) 294-2910	

Advanced surety system components are being developed which require new candidate materials both as ES&H driven replacements and as substitutes to increase the margin of safety in abnormal environments, such as accidents involving fuel fires and conditions under which materials may be degraded from exposure to elevated temperature conditions. Design guidance for materials selection and evaluation requires the understanding of the interactions between materials and the ability to survive normal and abnormal stockpile conditions. Appropriate projects are initiated to evaluate the compatibility of new material combinations in accelerated aging tests, to design appropriate moisture control for the entire PRESS/CM system, to determine molten metal interaction

rates, and to evaluate lightning burn through resistant coatings for exclusion region materials. These activities are coordinated with the corporate activities for Reliability, Safety, Security, Production, Enhancements for Enduring Stockpile, including Manufacturing, Electrical & Electronic MCM related Materials Issues where ever possible. Materials analysis and testing, including mechanical property and fatigue testing, and microstructureproperty relationships for solid and foamed/porous materials are provided as needed.

Keywords: Metals, Coating, Composite, Failure, Melting, Net Shape, Packaging

300.	<u>Material</u>	s Replacement Engineering for the Stockpile	<u>FY 1994</u>
			\$1,084,000
DOE	Contact:	G. J. D'Alessio, (301) 903-6688	

Components are regularly remanufactured and replaced in weapons system in the stockpile for a number of reasons, including the designed limited lifetime for special components such as neutron generators. Because of environmental, safety and health considerations, old technologies no longer available, and the ability to upgrade the performance of non-nuclear components, new materials and processes are needed to support the Stockpile Management Program. Engineering has been done to incorporate MDA-free epoxies in encapsulant applications, provide support from development through specification for foams and rubbers, procure o-rings, correct cleaning activities for environmental protection, and provide materials and process consulting for the reclamation of returned hydrogen reservoirs. There have been a wide range of support services provided including radiography, metallography, chemical analysis, surface analysis, welding, and metal finishing.

Keywords: Metals, Corrosion, Cleaning, Coating, Failure

SNL Contact: Bennie C. Odegard, (510) 294-2789

301. <u>SMARTWELD</u>

<u>FY 1994</u> \$131,000

DOE Contact: G. J. D'Alessio, (301) 903-6688 SNL Contact: Kim W. Mahin, (505) 844-2222

SMARTWELD is a concurrent engineering system which integrates product design and processing decisions within an electronic desktop engineering environment. It is being developed to provide the designer with transparent access to people, information tools and past experience. Empirical understanding along with process models are synthesized within a knowledge-based system to identify the best fabrication procedures based on cost, schedule, performance or environmental impact. Integration of process simulation tools with design tools will enable the designer to rapidly assess a number of design and process options on the computer, rather than on the manufacturing floor. Task models and generic process models are being embedded within user friendly graphical user interfaces to enable customers to use the system without extensive training. The integrated system architecture under development will provide interactive communications and shared application capabilities across a variety of workstation and PC-type platforms locally and at remote sites.

Keywords: Metals, Bond, Joining, Modeling, Weld

302.	Advanced Gas Transfer Materials Studies	<u>FY 1994</u>
		\$474,000
DOE	Contact: G. J. D'Alessio, (301) 903-6688	
SNL (Contact: Bernice E. Mills, (510) 294-3230	

For improved gas transfer systems, materials development supports the component engineers in materials processing, characterization, and cleaning studies. The performance of gas transfer systems strongly depends on the properties and compatibility of gas storage materials. The aging behavior of materials is also critical to the reliability of gas transfer systems. Our project is designed to address these issues by developing processes and establishing WR specifications for new materials with well-characterized properties to be used for gas transfer systems. We are also developing cleaning procedures for these materials through concurrent engineering with the design engineers.

> <u>FY 1994</u> \$475.000

Keywords: Organics, Gas-Transfer, Aging, Cleaning, Materials Characterization

303.	Inertial	Confinement	Fusion	Target Fa	<u>brication</u>
DOE	Contact:	G. J. D'Ales	sio, (30)	1) 903-668	8
SNL (Contact:	James H. Au	bert, (5	05) 844-44	81

In this project we have developed materials and fabrication techniques to prepare complex targets for Sandia's inertial confinement fusion program (ICF). This program is studying the interactions of energetic lithium ions, produced in Sandia's particle beam fusion accelerator (PBFA II), with materials and the resulting radiating plasmas. The recent campaigns involved targets composed of 1 μ m thick gold wall hohlraums containing a very low density foam, 0.005g/cm3. The gold is fairly transparent to the high energy lithium ions but the foam is efficient at stopping them and adsorbing their energy. Hohlruam temperatures as high as 60 eV were obtained. In the future, such hot plasmas will be used to drive fuel capsules contain deuterium and tritium fuel.

Keywords: Organics, ICF, Fabrication, Foam, Foil

Instrumentation and Facilities

304. Noninvasive Blood Alcohol Monitor	<u>FY 1994</u>
	\$135,000
DOE Contact: G. J. D'Alessio, (301) 903-6688	1
SNL Contact: Ann M. Bouchard, (505) 845-0552	. 1

Current methods for the quantitative analysis of blood alcohol is accomplished through so-called "breathalyzers." For a variety of reasons, these instruments are unreliable and sometimes inaccurate. We have developed a method for using near infrared spectroscopy through the finger combined with chemometrics for data analysis which can determine the alcohol concentration in a patient's blood noninvasively. The methods to reduce this to commercial feasibility are currently being investigated.

Keywords: Analysis, Spectroscopy, Chemometric

305. Noninvasive Blood Glucose Monitor

DOE Contact: G. J. D'Alessio, (301) 903-6688 SNL Contact: James A. Borders, (505) 844-8855

There are currently 2.5 million diabetic patients in the United States who must monitor the glucose concentrations in their blood. Compliance is poor due to the pain of drawing blood. Improved compliance would result in a decrease in the secondary effects of diabetes which are the most debilitating and costly. We have developed a method for using near infrared spectroscopy through the finger combined with chemometrics for data analysis which can determine the glucose concentration in a patient's blood noninvasively. A fully funds in CRADA has been established with Rio Grande Medical Technologies to commercialize the technology in partnership with the University of New Mexico School of Medicine.

Keywords: Analysis, Spectroscopy, Chemometric

306. <u>Laser Welding Diagnostics</u>

DOE Contact: G. J. D'Alessio, (301) 903-6688 SNL Contact: Marcelino Essien, (505) 845-0574

In order to optimize the laser welding process, it is necessary to characterize the propagation of the laser beam and the interaction of the beam with the metal. Critical to this optimization are knowledge of the laser parameters and a knowledge of the response of the metal to the laser radiation. Characterization of continuous-wave and pulsed

<u>FY 1994</u> \$150,000

<u>FY 1994</u> \$600,000
Nd:YAG laser beams is a central focus of this project, as well as a study of the propagation of these laser systems through focusing optics. This projects entails characterization of Nd:YAG laser radiation in terms of pertinent laser parameters, as well as identification of the factors which limit the focusibility of the laser radiation, including plume refraction of the laser beam.

Keywords: Metals, Optics

Materials Preparation, Synthesis, Deposition, Growth or Forming

307. <u>Advanced Materials for Biomedical and Aerospace</u> <u>Applications</u>

FY 1994 \$350,000

DOE Contact: Maurice Katz, (202) 586-5799 SNL Contact: Richard K. Brow, (505) 845-8047

Advanced aerospace electronic components and commercial biomedical electronic components, such as pace makers, require glasses which are capable of forming reliable hermetic seals with titanium metal. Currently, the compositions of most commercial sealing glasses are based on silicates which undergo deleterious interfacial reactions with Ti metal thus rendering them unreliable. Consequently, the development of such technologies is hampered by the lack of appropriate commercial sealing glasses. We have, however, discovered that certain glasses whose compositions are based on borates offer considerable advantages over silicates. We are currently working on (1) the development of new borate based sealing glass compositions, (2) the appropriate sealing technologies and (3) the manufacturing of reliable hermetic titanium glass-to-metal seals.

Keywords: Ceramics, Glass, Electronic, Modeling, Packaging, Structure

308.	Biomimetic Processing of Oriented Crystalline Ceramic Films	<u>FY 1994</u>
		\$300,000
DOE	Contact: Maurice Katz (202) 586-5799	

DOE Contact: Maurice Katz, (202) 586-5799 SNL Contact: Michael J. Hurst, (505) 845-0809

The performance of optoelectronic ceramic films for optical memories, computers, and displays depends on crystalline, oriented material. Biomimetic growth, Nature's pathway for fabricating oriented films, uses an organic template to nucleate inorganic crystals, e.g. protein-controlled growth of bone. In our biomimetic technique to grow oriented cadmium sulfide (CdS) on gold-coated silicon, Langmuir-Blodgett (LB) films of cadmium stearate serve as a 100μ -thick organic template, and CdS grows on the LB film from solutions with

the assistance of an alternating electric field. Atomic force microscopy reveals that CdS crystals are templated to the underlying LB film.

Keywords: Ceramics, Biometric, Film, Membrane

309. Novel Approach to the Production of Thick. Patterned Diamond Films FY 1994

\$200,000

DOE Contact: Maurice Katz, (202) 586-5799 SNL Contact: Michael J. Hurst, (505) 845-0809

Thick, stress-free diamond coatings and free-standing pieces with tailored surface topographies can be formed economically in short processing time by adapting techniques developed for thick-film screen printing. We used artificial diamond powder precursors from diamond ink, then densified this powder deposit in a chemical vapor deposition (CVD) diamond reactor. A number of factors define limits of the product. The porosity of the powder has a major effect on the in the CVD reactor: high density precursors with small pores densify more readily. System geometry and operating conditions are important to the amount of diamond relative to other forms of carbon present. Variations in the fluorescence bands indicate silicon and boron impurities (from the doped substrate) and defects in the diamond lattice. Under some conditions we observed the growth of euhedral, homogeneous, 20μ m-diameter diamond spheres and hemispheres.

Keywords: Ceramics, Diamond, CVD, Film

310. <u>Scalable, Flat-Flame Technology for the Synthesis of</u> <u>Diamond Films</u>

<u>FY 1994</u> \$415,000

DOE Contact: Maurice Katz, (202) 586-5799 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. Flat-flames based on inherently scalable stagnation flows give rapid and uniform diamond growth. A novel flow manifold, called a "trumpet bell," is used to produce all the ideal properties of an infinite stagnation flow, but on a finite scale that maximizes the use of reagent gas. Computational modeling is used to understand and optimize the deposition process and to investigate potentially advantageous but high risk processes. In the near future, we will take our technology to the point where it can be quantitatively evaluated against competing technologies.

Keywords: Ceramics, Diamond, Film, Modeling

311. Surface. Interface. and Bulk Properties of Advanced Ceramics

<u>FY 1994</u> \$179,000

DOE Contact: G. J. D'Alessio, (301) 903-6688 SNL Contact: Kevin F. McCarty, (510) 294-2067

The major focus of this program is the synthesis of novel thin ceramic films using pulsed laser deposition. We strive for a fundamental understanding of the film growth process, including the microscopic mechanisms controlling phase selection in the boron nitride system. In addition, we study the microstructure, phonon spectrum, and electronic defect structure of advanced ceramics with emphasis on ultrahard materials and wide bandgap semiconductors. We emphasize the techniques of Raman spectroscopy, infrared spectroscopy, photoluminescence, and transmission electron microscopy.

Keywords: Ceramics, Nitride, Film, Microstructure

312. <u>Synthesis and Microstructural Development of Oxide Thin Films</u> <u>FY 1994</u> \$345,000

DOE Contact: G. J. D'Alessio, (301) 903-6688 SNL Contact: Duane B. Dimos, (505) 844-6385

Sol-gel processing is a versatile technique for fabricating multicomponent oxide thin films. To develop an intelligent approach to sol-gel processing, the effects of various ligands, chelating agents, and solvents are studied. Furthermore, side reactions and hydrolysis that occur in solution need to be taken into account. These solution effects are being studied for three model multicomponent perovskite systems, $Pb(Zr,Ti)O_3$, $Pb(Mg,Nb)O_3$ and $(Ba,Sr)TiO_3$. In addition, the performance and reliability of devices based on ferroelectric thin films depends on producing films with optimized microstructures. The main issue that governs microstructural development of these films is control of the nucleation and growth of the perovskite phase. The influence of the substrate on nucleation and growth are determined by studying microstructural evolution of $Pb(Zr,Ti)O_3$ films as a function of substrate type, morphology, orientation, and grain size. To achieve additional control of film microstructure, the effects of firing conditions (temperature, heating rate) and processing environments (oxygen partial pressure, lead partial pressure) are also investigated.

Keywords: Ceramics, Ferroelectric, Film, Sol Gel

313. Synthesis of Ceramics Using Supercritical Fluids

FY 1994 \$356.000

DOE Contact: Maurice Katz, (202) 586-5799 SNL Contact: Carol L. Jones Adkins, (505) 845-9119

Supercritical fluids such as H₂O, CO₂, NH₃, etc., have unique solvation properties that make them appealing for the synthesis of materials that cannot be made by conventional means. If a solute-laden supercritical fluid is rapidly expanded through a nozzle, a powder is produced as the fluid expands. The rapid expansion of the fluid can lead to the production of unusual, nonequilibrium phases of the solute that might prove to be more readily sinterable. This technique combines the benefits of gas-phase powder synthesis with the high throughputs possible using spray technology. Waste minimization is automatic since the working fluid can be recycled. We are exploring the use of supercritical fluids to synthesize novel (e.g., ultrafine, more reactive) ceramic powders. The synthesis and reactivity of materials leading to the formation of ceramic powders in supercritical water is being investigated. In addition, we are examining the possibility of using surfactants to facilitate the formation of ceramics of interest in supercritical carbon dioxide -- a easier supercritical fluid to work with.

Keywords: Ceramics, Synthesis, Powder, Super Critical

314. Advanced Brazing Technology Development

FY 1994 \$200,000

DOE Contact: G. J. D'Alessio, (301) 903-6688 SNL Contact: John J. Stephens, (505) 845-9209

This program is aimed at developing the technology required to manufacture ultra high reliability nuclear weapons hardware. Included in this program is a project that will develop and characterize active metal brazing processes and materials for hermetic cermet/metal braze joints. Other projects characterize and correlate the microstructure in titanium alloy braze joints with the resultant mechanical properties, and characterize the evolution of braze joint microstructure subject to long time, high temperature environments.

Keywords: Metals, Joining, Alloy, Bond, Braze, Microstructure, Modeling

315.	Advanced	Laser	Processing	Technology

DOE Contact: G. J. D'Alessio, (301) 903-6688 SNL Contact: David M. Keicher, (505) 845-8365

The goal of this project is to develop a fundamental understanding of the process controlling parameters associated with laser welding, soldering, and machining. Specific

FY 1994 \$150,000

Office of Defense Programs

tasks include: calorimetric study of energy transfer during laser welding of aluminum alloys and stainless steels, design and development of frequency multiplied solid state laser systems, the development of unique laser focusing optics for specific applications, and optics modeling of the spatial distribution of laser energy for commercial focusing optics.

Keywords: Metals, Joining, Laser, Modeling, Solder, Weld

316. <u>Advanced Welding Technology</u>

DOE Contact: G. J. D'Alessio, (301) 903-6688 SNL Contact: Phillip W Fuerschbach, (505) 845-8877

This program is aimed at developing the technology required to manufacture ultra high reliability nuclear weapons hardware. Included in this program are projects that will model the solidification and mechanical behavior of weld joints, assess the weldability of advanced gall-resistant stainless steels, establish a process for friction joining metals to ceramics, and develop a model for energy transfer efficiency during CO_2 and Nd:YAG laser welding of stainless steel and aluminum alloys.

Keywords: Metals, Weld, Joining, Laser, Microstructure

317. Development of Novel Laser Coating and Joining Technology

<u>FY 1994</u> \$180,000

DOE Contact: J. L. VanFleet (202) 586-5782 SNL Contact: David M. Keicher, (505) 845-8365

Laser deposition of metallic materials is an emerging technology which will allow material properties of various hardware components to be tailored to specific requirements. Hard, wear resistant surfaces can be selectively deposited onto ductile components to enhance the lifetime of these components without compromising the overall metallurgical properties of the entire component. Other materials can be deposited to enhance corrosion resistance, weldability, etc. The localized heating properties associated with lasers allow materials to be deposited with a minimum heat affected zone or alloying in the base material. As part of this effort, we have now established a capability at Sandia to perform laser powder deposition in a controlled atmosphere. We are presently performing tests to evaluate our system and then will use statistically designed experiments to develop response surface models of the laser deposition process. These results will lead to a fundamental understanding of the process and identify key parameters for use in process control. This technique will allow placement of metal during manufacturing to obtain high strength welds

<u>FY 1994</u> \$500,000 on weapons hardware and allow development of near-net shape components from powder metals. This project is a CRADA with Pratt & Whitney.

Keywords: Metals, Alloy, Coating, Corrosion, Joining, Laser, Net Shape, Surface, Weld

318. Electro-Slag Remelting - Fundamentals and Controller DevelopmentFY 1994\$1,175,000\$1,175,000DOE Contact: J. L. VanFleet, (202) 586-5782

SNL Contact: M. Eric Schlienger, (505) 845-3105

Electro-Slag Remelting is a melt refining process used by the Specialty Metals Processing Consortium members to remove unwanted impurities from high performance steels and nickel-based alloys. The process melts an electrode suspended in a bath of molten slag which is heated by passing current from the electrode through the slag and into an ingot, formed below the slag pool. This project includes research into fundamental process phenomena and application to design and optimize process controls. Aspects of the process such as current pathways, impedance spikes, slag metal interfaces, and fluid flows can significantly impact process stability. Lack of stability can cause solidification defects and ingot surface quality problems, both of which affect product yield. The goal of this project is to derive and optimize process control methodologies to extend the operating window for process stability. Laboratory and industrial experiments are combined with process modeling to optimize process controls.

Keywords: Metals, Melting, Modeling

319. FASTCAST Rapid Prototyping Development

<u>FY 1994</u> \$250,000

DOE Contact: J. L. VanFleet, (202) 586-5782 SNL Contact: Michael C. Maguire, (505) 845-3105

Rapid prototyping technologies have developed dramatically over the past several years. The ability to rapidly produce a functional representative of a design in a day is now a reality. However, to use these parts in the investment casting process requires substantial process development. The use of stereolithography or selective laser sintering, two of the most advanced technologies for rapid prototyping, in investment casting has resulted in significant lead time reduction for first run parts. This project was focused on how to incorporate the new pattern materials into investment casting, improvements in build parameters and post processing to improve surface finish, and dimensional accuracy studies to benchmark the performance of these processes.

Keywords: Metals, Fastcast, Net Shape

320. FASTCAST Software Development and Experiments

FY 1994 \$750,000

DOE Contact: G. J. D'Alessio, (301) 903-6688 SNL Contact: Michael C. Maguire, (505) 845-3105

The FASTCAST consortium was formed this year from 17 industrial partners to advance the science of investment casting process simulation, and to improve the performance of rapid prototyping technologies. The work to achieve these goals started in 1990 with the development of an integrated software environment to combine casting design, simulation, and production. The ultimate goal of the project is to provide software and hardware solutions to member companies that will improve the quality and reduce the lead time for investment castings.

Keywords: Metals, Fastcast, Modeling

321. Lightweight Materials for Automotive Applicatio	ons <u>FY 1994</u>
	\$560,000
DOE Contact: J. L. VanFleet, (202) 586-5782	
SNL Contact: Michael C. Maguire, (505) 845-3105	

This is a multi-lab CRADA with General Motors, Sandia National Laboratories, Oak Ridge National Laboratory, and Lawrence Livermore National Laboratory. Each laboratory has an individual CRADA with GM. There is a increasing demand both in the automobile industry and the weapons community for new alloys and processes for production of lightweight, wear resistant aluminum castings. The resulting casting can be used effectively to reduce size, fuel consumption, and weight while maintaining crash worthiness and performance standards. Sandia is studying the casting production processes by evaluating porosity in green sand cast aluminum over varying casting conditions, using fusible salt cores to produce localized regions of increased wear resistance, and using real-time X-ray radiography to validate gating design and modeling efforts to predict mold filling.

Keywords: Metals, Alloy, Melting, Microstructure, Porosity, X-ray

322.	Materials Projects in the Former Soviet Union	<u>FY 1994</u>
	-	\$660,000
DOE	Contact: G. J. D'Alessio, (301) 903-6688	
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D SNL Contact: Frank J. Zanner, (505) 845-3085

During the past year a program was funded and implemented to invest in science and technology in the former Soviet Union (FSU) for the purposes of commercialization. For Sandia's part of this US Lab-to-FSU Institute program, 20 contracts were written with Russian Institutes and 10 contracts were written with Ukrainian Institutes to work on materials technologies involving coating processes and metals processing. These contracts were placed and the work is currently underway.

Keywords: Metals, FSU, Coating, Liquid Metal Processing

323. Materials Projects in the Ukraine and Russia

<u>FY 1994</u> \$870,000

DOE Contact: G. J. D'Alessio, (301) 903-6688 SNL Contact: Frank J. Zanner, (505) 845-3085

Under the auspices of the Specialty Metals Processing Consortium (SMPC), materials technology projects of interest to SMPC members were initiated with Ukrainian and Russian Institutes. These projects include porous metal technology, Alloy 718 phase relationships, and characterization of Al-Si hypereutectic alloys at the Dnepropetrovsk Metallurgical Institute in Dnepropetrovsk, electron beam casting of fine grain ingots at the Paton Electric Welding Institute in Kiev, measurement of liquid metal temperature with a sapphire window at the Institute of Foundry Problems in Kiev, and gyrotron microwave processing technology at the Institute of Applied Physics in Nizhniy Novgorod. As the equipment and technology is received from Russia and the Ukraine it will be tested in SMPC member plants.

Keywords: Metals, FSU, Liquid Metal Processing, Microwave Processing, Sensors

324. <u>Solidification Studies</u>

<u>FY 1994</u> \$114,000

DOE Contact: G. J. D'Alessio, (301) 903-6688 SNL Contact: James A. Van Den Avyle, (505) 845-3105

The process response and performance of nickel-base superalloys are strongly affected by their solidification structures, as characterized by microstructural scale, amounts of microconstituents, overall homogeneity, extent of micro and macrosegregation, and occurrence of solidification defects. Solidification processes such as ingot growth, welding, and casting are carried out under characteristic conditions which produce varying structures. The goal of this study is to characterize the response of a superalloy, Alloy 718, over a wide range of controlled solidification conditions. Experiments are conducted in a controlled directional solidification furnace under thermal gradients and growth rates representative of those observed in industrial scale remelting processes. Microstructural analyses include dendrite structure, compositional variations by X-ray analysis, and distribution of intermetallics and melt defects.

Keywords: Metals, Alloy, Melting, Microstructure, X-ray

325. <u>Titanium Facecoat Development</u>

DOE Contact: Maurice Katz, (202) 586-5799 SNL Contact: Michael C. Maguire, (505) 845-3105

The titanium investment casting industry has suffered from the formation of a brittle surface layer on the castings owing to a mold/metal reaction. This brittle layer, termed alpha case, is usually removed by chemical milling. The existence of this layer has limited the use and increased the cost of investment cast titanium parts. This project is aimed at first determining which components of the investment casting mold material contribute to the alpha case, and then develop materials that reduce the formation of the layer.

Keywords: Metals, Net Shape

326.Titanium Nitride Dissolution in Molten TitaniumFY 1994\$200,000\$200,000DOE Contact:J. L. VanFleet, (202) 586-5782

SNL Contact: Michael D. Baldwin, (505) 845-3105

A common problem associated with the production of titanium alloys is the retention of titanium nitride inclusions through melt processing. These inclusions can act as initiation sites for low cycle fatigue failures in rotating parts for aircraft engines. Research currently being conducted under the Specialty Metals Processing Consortium is directed toward understanding the dissolution kinetics of TiN in molten titanium. The goal of this study is to predict the dissolution rate and characterize the diffusion mechanism. The variables in the study include type and nitrogen content of the TiN seed and time. The study will be conducted using a levitation furnace, computer tomography and microprobe analysis.

Keywords: Metals, Melting, Microstructure, Nitride

327. <u>Vacuum Arc Remelting Process Control</u>

<u>FY 1994</u> \$1,068,000

DOE Contact: J. L. VanFleet, (202) 586-5782 SNL Contact: Rodney L. Williamson, (505) 845-3105

Vacuum arc remelting (VAR) is a process used throughout the specialty metals industry in the production of reactive and segregation sensitive alloys. The process must be carefully controlled to minimize or eliminate transient conditions in the solidification zone of the ingot formed during remelting. In general, this is difficult to achieve because of random disturbances in uncontrolled state variables. The goal of this project is to better characterize these disturbances and to design process control responses that minimize their effects on the solidifying ingot, and to transfer this technology to our industrial partners in

FY 1994 \$250,000 the Specialty Metals Processing Consortium. The problem is being addressed theoretically, using computer simulations, and experimentally, by carrying out both laboratory-scale and industrial-scale experiments.

Keywords: Metals, Alloy, Melting, Modeling

328. <u>Welding and Processing of an Advanced Titanium Alloy</u> FY 1994

DOE Contact: G. J. D'Alessio, (301) 903-6688 SNL Contact: Gerald A. Knorovsky, (505) 844-1129

The goal of the project (a CRADA with United Technologies Corp.) is to enhance the commercial and defense application of the advanced alloy under study (Titanium Alloy C, Ti-35V-15Cr) by characterizing its processing metallurgy, weldability and formability. This alloy is of interest because of its atypical (in Ti alloys) resistance to combustion in combination with attractive high temperature mechanical properties. Despite generally favorable initial experience in secondary processing and welding, a grain boundary separation phenomenon has been encountered in the weld fusion zone and during deformation processing which is as yet incompletely understood. Our investigation of this alloy will employ the tools of differential thermal analysis, weldability testing, kinetic investigations of phase transformation behavior and Analytic Electron Microscopy

Keywords: Metals, Alloy, Joining, Melting, Microstructure, Weld

329. Advanced Materials Synthesis

FY 1994 \$300,000

\$200,000

DOE Contact: G. J. D'Alessio, (301) 903-6688 SNL Contact: Roger Lee Clough, (505) 844-3492

Microengineered materials offer the possibility of controlling material properties in very specific ways, and should allow the production of advanced materials having higher strength, or controlled porosity. We are developing micro-phase-separated ceramic-polymer $(SiO_2$ -epoxy) composites for encapsulation of electronic components. Compared with conventional composites now in use, these advanced materials offer the advantages of: wider processing latitude, more consistent batch-to-batch properties, and curing chemistry involving non-toxic materials. We are also synthesizing nanoporous silsesquioxane materials which will allow the production of high-efficiency, lower cost battery membranes and hydrogen getters.

Keywords: Organics, Encapsulant, Membrane, Microporous, Polymer

330. Development of Sticky Foams Without Chlorofluorocarbons

<u>FY 1994</u> \$200,000

DOE Contact: G. J. D'Alessio, (301) 903-6688 SNL Contact: Peter B. Rand, (505) 845-8695

Sticky foam is a unique one-container foam developed as a dispensable deterrent to protect nuclear weapons and materials. The original material used dichlorodifluoromethane (R-12) as the solvent/foaming agent. It is necessary to replace the R-12 to protect the ozone layer. Requirements for the replacement include: non flammability, boiling point below -20°C, adequate solvent for the resin blend, and slow diffusion through the foam structure to prevent rapid collapse. A wide variety of low boiling halocarbons and hydrocarbons have been evaluated as potential solvent/blowing agents for this foam. The only materials which meet all the requirements were the hydrofluorochlorocarbons such as difluorchloromethane. Resin reformulation was necessary to regain the foam volume stability required for this application. The new hydrochlorofluorocarbon formulations have been evaluated and are ready for use.

Keywords: Organics, Foam, Polymer

331.	Engineered Monodisperse Porous Materials	<u>FY 1994</u>
		\$320,000
DOD	C. test. C. I. D'Alest. (201) 002 ((00	

DOE Contact: G. J. D'Alessio, (301) 903-6688 SNL Contact: Randall S. Saunders, (505) 844-1760

Porous materials are available with pore sizes ranging from Angstroms to hundreds of microns. However, above 1.5 nm it is difficult to obtain complete control over pore size, size-distribution, and ordering. This project is using the novel properties of block copolymers to create monodisperse, controllable, ordered porous materials spanning the nanoporous range (2-50 nm). The blocks of a block copolymer want to phase separate from each other but are limited by the chemical attachment. This results in well-ordered, monodisperse, nm-size domains of one polymer surrounded by the other. We are synthesizing block copolymers by Ring Opening Metathesis Polymerization (ROMP). Our synthesis will allow one phase to be crosslinked and the other phase to be either chemically or thermally removed. This will lead to unique nanoporous materials. These materials could impact several technologies including polymer and gas separations, remote sensor and bio-sensor materials, and catalyst supports.

Keywords: Organics, Foam, Microporous, ROMP, Separations

332. Environmental Conscience Manufacturing Technology

<u>FY 1994</u> \$672,000

DOE Contact: G. J. D'Alessio, (301) 903-6688 SNL Contact: Linda A. Domeier, (510) 294-2350

This project consists of two sub-projects: MDA Free Epoxy Formulations and Environmentally Optimized Chemical Processing for CAP Assemblies. For the first subproject, we developed new epoxy formulations with improved properties to replace methylene dianiline (MDA), which is an OSHA regulated aromatic diamine, in epoxy encapsulants, for neutron generators, thermal batteries, and other applications. For the second sub-project, we address the current environmental issues involving chemical processes for cleaning, etching, passivation and plating on heater and gas transfer system CAP assemblies. We identified several ES&H and stockpile problems concerning hazardous materials and developed processes to eliminate or minimize the use of these materials.

Keywords: Organics, MDA, CAP, ECM, Encapsulant, Gas-Transfer

333. Fullerene-Based Materials

DOE Contact: Maurice Katz, (202) 586-5799 SNL Contact: Paul A. Cahill, (505) 844-5754

Carbon-in the form or diamond or graphite-provides key properties for many commercial and defense materials technologies. A third form of carbon-the fullerenes-are soluble, roughly spherical molecular form of carbon with the potential to be a building block for new materials. Work this year supported investigations into the fundamental aspects of the chemistry and physics of fullerenes and was focused on four topics: (1) polymer science of fullerenes, (2) experimental investigations of the fundamental aspects of the chemistry of C_{60} and C_{70} , (3) computational/theoretical models of the relative stability of fullerene derivatives, and (4) measurement of the rotational correlation time constant of C_{60} H₂. Sandia researchers have largely defined the fundamental nature of the chemistry of C_{60} and C_{70} , and recommended further investigations into the use of fullerenes in composite materials.

Keywords: Organics, Fullerene, Modeling, Polymer

<u>FY 1994</u> \$420,000

DOE Contact: G. J. D'Alessio, (301) 903-6688 SNL Contact: Tamara A. Ulibarri, (505) 844-5279

Since silicone materials are inherently weak, reinforcement methods are required. However, while current these methods are effective, they are costly since they involve the ex situ preparation of pyrogenic silica and energy intensive mixing steps. Our work seeks to develop a new manufacturing process for reinforced elastomers. The basic strategy is to use our existing knowledge of silica sol-gel chemistry to control the condensation and phase separation of silica produced in a silicone matrix. The project is designed to develop the scientific and engineering knowledge base required for the successful production of in situ silica reinforced silicone elastomers.

Keywords: Organics, Composite, Polymer

Office of Defense Programs

334.	Low-Dielectric Insulating Films for Microelectronics	<u>FY 1994</u> \$175,000
DOE	Contact: Maurice Katz, (202) 586-5799	. ,
SNL (Contact: Randall S. Saunders, (505) 844-1760	

Thin low-dielectric constant and high-temperature films are used to separate multiple layers of patterned conductors in multichip module packaging. Significant improvements in processing speed could be obtained from the use of lower dielectric constant material. In this project, we obtain lower dielectric constant material by preparing porous polymer films. Since the dielectric constant of air is about 1.0, incorporation of porosity into the insulating film reduces the average dielectric constant in proportion to the amount of porosity. Porous polyimide films are prepared by spin coating polyimide/solvent films and then phase separating the polyimide/solvent film by exposure to a nonsolvent. After removal of the solvent and nonsolvent a porous film results. Control over the porosity is obtained primarily by controlling the phase separation process. We are measuring the complete phase diagram for the ternary polyimide system under study in order to optimize the phase separation process and resulting microporous structure.

Keywords: Organics, Dielectric, Electronic, Foam, Microporous, Packaging

335. Microengineered Materials

<u>FY 1994</u> \$350,000

336. Microporous and Composite Materials

<u>FY 1994</u> \$1,774,000

DOE Contact: G. J. D'Alessio, (301) 903-6688 SNL Contact: Jill M. Hruby, (510) 294-2596

This activity consists of two independent projects: microporous materials research, and composite materials research. In the microporous materials project, research on the synthesis, processing, and characterization of microporous materials is conducted to achieve the basic knowledge to tailor the structure and properties of the materials. In addition, a fundamental understanding of the materials in their potential applications is also developed. The emphasis is on polymer and carbon materials. Potential applications include electrodes for electrochemical storage, chemical or physical separations, low dielectric materials, encapsulents, etc. In the composite materials project, the activities are centered on (1) understanding improved chemical vapor infiltration processing of carbon-carbon materials, and (2) embedded sensors in organic composites.

Keywords: Organics, Microporous, Composite, Polymer

337. <u>New Adhesive Systems Based on Functionalized Block Copolymers</u> FY 1994

\$228,000

DOE Contact: G. J. D'Alessio, (301) 903-6688 SNL Contact: Michael S. Kent, (505) 845-8178

The need to control and optimize the properties of polymer/solid interfaces is critical in a host of technologies. Often the adhesive strength of the interface, the resistance to moisture, and the ability to transfer stress through the interface are critical to the overall performance of the product. Recent evidence indicates that the adhesive failure often occurs a very short distance into the polymer matrix, typically 10-100nm. This "interphase" region has proved difficult to design from first principles. In this project we are designing and testing (by X-ray and neutron reflectivity) new adhesives systems based upon block copolymers, where one block (A) attaches to the surface while the second block (B) is compatible with and bonds to the polymeric matrix. An important advantage of a block copolymer is that the B block can easily be made long enough to span the weak region of 10-100nm and form a strong interlock with the matrix. These systems may lead to improved adhesion and a more systematic design of the interphase region.

Keywords: Organics, Adhesive, Bond, Copolymer, Reflectivity

338. Organic Electronic and Optical Materials

<u>FY 1994</u> \$400,000

DOE Contact: G. J. D'Alessio, (301) 903-6688 SNL Contact: Roger Lee Clough, (505) 844-3492

Electronic devices are critical parts of weapon systems. The technology for highspeed, advanced capability electronic and optoelectronic materials is advancing rapidly. We are developing organic light-emitting diodes which could make possible the production of large, flat panel displays for computer monitors, video sets, etc. This work involves developing an understanding of the fundamental physics of the light emission process in these devices (particularly charge-transport in the materials), and the synthesis of new polymeric materials designed for longer lifetime in the application. We are also developing resist materials, based on new silvlation techniques, which function efficiently in the deep-U.V. range, thus permitting smaller feature sizes in microelectronic devices. We are developing new polymeric nonlinear optical materials, for use in interconnects between computer chips, which will make data transmission between chips, in multi-chip modules, more efficient.

Keywords: Organics, Electronic, Electrooptic, Nonlinear, Polymer

339.	Polymeric Nonlinear Optical Materials and Devices Development	<u>FY 1994</u>
		\$355,000

DOE Contact: J. L. VanFleet, (202) 586-5782 SNL Contact: Paul A. Cahill, (505) 844-5754

Optical interconnects, for example between chips on a board, between boards in a parallel processor, or between a central database and the home, will require a means of modulating light within a fiber or waveguide. This CRADA with Amoco Chemical Co. combines Amoco's polyimide technology with Sandia's modeling and synthesis capabilities to produce new electrooptical compositions for this emerging optical interconnect market. A change in the market for optical interconnects has forced a change in the direction of this project toward passive interconnects based on Amoco polyimides and a Sandia developed photosensitive dye. This project is focused on the design and fabrication of optical devices such as splitters, bi-directional transmitters, and fiber-to-guide couplers using these new jointly developed compositions.

Keywords: Organics, Polymer, Electrooptic, Modeling, Nonlinear, Optical

340. Polyphosphaacetylenes: New Organic-Inorganic Electrical Conductors FY 1994

\$300,000

DOE Contact: Maurice Katz, (202) 586-5799 SNL Contact: Clifford L. Renschler, (505) 844-0324

A large effort has been expanded worldwide on the development of electrically conducting organic materials. This extraordinary level of interest is due to the high degree of flexibility and control such materials would lend to both electrical and mechanical properties. However, the promise of these materials has yet to be realized, largely due to myriad processing problems associated with the materials classes studied thus far. In this project, we are developing a new class of formable, electrically conducting hybrid organicinorganic materials, the polyphosphaacetylenes, that should display the high conductivity of doped organic conductors with much better processing characteristics. Our approach is to take advantage of the high reactivity of low-coordinate phosphorus-carbon triple bonds under favorable reaction conditions to induce polymerization to form polyene-analogous backbones bearing solubilizing substituents. This project utilizes Sandia's expertise in computer-aided molecular design and hybrid synthesis and characterization.

Keywords: Organics, Electronic, Modeling, Polymer

341. Polysilane Photoresist Technology

DOE Contact: G. J. D'Alessio, (301) 903-6688 SNL Contact: Clifford L. Renschler, (505) 844-0324

Printed Wiring Boards are used to make the necessary interconnects between integrated circuit chips in modern electronic assemblies for computers, telecommunications, consumer electronics, and military and automotive applications. The photoresists used to define the conductive traces produce large volumes of organic and aqueous waste. A much more environmentally friendly process would result from a resist that could be applied to the board using only an alcohol solvent, and imaged without any further use of solvent. Polysilanes are a class of materials that can be used as self-developing resists, i.e. resists in which the imaging and development steps occur simultaneously via volatilization of the resist material. Working in collaboration with Stanford University, we are developing specific polysilanes that have not been previously synthesized, and whose properties can be optimized for this application. An added advantage of our approach is that the materials produced by the new synthetic method can be made much more safely than conventional polysilanes.

Keywords: Organics, Electronic, Lithography, Packaging, Polymer

<u>FY 1994</u> \$250,000

Materials Structure and Composition

342. <u>Phase Identification in a Scanning Electron Microscope</u>

<u>FY 1994</u> \$304,000

DOE Contact: G. J. D'Alessio, (301) 903-6688 SNL Contact: Joseph R. Michael, (505) 844-9115

Phase identification is classically accomplished using diffraction, either electron or X-ray. In very small particles or thin films, electron diffraction in a transmission electron microscope is normally used, but this involves time-consuming and sometimes unsuccessful sample preparation. We are developing a method for phase determination by analyzing backscattered electron Kikuchi patterns in a scanning electron microscope using a Sandia-designed charge-coupled device based detector system. We have shown that the addition of a special electron filter to the CCD detector system permit high quality X-ray Kossel patterns to be obtained. Using this system crystallographic parameters can be measured with an accuracy of better than one part in 10,000.

Keywords: Analysis, Microstructure, Microscopy, X-ray

343. <u>Pyrolytically Derived Carbon</u>

DOE Contact: G. J. D'Alessio, (301) 903-6688 SNL Contact: Clifford L. Renschler, (505) 844-0324

This project develops carbon films with well-controlled properties via pyrolitic decomposition of organic polymers. We have developed methods to produce pyrolitic carbon films with well-controlled electrical conductivity, adhesion, and morphology. Applications have been identified in electronic devices, protective coatings, fuel cell fabrication, as well as direct weapon applications. In collaboration with New Mexico State University, we have developed extremely small, robust, carbon film electrodes (termed "nanoband" electrodes) for metals analysis in remote, harsh environments. We recently set "world records" for the smallest volume sample ever characterized electrochemically (500 nanoliters) and the smallest total analyte ever determined electrochemically (500 attomoles of lead).

Keywords: Analysis, Electronic, Polymer

<u>FY 1994</u> \$200,000

FY 1994

344. Thin Film X-ray Diffraction Development

<u>FY 1994</u> \$180,000

DOE Contact: G. J. D'Alessio, (301) 903-6688 SNL Contact: Michael O. Eatough, (505) 844-7761

Residual strain in thin films can affect the properties of the films. Current methods measure only average strain throughout the film. There are currently no methods for the determination of the anisotropic strain distribution as a function of film depth. Such a capability would particularly benefit the development of nonvolatile optical and electronic memories where thin films are extensively used. Grazing incidence X-ray diffraction is being investigated and a microdiffractometer is being constructed using a two dimensional detector and total reflection collimation for the analysis of 10-1000 micrometer diameter areas. Proof of principle has been attained for this strain profiling technique.

Keywords: Analysis, Diffraction, X-ray

345. <u>X-ray Micro-Tomography</u>

DOE Contact: G. J. D'Alessio, (301) 903-6688 SNL Contact: Monte C. Nichols, (510) 294-2906

Advanced materials exhibiting micro-nonhomogeneity such as ceramic matrix composites are increasingly used in high technology applications. The fabrication of these materials requires a better understanding of processing variables and how they control the development of the composite microstructure. We have developed high-resolution methods of X-ray tomography to measure density and porosity in such materials. This information can be used to adjust the processing variables to achieve the desired microstructure. A load frame associated with the X-ray tomography apparatus is enabling us to understand the fundamental mechanisms associated with the fracture process in continuous fiber composites.

Keywords: Analysis, X-ray, Microstructure, Porosity

346. Defect Studies of ZnO Phosphors

DOE Contact: G. J. D'Alessio, (301) 903-6688 SNL Contact: Duane B. Dimos, (505) 844-6385

Low-voltage phosphor materials for red, green, and blue light are required for improved flat-panel displays. Based on its electrical properties, ZnO is the most promising candidate material for developing low-voltage phosphors. Fabrication of phosphors requires doping of the ZnO to suppress the intrinsic luminescence and to enhance luminescence of

<u>FY 1994</u> \$300,000

<u>FY 1994</u> \$136,000 the desired wavelengths. To develop an understanding of the origin of the background luminescence and the role of potentially useful dopants, the defect states of intrinsic point defects and dopants need to be studied. Defect studies using electron paramagnetic resonance and photothermal deflection spectroscopy will be used to determine the defect structures and energy levels of dopants used to enhance electroluminescence of ZnO.

Keywords: Ceramics, Electronic, Optical

SNL Contact: Steven H. Goods, (510) 294-3274

347.	<u>Containm</u>	ent Materials for Transferable Explosives	<u>FY 1994</u>
		-	\$409,000
DOE	Contact: (G. J. D'Alessio, (301) 903-6688	

First-wall materials must be identified for containment vessels that can withstand prolonged exposure to transferable paste explosives, prevent permeation of liquid constituents and function properly on demand for transfer of energetic fluids. We are evaluating the compatibility of energetic fluids with candidate containment materials. The energetic fluids are constituents of various extrudable explosives developed by Lawrence Livermore National Laboratory. These paste-like explosives consist of explosive particulates (HMX, TATB for example) suspended in mixtures of energetic liquids and are designed to remain extrudable over a wide temperature range for many years. It is important to preclude or minimize interactions between the constituents of the paste and the containment materials since such interactions could result in decreased reliability or failure of the containment vessel as well as intrinsic changes in the flow or explosive characteristics of the This work focuses on one specific paste formulation: RX-52-AE, composed paste. principally of the solid explosive TATB and the energetic liquid, FEFO (BIS-(2-FLUORO-2,2-DINITROETHYL) Formal). Compatibility between a number of organic and metallic materials with neat FEFO has been evaluated.

Keywords: Metals, Corrosion, Coating, Embrittlement, Failure

348. Polymer Blends and Interfaces

<u>FY 1994</u> \$350,000

DOE Contact: G. J. D'Alessio, (301) 903-6688 SNL Contact: Roger Lee Clough, (505) 844-3492

Preparation of materials through the blending of two or more different polymers offers the ability to tailor materials properties for specific application requirements. However, polymers exhibit very limited solubility in one another, thereby limiting the usefulness of this approach to advanced materials development. A closely related problem involves the adhesion between two different organic materials; here, the interaction of polymer chains at the interface is of paramount importance. We have developed successful models for predicting the phase diagrams of polymer blends. This work is being applied to the development of polymer-based additives to enhance the solubility and bondability of polymeric materials. Scattering techniques are being applied to verify the degree of intermixing of polymers at the interfaces of surfaces and phase boundaries.

Keywords: Organics, Adhesive, Modeling, Polymer

349. Polymer Degradation and Lifetime

<u>FY 1994</u> \$350,000

DOE Contact: G. J. D'Alessio, (301) 903-6688 SNL Contact: Roger Lee Clough, (505) 844-3492

Prediction of material lifetimes is of extreme importance to the viability of the stockpile. Polymers undergo a steady aging process, which leads to a deterioration of their properties, over the course of years. This deterioration carries with it the potential of failure of the device in which the material is incorporated. Aging predictions, which are based on accelerated aging tests, are prone to incorrect conclusions due to the fact that the nature of the aging process may be fundamentally different under accelerated (laboratory) conditions versus real-world aging conditions. We are developing advanced accelerated aging methodologies based on the use of highly sensitive techniques (microcalorimetry, oxygen consumption) that allow us to monitor degradation rates under both application conditions and accelerated aging conditions. This approach will allow us to verify extrapolations of aging rates based on accelerated tests.

Keywords: Organics, Modeling, Polymer

Materials, Properties, Behavior, Characterization or Testing

350. <u>Chemometric Development</u>

DOE Contact: G. J. D'Alessio, (301) 903-6688 SNL Contact: David M. Haaland, (505) 844-5292

Chemometrics involves the use of modern statistical methods to analyze chemical data. The deconvolution of a peak into overlapping constituent peaks and the smoothing of noisy data are very simple and classical examples. At Sandia, we have been working for over 15 years to develop new methods which can increase the information which we can glean from chemical data. Techniques are being developed and refined for the quantitation of chemical species from infrared spectroscopy, for frequency selection in applying multivariate calibration and prediction methods to infrared and near-infrared spectroscopy and for the reduction of data from "two-dimensional" or "hyphenated" methods (e.g. TGA-FTIR). We have developed transfer of calibration algorithms to use models developed on

FY 1994 \$300.000 one spectrometer on another. Applications of the software developed have ranged from more sensitive analysis of gases evolving from explosive components used in missiles to methods for the on line analysis of passivating dielectrics films used on integrated circuits to the instruments for noninvasive blood chemistry determinations.

Keywords: Analysis, Chemometric, Spectroscopy

351. <u>Dismantled Weapon Hardware - Characterization and Analysis</u> FY 1994

\$180,000

DOE Contact: G. J. D'Alessio, (301) 903-6688 SNL Contact: William B. Chambers, (505) 844-3849

The waste characterization issues surrounding the disposition of excess component hardware from dismantled weapons are a potential regulatory bottleneck that could impact the dismantlement schedule. The functional design characteristics of complex electronic assemblies are well known, however, the quantitative material composition of electronic parts was not well documented if not specific to the function. Our project has focused on analyzing the chemical and material characteristics of electronic hardware which dictate the disposal options. Inductively Coupled Plasma (ICP) and X-ray Fluorescence spectroscopic analyses have shown that the majority of components tested contain enough lead and cadmium to be considered hazardous solid waste which requires controlled disposal in a chemical waste landfill. Analyses have also shown that these same components contain sufficient precious metal (Au, Ag, Pd) to warrant reclamation through pyrometallurgical processing. The reclamation option provides for a disposal route which is not only economical but promotes waste minimization through material resource recovery.

Keywords: Analysis, Chemical, Metals, Spectroscopy, X-ray

352. <u>Materials Characterization Using Ultrafast Optical Techniques</u> \$250,000

DOE Contact: G. J. D'Alessio, (301) 903-6688 SNL Contact: Richard H. Stulen, (510) 294-2070

The long term objective of this task is to apply techniques of optical spectroscopy to the characterization of materials, especially wide band gap materials whose utility can be related to their optical properties. We currently focus on materials used as photoconductive sensors for radiation detectors, and also on novel materials synthesized in a companion task, "Surface, Interface, and Bulk Properties of Advanced Ceramics." Successful application of photoconductive radiation sensors depends critically on the dynamics of charge carriers photogenerated within the bulk of the material; this charge must be efficiently collected if the detector is to function properly. These charge carriers lose energy, evolve into collective pseudoparticles, fall into traps, and recombine in sub-picosecond time scales. Thus we utilize ultrashort laser pulses, extending into the femtosecond regime, and ultrafast detectors to determine the detailed dynamics of charge carriers in pure materials, and in those containing dopants, impurities, and defects. The objective of such characterization is to enhance charge collection efficiency by determining the mechanisms limiting the lifetime and mobility of charge carriers in such materials. Also, novel materials synthesized in the companion task are probed via photoluminescence spectroscopy to characterize impurity and structural defects, and to determine band gap structure.

Keywords: Analysis, Semiconductor, Compound, Spectroscopy

353.	Materials Identification for Weapon Dismantlement	<u>FY 1994</u>
		\$229,000
DOE	Contact: G. J. D'Alessio, (301) 903-6688	
SNL	Contact: Mark W. Perra, (510) 294-2093	

Sandia/California is developing and applying materials chemical analysis methods to obtain needed materials identification for California weapons components. We use these methodologies when we cannot adequately define required information through reviews of drawings, reports and specifications. When ambiguity or uncertainty exists, we assist in materials specification interpretation and provide independent confirmation by analysis of materials to assure the accuracy and integrity of information in the dismantlement database. Sandia/California measures and assesses the significance of service contamination, including residual tritium contamination on and within California weapon components. (The component specifications will not reflect this contamination.) Lastly, we will identify materials from on-site, undocumented development hardware and from WR-like components.

Keywords: Analysis, Chemical, Diffraction, Microscopy, Microstructure, Spectroscopy

354.	Metal Deposition on Semiconductor Surfaces	<u>FY 1994</u>
	•	\$150,000
DOE	Contact: G. J. D'Alessio, (301) 903-6688	
SNL	Contact: Victoria E. Granstaff, (505) 844-8789	

Metal contaminant deposition on semiconductor wafer surfaces is a primary cause of defects which leads to lower yields of functional devices from a wafer. Very low levels of metallic impurities in chemicals used in integrated circuit processing can be a source of this contaminant deposition. Understanding the mechanism of deposition may allow easily implemented steps to be taken to reduce or eliminate the deposition. Electrochemical studies have been undertaken to understand these mechanisms. Methods for the analysis of very low level impurities in these chemicals either do not exist or are exceedingly timeconsuming and labor- intensive. New Inductively-coupled-plasma/mass spectrometry techniques are being investigated as a relatively rapid method for the quantitation of metallic species to the part/per/trillion level.

Keywords: Analysis, Surface, Chemical

355. <u>Non-Nuclear Laboratory Operation Reconfiguration Support</u> FY 1994

DOE Contact: G. J. D'Alessio, (301) 903-6688 SNL Contact: James R. Brangan, (505) 844-1832

We are supporting the transfer of neutron generator and neutron tube manufacturing from the DOE's Pinellas Plant. This support includes all non-radioactive materials analysis for the development and production of the new and recertified generator and tube components. During FY94, a project plan was developed to allow for the implementation of a materials qualification program that is fully compliant with DOE requirements, addressing the needs for documentation; identifying all applicable requirements, and QA/QC needs. In addition, this program seeks the fulfillment of customer needs, defining and designing processes for WR qualification of materials including equipment calibration, identifying the needed resources of manpower and equipment, and teaming with Neutron Generator Manufacturing Facility personnel to provide seamless laboratory support.

Keywords: Analysis, Reconfiguration

356. <u>Process Applications</u>

<u>FY 1994</u> \$667,000

\$230,000

DOE Contact: G. J. D'Alessio, (301) 903-6688 SNL Contact: Mark W. Perra, (510) 294-2093

Sandia/California is acquiring, developing, extending and applying materials capabilities required to execute core DP missions in science-based stockpile stewardship, strategic surety and product realization. Specifically, we use materials and process capabilities to quickly diagnose and understand failures in the stockpile, replace limited life components, as well as to maintain, upgrade and dismantle weapons. We support the product realization process for components and subsystems. We develop analytical tools needed to meet DP requirements in production support and problem solving. To understand and validate predictive models of aging stockpile materials, we develop, demonstrate and extend specialized materials characterization tools.

Keywords: Analysis, Chemical, Diffraction, Microscopy, Microstructure, Spectroscopy

357. <u>A Mechanical Test for Qualifying Ceramic Granules</u>

<u>FY 1994</u> \$92,000

DOE Contact: G. J. D'Alessio, (301) 903-6688 SNL Contact: S. Jill Glass, (505) 845-8050

Lightning arrestor connectors (LACs) provide protection for electronic components from over voltages. Ceramic granules which are fabricated from zinc oxide, rutile and lead magnesium niobate-lead titanate, play an important role in the operation of LACs. While these granules must meet specified electrical requirements, there are important mechanical requirements which they must satisfy. They should exhibit sufficient mechanical integrity so that they do not fracture under specified vibrational and shock loading conditions. A loss of granule fragments as a result of fracture could lead to a loss of protection. This project is developing a reliable mechanical test and doing the subsequent testing of the granules to ensure the mechanical integrity of the granules during service.

Keywords: Ceramics, Varistor, Fracture

358.	Analysis of Glass Properties for Stockpile Components	<u>FY 1994</u>
		\$118,000

DOE Contact: G. J. D'Alessio, (301) 903-6688 SNL Contact: Richard K. Brow, (505) 845-8047

Glass in stockpile components experiences mechanical stresses which arise from handling and, more importantly, the service environment. The nature of the stresses that arise from handling differ fundamentally from those it experiences during service. One significant problem is the occurrence of surface defects which ultimately affect the reliability of the material since the material can potentially fail at lower than anticipated stresses when handled. Consequently, a need for fractographic analysis is essential in order to get a better estimate of the overall reliability of the material. The nature of the service environment is such that the molecular structure of the glass is affected. Consequently, spectroscopic techniques, such as nuclear magnetic resonance and Raman spectroscopy, are being combined with the studies of the mechanical properties of aged and unaged materials in order to get a better understanding of the behavior of the material and its potential service life.

Keywords: Ceramics, Glass, Fracture, Structure

359. Electrical and Optical Properties of Ferroelectric Thin Films

<u>FY 1994</u> \$325,000

DOE Contact: G. J. D'Alessio, (301) 903-6688 SNL Contact: Duane B. Dimos, (505) 844-6385

Although psuedo-cubic ferroelectrics can exhibit 90° domain switching, 90° switching appears to be suppressed in thin films. However, obtaining 90° switching is critical for good electrooptic responses. The influence of potential constraints, such as grain size, stress, and film thickness, on 90° switching is evaluated by varying these parameters and by using X-ray diffraction and optical birefringence measurements to determine the switching characteristics. High-quality ferroelectric thin films are also appropriate for smart electronics applications that require integrated piezoelectric materials. However, initial work suggests that thin films may exhibit smaller piezoelectric responses that bulk ceramics. The influence of thin-film clamping stresses and polarization relaxation on piezoelectric activity are studied. The piezoelectric response is determined directly using optical methods and indirectly using SAW devices. In addition, the effect of microstructure and porosity on electromechanical losses is investigated. Electron paramagnetic resonance studies and bandstructure calculations are used to develop an atomistic description of the ferroelectric behavior of Pb-based ferroelectrics.

Keywords: Ceramics, Electrooptic, Ferroelectric, Film, Piezoelectric, Sol Gel

360. Ferroelectric Read/Write Optical Disc

<u>FY 1994</u> \$550,000

DOE Contact: G. J. D'Alessio, (301) 903-6688 SNL Contact: Duane B. Dimos, (505) 844-6385

Optical memories are an important technology for mass data storage because they have very high storage densities, are removable/archivable, and can be used in harsh environments. However, magnetooptic materials, which are the current state-of-the-art for read/write optical memories, have a variety of technical limitations. Ferroelectric, lead lanthanum zirconate titanate (PLZT) thin films are being developed as an alternative optical memory medium, since they have larger Kerr effects, greater temperature stability, and lower power requirements. To optimize the electrooptic response in a memory, which improves the signal-to-noise ratio, a high reflective coating stack that is compatible with PLZT thin film processing is being developed. Ellipsometry and waveguiding refractometry are used to characterize and optimize the electrooptic response. PLZT 9/65/35 films are also being developed to optimize the intrinsic electrooptic response of the ferroelectric. To permit optical storage at laser diode wavelengths, appropriate photoconductive polymers are being evaluated. Finally, light scattering and spatially-resolved electrooptic measurements are being done to characterize the uniformity and optical quality of PLZT thin films.

Keywords: Ceramics, Electrooptic, Ferroelectric, Film, Optical, Sol Gel

361. Lead Magnesium Niobate-Lead Titanate Granules

<u>FY 1994</u> \$105,000

DOE Contact: G. J. D'Alessio, (301) 903-6688 SNL Contact: Bruce A. Tuttle, (505) 845-8026

Zinc oxide varistor materials and rutile have been used to fabricate ceramic granules for lightning arrestor connectors (LACs). The granules are an important factor in the reliability and performance of LACs which provide protection for components from over voltages. The granules in a LAC must meet certain requirements. In addition to mechanical integrity, the granules must maintain a certain level of insulation resistance and fast rise breakdown voltage even after prolonged exposure to temperature and humidity. Recently developed granules based on lead magnesium niobate-lead titanate (PMN-PT) offer important advantages relating to reliability over rutile, ZnO or mixed oxide based granules. Studies are underway to identify composition ranges and processing parameters that will ensure the reliable production of PMN-PT granules that will offer improved performance over granules currently used in LACs.

Keywords: Ceramics, Varistor, Electronic

362. A Novel Technique for the Mechanical Characterization of Thin FilmsFY 1994
\$307,000DOE Contact: G. J. D'Alessio, (301) 903-6688

SNL Contact: Roy J. Bourcier, (505) 844-6638

We are developing novel test methods, through the combined use of ultralow load mechanical testing and large-strain finite element analysis, which will accurately characterize the elastic and plastic mechanical response of thin films. The accurate characterization of film properties will help guide film alloy development efforts and improve prediction of film behavior in engineering components. In developing these test methods, we are using micromachining techniques to fabricate isolated film features which are being mechanically tested using our ultralow-load indentation test system. Finite element analysis has been employed to optimize the design of the geometric features of the film to be tested. Finite element analysis will also be used, as necessary, to deconvolute the observed test specimen response to extract the constitutive response of the film. This test method will have an immediate impact on our ability to understand the behavior of IC interconnect metallizations, the mechanical response of micromachined devices, and the characterization of ion implanted films.

Keywords: Metals, CVD, Failure, Film, Fracture, Modeling, Packaging, Surface

363.	Development of Alternatives for Lead Based Solders	<u>FY 1994</u>
	•	\$278,000
DOF	Compared: J. J. MamElant (202) 596 5792	

DOE Contact: J. L. VanFleet, (202) 586-5782 SNL Contact: Paul T. Vianco, (505) 844-3429

The objectives of this CRADA project (with NCMS) are to evaluate and select alternative alloys for lead-based solders used for electrical and electronic assembly interconnections. These alternative alloys will have physical and electronic properties selected for specific applications. The selection of candidate lead-free solder alloys for evaluation will be based on several factors including technical, economic, environmental, and human factor considerations. Additionally, the selected alloys will be required to meet performance requirements at operating environments from -70°C to 180°C. Sandia will perform most of the initial alloy design, preparation, and screening and will assist the industrial participants in assessing manufacturing issues pertaining to the new alloys. This includes model joint testing, test hardware development and manufacture, environmental stress testing, and testing of manufactured printed wiring boards.

Keywords: Metals, Solder, Alloy, Joining, Joint, Packaging

364.	NCMS Printed Wiring Board Surface Finishes Program	<u>FY 1994</u>
		\$650,000
DOF	Contact: J. J. VanEleet (202) 586-5782	

SNL Contact: Frederick G. Yost, (505) 844-5278

The goal of the Printed Wiring Board Interconnect Systems Program is to develop advanced technology to enable the U.S. Printed Wiring Board (PWB) industry to maintain its position at the leading edge of this crucial technology. The program addresses critical areas of generic, pre-competitive technologies needed to enable the utilization of next generation electrical components. As the operating speed and number of interconnections of individual electronic devices has increased, PWB technology has been challenged to keep pace and the fundamental limits of existing PWB manufacturing technologies are becoming increasingly apparent. The Surface Finishes component of this program emphasizes development of solderability test methodologies and development of "leap frog" technologies that provide more robust assembly processes with a more benign environmental impact. The Surface Finishes project activities are divided into 5 parts. Solderability Assessment focuses on solderability measurement and understanding the fundamental aspects of wetting behavior. Solderable Finish Stressing explores the results of aging and accelerated stressing on the shelf life of PWB surfaces. Baselining and Benchmarking attempts to compare PWB product from the participating companies in order to facilitate improvements. Surface Finish Improvements seeks to implement identified process enhancements. Surface Finishes for New Assembly Technologies anticipates emerging assembly technologies, such as Ball Grid Array technology, and investigates new and compatible surface finishes.

Keywords: Metals, Solder, Coating, Modeling, Packaging, Surface

365.	Specialty Metals Product Characterization and Ouality	<u>FY 1994</u>
		\$695,000
DOE	Contact: J. L. VanFleet, (202) 586-5782	
SNL	Contact: James A. Van Den Avyle, (505) 845-3105	

This project, conducted for the Specialty Metals Processing Consortium (SMPC), addresses issues of ingot and final product quality for alloys produced by vacuum arc remelting or electroslag remelting processes. The effort includes metallurgical ingot analyses to evaluate solidification conditions produced by differing melt control strategies, to verify process modeling predictions, and to study melt defect formation. New X-ray analytical techniques to measure ingot composition variations are being developed. The project includes fundamental studies of micro-scale solidification processes and how they relate to melt defect formation. To assess the final product quality of Alloy 718 billets, the effects of solidification defects on fatigue properties are being evaluated.

Keywords: Metals, Alloy, Melting, Microstructure, Modeling, X-ray

366. Welding of AerMet 100

<u>FY 1994</u> \$225,000

DOE Contact: J. V. VanFleet, (202) 586-5782 SNL Contact: Charles V. Robino, (505) 844-6557

AerMet 100 is a recently developed high strength, high fracture toughness alloy designed for use in structural components in aerospace applications. The alloy is basically a precipitation hardenable martensitic steel with strength levels exceeding that for AF 1410, while toughness is intermediate between AF 1410 and Marage 250. As a result of this combination of very high strength and toughness, the alloy has a number of potential applications in weapon systems. However, the ability of the welded alloy to meet service requirements for mechanical properties, corrosion resistance, *etc.*, has not been characterized. The suitability of AerMet 100 for application in welded structures, and the processing requirements for confident application, are being addressed in this CRADA. Weld test panels are being fabricated for determination of the effects of weld processing parameters on mechanical properties of the weld fusion and heat-affected zones. In addition, weld simulation studies are being used for determination of the kinetics of microstructural evolution in the heat-affected zone. It is expected that knowledge of the kinetics of microstructural changes (and mechanical property changes) will allow for selection of optimal weld processing schedules. (This project is a CRADA with Carpenter Technology Corp.)

Keywords: Metals, Weld, Joining, Steel

367. Carbons for Electrochemical Energy Storage

FY 1994 \$298,000

DOE Contact: G. J. D'Alessio, (301) 903-6688 SNL Contact: Jill M. Hruby, (510) 294-2596

Advanced concepts for lithium secondary batteries and supercapacitors require microporous carbon materials as an electrode or composite electrode. The advanced batteries and capacitors will enable new power supplies for weapons as well as new surveillance and monitoring techniques. For lithium batteries, the carbon is intercalated with lithium to allow for high energy storage and long lifetimes. For supercapacitors, the carbon serves as an electrode and enables small, lightweight, high capacitance devices to be developed. In this activity we engineered microporous carbons from a variety of polymer precursors, processed the carbons using different conditions, and measured their performance as battery or supercapacitor materials. The most promising carbons were used in prototype devices and the overall component performance measured.

Keywords: Organics, Microporous, Polymer, Carbon

368. <u>Catalytic Carbon Foam Filters</u>

DOE Contact: Maurice Katz, (202)586-5799 SNL Contact: James C. F. Wang, (510) 294-2786

Activated carbon catalytic foam materials with low back pressure have many applications in the energy generation and storage as well as in waste minimization areas. An example is carbon foam filters that are capable of converting ozone produced in copy machines into harmless oxygen; similar filters may be used for applications in commercial airliners, the space shuttle, and the space stations. Catalytic carbon foams may also be used in converting natural gas into low-polluting liquid fuels for various users such as transportation. This project is to develop manufacturing processes of catalytic carbon filters based on our expertise in engineering of microporous foams for various energy and environment related applications.

Keywords: Organics, Catalytic, Carbon, Filter, Foam

<u>FY 1994</u> \$338,000

369. <u>Chlorinated Polyethylene</u>

<u>FY 1994</u> \$358,000

DOE Contact: J. L. VanFleet, (202) 586-5782 SNL Contact: James H. Aubert, (505) 844-4481

This project includes a CRADA with an industrial partner which is a major producer of chlorinated polyethylene (CPE). The polymer is used as an impact modifier for polyvinylchloride and acrylonitrile-butadiene-styrene copolymer and as an elastomer for wire cable coatings and automotive parts. We are working towards an understanding of the relationship between the molecular structure of CPE (chlorine content, chlorine distribution, molecular weight) and the solid and liquid state structures (phases present, percent crystallinity, crystal structure, morphology). This architecture will then be related to the conditions in the reactor used to produce this product with its' unique properties. In this way we and our industrial partner can utilize these relationships to optimize CPE plant operations and expand their customer base. We are relying on many analytical techniques to develop these relationships including NMR, X-ray and neutron scattering, diffraction, and calorimetry.

Keywords: Organics, Scattering, CRADA, NMR, Polymer

370. <u>High Density Electronic Interconnects</u>

<u>FY 1994</u> \$890,000

DOE Contact: G. J. D'Alessio, (301) 903-6688 SNL Contact: Clifford L. Renschler, (505) 844-0324

As integrated circuits with ever larger pin-outs come into use, the interconnect density of printed wiring boards (PWBs) is increasing beyond the point at which current materials and processes can be economically used. In this program, we are working with the National Center for Manufacturing Science and member companies Texas Instruments, IBM, AT&T, GM-Hughes, United Technologies, and Allied Signal to develop the next generation materials for PWB fabrication. We are working in four general areas in support of this program: enhanced control of plasma processing of boards, improved strength between the copper/resin and glass/resin interfaces, modeling of multilayer boards, and development of board substrates with non-woven reinforcement.

Keywords: Organics, Composite, Electronic, Modeling, Plasma, Polymer

371. Materials for Improved Tire Technology

<u>FY 1994</u> \$1,000,000

DOE Contact: J. L. VanFleet, (202) 586-5782 SNL Contact: Roger Lee Clough, (505) 844-3492

We are working with an industrial partner on a highly integrated program to provide elastomeric materials having improved performance and high reliability. We are working to improve filler-elastomer interaction in conventional materials to enhance durability and mechanical performance. We are developing enhanced methodologies for lifetime prediction of elastomeric materials, based on the analysis of degradation rates and mechanisms under accelerated aging conditions. We are evaluating new filler types, with regard to molecular structure and macroscopic properties. We are applying principles of chemometrics to rapid analysis of materials formulations.

Keywords: Organics, Polymer, Modeling

372. Applica	tion of IRIS to Semiconductor Processing	<u>FY 1994</u>
	•	\$175,000
DOE Contact	G. J. D'Alessio, (301) 903-6688	
SNL Contact:	Clifford L. Renschler, (505) 844-0324	

Sandia researchers have recently developed a technique known as IRIS (Imaging of Radicals Interacting with Surfaces). To take an IRIS measurement, a molecular beam is extracted from a plasma and scattered off the substrate of interest while molecules in the beam are simultaneously probed before and after scattering from the substrate with laser-induced fluorescence. IRIS is currently the only technique available, worldwide, to measure the surface reaction probabilities for plasma radicals impinging on a depositing film. Accurately known reaction probabilities are essential for the development of robust plasma process control models of the type that will be required for future computer-controlled, ultra-high throughput semiconductor manufacturing. In a CRADA with Texas Instruments, Inc. (TI), we measured the surface reactivities of the OH and NH radicals that are important in the deposition of silicon dioxide and silicon nitride films during integrated circuit manufacture. These data were incorporated into plasma process control models at one of TI's manufacturing facilities. In addition, we incorporated Sandia's patented gas phase metal precursor sensor technology into TI's process line.

Keywords: Semiconductor, Coating, Film, Plasma

Lawrence Livermore National Laboratory

Materials Preparation, Synthesis, Deposition, Growth or Forming

373. Engineered Nanostructure Laminates

<u>FY 1994</u> \$1,300,000

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 500μ m thick samples have been synthesized for mechanical property studies of multilayer structures.

These unique man-made materials have demonstrated extremely high mechanical performance as a result of the inherent ability to control both composition and structure at the near atomic level. Also, mechanically active flaws that often limit mechanical performance are controllable so that the full potential of the structural control available with multilayer materials is accessible. Systematic studies of a few multilayer structures have resulted in free-standing foils with strengths approaching those of whiskers, approximately 70 percent of theory. Also, new mechanisms for mechanically strengthening materials are accessible with nanostructure laminates.

Applications now under development include: coatings for aircraft gas turbine engines; EUV, soft X-ray and X-ray optics spectroscopy and imaging; high performance capacitors for energy storage; capacitor structures for industrial applicatons; high performance tribological coatings; coatings for aircraft gas turbine engines; ultra-high strength materials; integrated circuit interconnects; magnetic transducers/GMR.

Keywords: Thin Films, Multilayer Technology

374. Sol Gel Coatings

FY 1994 \$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 high reflection (HR) coatings using colloidal SiO_2 with either HfO_2 or ZrO_2 . We have found that the

incorporation of an organic polymer binder such as polyvinyl alcohol or polyvinyl pyrolidinone into the high index component has resulted in an increase in the damage threshold and a decrease in the number of layer pairs required for high reflection.

A laboratory size meniscus coater was evaluated and found to produce mirrors of high optical performance and adequate damage threshold. This is now the preferred method of application, and a large machine capable of producing Beamlet and NIF size mirrors is to be delivered in early FY 1994.

Keywords: Sol Gel Coatings, Meniscus Coater, HR Coatings

375. KDP Growth Development

<u>FY 1994</u> \$900,000

DOE Contact: G. J. D'Alessio, (301) 903-6688 LLNL Contact: J. J. De Yoreo, (510) 423-4240

Potassium dihydrogen phosphate (KDP) and its deuterated analog (DKDP) are important nonlinear crystals used both for frequency conversion as well as for a large Pockels cell. These crystals are very expensive, due in part to the very long times required to grow large boules (2-3 years) and the cost of D_2O for growing DKDP. We are developing alternative growth techniques to dramatically increase the growth rate of these crystals.

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 have recently completed a station for the growth of 50x50x50cm³ crystals and are currently testing its capabilities. 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

376. Advanced Finishing Development

<u>FY 1994</u> \$300,000

DOE Contact: G. J. D'Alessio, (301) 903-6688 LLNL Contact: J. S. Taylor, (510) 423-8227

Advanced optical fabrication methods will 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.

In addition, we will be working with LANL to characterize and optimize the use of synthetic pads as a polishing lap material on continuous polishing machines. Successful development of synthetic pad polishing is of primary importance in our quest to lower fabrication times, and hence costs, of large, precision, flat optics for future ICF lasers.

Keywords: Optical Finishing, Synthetic Pad Polishing, Cost Reduction, Manufacturing, ICF, NIF

377. Doped Polymers for ICF

<u>FY 1994</u> \$50,000

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

378. <u>ICF Capsule Ablators via Plasma Polymerization</u>

<u>FY 1994</u> \$428,000

DOE Contact: G. J. D'Alessio, (301) 903-6688

LLNL Contacts: R. Brusasco, (510) 422-3111, R. Cook, (510) 422-3117 and S. Letts, (510) 422-0937

Our group uses plasma polymerization to prepare conformal coatings of organic polymer for use as ICF capsule ablators. These coatings have some unique and stringent requirements, such as a surface roughness of the order of 10 nm rms or less and the strength

to hold fuel pressures of from 50 to 100 atm. This project supports development of methods to incorporate high Z dopants (e.g., germanium) into the polymer structure, development of coating procedures which efficiently produce useable target mandrels and basic studies to understand the mechanism of roughness evolution during deposition. A coating system with a computer interface has increased production throughput and aided the optimization of the coating process. In addition, new mass spectrometric tools are being used to increase our fundamental knowledge of the deposition mechanisms.

Keywords: Plasma, Polymer, Germanium, Fusion

379. Excimer Laser Micromachining

<u>FY 1994</u> \$100,000

<u>FY 1994</u> \$200,000

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

380. Advanced Synchrotron Radiation Study of Materials

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-ofthe-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 subsecond 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 *in-situ* mapping of phase boundaries 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. The latter activity has been awarded a lab-wide LDRD at start of FY94. Since January 1994, Dr. Michael Fröba, a physical chemist recently graduated from the university of Hamburg, Germany, and awarded a prestigious Humboldt postdoctoral fellowship has joined our soft X-ray experimental effort. The theoretical effort in calculating and elucidating the fine structure features in the soft X-ray XANES spectra has been undertaken by Dr. Eiichi Tamura.

Keywords: Synchrotron Radiation, Fusion Welds, Phase Transformation, QEXAFS Monochromator

381. Structural Transformations and Precursor	Phenomena FY 1994
	\$169,000
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
382. Very High Energy Density Materials

<u>FY 1994</u> \$1,060,000

> <u>FY 1994</u> \$300,000

DOE Contact: G. J. D'Alessio, (301) 903-6688 LLNL Contacts: R. L. Simpson, (510) 423-0379

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.

LDRD: High Explosive Alloys (\$150K): We are investigating the development of high energy explosives which are made through co-crystallization of energetic components. A highly oxidized molecule is stablized in the lattice with an oxygen deficient molecule.

WSR: Synthesis of TATB (\$210K): Alternate synthesis route to 1,3,5-triamino-2,4,6-trinitrobenze (TATB) using picrates instead of 1,3,5-trichlorobenzene.

Keywords: Hard Structure Munitions

383. Interfaces, Adhesion, and Bonding

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 semiempirical embedded atom method (EAM), which uses modified two-body potentials with molecular dynamics, molecular statics, or Monte Carlo techniques to determine atomic rearrangements.

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

384. Laser Damage: Modeling and Characterization

<u>FY 1994</u> \$400,000

DOE Contact: G. J. D'Alessio, (301) 903-6688 LLNL Contact: M. R. Kozlowski, (510) 424-5637

We have been working to understand the damage mechanism in thin film coatings used on Nova 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

385. <u>KDP Characterization</u>

<u>FY 1994</u> \$400,000

DOE Contact: G. J. D'Alessio, (301) 903-6688 LLNL Contact: J. J. DeYoreo, (510) 423-4240

We require very large, high quality crystals of potassium dihydrogen phosphate (KDP) and its deuterated analogue (DKDP) for present and advanced high power lasers in the ICF Program. The performance of these crystals is limited by strain which induces anomalous birefringence and wavefront distortion. 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 and inhomogeneous impurity distributions due to anisotropies in growth kinetics. 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 these characterization techniques to relate the severity of these defects to the growth conditions.

Keywords: KDP, Strain, Crystal

386. Damage Testing

<u>FY 1994</u> \$800,000

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 fullsized 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

387.	Energy Transfer Dynamics in Energetic Materials	<u>FY 1994</u>
		\$120,000
DOE	Contact: G. J. D'Alessio, (301) 903-6688	
LLNI	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

388. <u>Processing-Structure-Property Correlation in Laminated</u> <u>Metal Composites</u>

<u>FY 1994</u> \$169,000

<u>FY 1994</u> \$390,000

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

389.	Scanning Tunneling	Microscopy (STM)	and Atomic Force
	Microscopy (AFM)		.*

DOE Contact: G. J. D'Alessio, (301) 903-6688 LLNL Contact: W. Siekhaus, (510) 422-6884

A small building standing separate from noise-generating machinery and hence having a low natural vibration background, has been refurbished to house all scanning probe instrumentation. The large stage scanning probe microscope that can perform scanning tunneling as well as contact and non-contact atomic force microscopy on the surface of objects as large as 6" in diameter, a small-stage non-contact AFM and STM, and a newly acquired ultra-high vacuum instrument that can perform non-contact AFM and STM measurements and STM spectroscopy (STS) have been moved into that facility.

UHV STM has been used to determine the XeF2-Si etching mechanism and its rate at room temperature and to perform nonolithography, i.e., creating nm-scale SiO₂ lines on Si. A new technique, nanostethoscopy, has been developed and used to determine the onset of biological biomechanical activity during the development of brine shrimp for cyst to nauplius. Nm-scale clusters of Si have been deposited by laser ablation onto the basal plane of graphite, and analyzed by STM and STS to study the physical basis for light-emission from Si. Tapping-mode AFM has been used to determine the morphology of novel gratings for NIF applications, and to determine the morphology of stress induced structural changes in aluminum thin films for microcircuitry. AFM in liquid has been used to determine the growth mechanism of KDP crystals. Large-stage AFM in air has been used to establish that inclusion-induced cones in multilayer antireflection and high-reflection optical coatings determine the laser damage threshold at 1.06 μ m if the diameter of the inclusion is above .6 μ m.

Keywords: NDE, Laser Damage, Optical Coatings, Optical Gratings, Nano-Lithography, Chemical Reaction, XeF₂, Etching, Nano-Stethoscope, Biomechanics, Si Light Emission, Stress Induced Grain Growth, Thin Films

390. <u>Thermoelectric Materials with Exceptional Figures of Merit</u>

<u>FY 1994</u> \$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. One approach to high ZT materials is the synthesis of two-dimensional quantum wells. We have synthesized several different thermoelectric multilayer films with the dimensions of quantum wells. These materials have been evaluated over a broad range of temperature, extending from the boiling point of liquid nitrogen to several hundred degrees centigrade. Though difficulties have been encountered with inadvertent doping of quantum wells by barrier layers, strategies are being developed to overcome this problem. Single layer thermoelectric thin films with very good electronic properties have been made. These single-layer films are now being incorporated into lightweight cooler designs for Boeing Defense and Space. We believe that such thin films can be used to make distributed coolers that have much less weight than comparable devices fabricated from bulk materials.

Keywords: Thermoelectric Materials

391.Capacitive Deionization as an Alternative to Ion ExchangeFY 1994

\$795,000

DOE Contact: Douglas Gish, DP 42, (202) 586-1741 LLNL Contact: J. C. Farmer, (510) 423-6574

A novel capacitive deionization process has been developed for the efficient removal of ionic contaminants from aqueous streams. Ions are 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 ($250 \text{ m}^2/\text{gm}$), <u>carbon aerogel</u> electrodes have been developed and are being used ($800 \text{ m}^2/\text{gm}$). This work is being funded by DOD SERDP (Strategic Environmental Research and Development Program). Collaborations are underway with a variety of government facilities including Tyndall Air Force Base, Idaho National Engineering Laboratory, and Westinghouse.

Keywords: Capacitive Deionization

392. <u>Trilayer Josephson Junctions (Technology Transfer Initiative)</u> FY 1994

\$425,000

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 third 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 perform microscopic investigations of interface quality and layer characteristics (LLNL), to select techniques for testing chemical homogeneity and surface regularity (LLNL) and to develop data for the processing data base. LLNL and Varian have performed all tasks described through the third sixmonth period milestones.

Varian Associates has delivered to LLNL researchers 22 trilayer wafers for evaluation, four of which were specially prepared for this TTI project. LLNL staff have completed Auger electron spectroscopy, X-ray fluorescence spectroscopy, transmission electron microscopy, ion microprobe spectroscopy, ion microscope spectroscopy, atomic force microscopy, scanning tunneling microscopy and Rutherford backscattering spectroscopy measurements on selected samples. Features observed in LLNL measurements have resulted in modifications of Varian procedures and Varian recently announced the most uniform array of electronic Josephson junctions ever produced in high temperature superconducting materials. Results have been transmitted on a regular basis to Varian participants through technical meetings.

Keywords: Superconductors, High Transition Temperature, Josephson Junction, Tri-Layers, Heteroepitaxy

393. Lithium Cell Development

<u>FY 1994</u> \$200,000

DOE Contact: Andre Cygleman, (202) 586-8814 LLNL Contact: John R. Kolb, (510) 422-6424

We continue to work on the development of a replacement electrolytic cell for the manufacture of lithium metal in support of the DOE Y-12 facility. Our development incorporates the introduction of a bipolar cell methodology where a bipolar electrode is one that is shared by two cells connected in electrical series. In the process being developed, lithium is electrodeposited in an aqueous cell at $\sim 30^{\circ}$ 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

394. <u>Environmentally Safe Disposal of Explosive Wastes: SERDP Project</u> <u>FY 1994</u> \$800,000

DOE Contact: Andre Cygleman, (202) 586-8814 LLNL Contact: John R. Kolb, (510) 422-6424

In collaboration with researchers at Los Alamos National Laboratory and the Pantex Plant, we are exploring options to support the Department of Energy and the Department of Defense in their quest to develop environmentally sound techniques for the destruction of residual high explosive remnants after dismantlement and demilitarization occur. We intend to pursue, and have demonstrated positively during this year, the capacity to minimize the amount of high explosive materials to be treated as waste and subsequently destroyed. We have chosen to manage the returning, surplus energetic material as an asset to be sold or given away in lieu of destruction. Through minimization of the amount of HE waste, we believe we can reduce, by an order of magnitude, the amount of material for which environmentally sound disposition techniques must be generated. We have focused on molten salt destruction, base hydrolysis and bioremediation as 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 1995. 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

395. Laminated Metal Composites for Aerospace Applications

<u>FY 1994</u> \$700,000

DOE Contact: Warren Chernock, (202) 586-7590 LLNL Contact: Donald Lesuer, (510) 422-9633

Laminated metal composites are materials in which two or more metal containing layers are deformation bonded. Previous work at LLNL has shown that these materials can have properties (such as fracture toughness, fatigue, damping capacity and impact behavior) that are superior to properties currently available in lightweight materials. These materials also offer the possibility to tailor properties to a prescribed application through the choice of component materials, relative volume fraction of the components, interface strength, etc. This project is funded through the Technology Transfer Initiative and is exploring the application of these materials to fan containment systems for commercial jet engines and to airframe structural components.

Keywords: Materials Properties, Behavior, Characterization or Testing

396.	Fatigue of	Metal Matrix Composites	· <u> </u>	FY 1994
DOF	Contact: 1	Varren Chernock (202) 586-7590	\$	450,000
LINI	Contact:	Densid Leaver (510) 422 0622		
LUNL	Contact:	Donald Lesuel, (310) 422-9033		

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

397.Molecular Dynamics Simulation Studies of Radiation Effects in SolidsFY 1994\$60,000\$60,000DOE 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

398. <u>Fundamental Studies of Particle-Solid Interactions</u>	<u>FY 1994</u>
	\$176,000
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 μ m technology.

Keywords: Ion Implantation, Semiconductor Processing, Dopant Diffusion, Computer Simulation

399.	Radiatio	n Effects in	Materials for	or Inertial	Confinement	<u>Fusion</u>	<u>FY 1994</u>
							\$50,000
DOE	Contact:	G. J. D'Ales	ssio, (301) 9	03-6688			

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

400.	Novel Materials for Optoelectronics and Photonics	<u>FY 1994</u>
		\$500,000
DOE	Contact: G. J. D'Alessio, (301) 903-6688	
LLN	L 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, organics (polymers), and aerogels. We have developed a type of nanocrystalline silicon (fabricated from porous silicon) that photoluminesces throughout 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 were also being studied. We have also fabricated arrays of miniature junction diodes from porous and nanocrystalline silicon that emit in the visible and near infrared. Silicon-based emitters are desirable because they integrate well with standard silicon-based microelectronics. Our studies on fullerenes showed their figures of merit 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 permit 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, Polymers, Electroluminescence, Flat Plan Displays, All-Optical Switching

Office of Defense Programs

401. Uranium Manufacturing Lead Lab Program

FY 1994 \$3,000,000

FY 1994 \$3,000,000

DOE Contact: Andre Cygleman, (202) 586-8814 LLNL Contact: Jeff N. Kass, (510) 422-4831

We are working 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 DOE Albuquerque Operations Office.

Manufacturing, Depleted Uranium, Uranium Alloy, Enriched Uranium, Waste Keywords: Minimization

402. Plutonium Manufacturing Lead Lab Program

DOE Contact: Andre Cygleman, (202) 586-8814 LLNL Contact: J. L. Robbins, (510) 422-7060

We are working with DOE, Los Alamos National Laboratory and Savannah River 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 for increased efficiencies. Funding for this effort is coming from SERDP and process development resources.

Keywords: Plutonium, Manufacturing, Casting, Machining, Waste Minimization

403.	Novel Materials Studies at High Pressures and Temperatures	
	by Using In-Situ X-ray Laser Heating Experiments in a DAC	<u>FY 1994</u>
		\$400,000

DOE Contact: Maurice Katz, (202) 586-5799 LLNL Contact: Choong-Shik Yoo, (510) 422-5848

The objective of this project is to integrate the synchrotron X-ray, laser heating, and diamond anvil cell technology together for the studies of material structure at the PVT conditions far beyond the reach of other technology. The feasibility of this experimental approach has already been demonstrated in the studies of iron phase diagram, providing crucial information for iron industry and for modeling the Earth core. The technique is now matured and is used for synthesis and characterization of novel materials such as super-hard materials and metastable energetic phases at high pressures and temperatures. Because the materials reactivity rapidly increases with pressure and temperature, in this study we have

been able to take a direct synthetic route between extremely inert molecules like nitrogen and hydrogen with many light elements like Li, Be, B, C, many of which combinations are potential for exotic novel materials like C_3N_4 and energetic metastable phases like LiH. Therefore, the success of this study would benefit to the US-industry by identifying one or more exotic novel materials and to DoD and DOE by providing a dual-use, state-of-the-art technology for studies of material properties at extremes of pressures and temperatures that can be carried out by a non-hazardous, table-top experiment.

- Keywords: Novel Materials Applications, Energetic Metastable Materials, Nitrides, Hydrides, Oxides, Ceramics, X-ray Laser Heating Experiments, High Pressures, Temperatures
- 404. <u>Advanced Molecular Dynamics Simulations of Molecular-Beam</u> <u>Induced Surface Processes</u>

<u>FY 1994</u> \$607,000

DOE Contact: Alex R. Larzelere, (202) 586-1101 LLNL Contacts: Christian Mailhiot, (510) 422-5873 and James F. Belak,

(510) 422-6061

The Wilson Center for Research and Technology of Xerox Corporation and Lawrence Livermore National Laboratory (LLNL) have begun work under a CRADA to develop fundamental scientific knowledge that will lead to improved performance in microelectronic devices used in a variety of industrial and consumer electronics products. LLNL's breakthrough atomic-level materials theory and modeling software extend Xerox's capabilities to study etching, passivation (making a surface less reactive chemically), growth of thin films, and other processes used in modern microelectronics. The project takes advantage of the breakthrough capabilities developed at LLNL in the area of advanced molecular dynamics simulations and the experimental capabilities to study supersonic molecular and reactive ion-beam-induced modifications of surfaces that have been developed at Xerox. In collaboration with Xerox, LLNL is developing and applying advanced molecular dynamics methods to examine energy transfer processes occurring in reactive gas/surface scattering as it relates to the etching, passivation and epitaxial growth of materials for microelectronics applications. These concurrent theoretical and experimental activities are synergistically coupled to validate LLNL's materials modeling methods and optimize Xerox's experimental processes.

Keywords: Atomic-level Materials Modeling, Ab-initio Electronic Structure Methods, Molecular Dynamics, Surface Science, Etching, Passivation, Tribology, Molecular Design

405. <u>High-Speed Tribology of the Head Disk Interface by</u> <u>Computer Simulation</u>

FY 1994 \$300,000

DOE Contact: Alex R. Larzelere, (202) 586-1101

LLNL Contacts: Christian Mailhiot, (510) 422-5873 and James F. Belak, (510) 422-6061

Lawrence Livermore National Laboratory (LLNL) and IBM's Almaden Research Center are collaborating under a CRADA on a research project that could help in the design of computer hard drives with greatly increased data storage capacity. Hard-drive technology currently allows storage of about 300 megabits of data per square inch of harddrive disk space. Researchers are trying to develop the components needed to store 10 gigabits (10 billion bits) per square inch. Increased data storage would allow hand-held or laptop computers to store more information, run software that could increase their usefulness many times over, and lead to smaller, more reliable hard drives that use less power. The team will use atomistic molecular dynamics modeling-describing the behavior of individual atoms of matter mathematically to better understand the chemical and physical processes at the point where the disk drive's read/write head meets the surface of the hard disk. By working interactively with the Almaden scientists who are developing new data storage technologies, the computer models can be checked for accuracy and assist IBM's engineer in the design and development of future generations of small and ultrasmall data storage products.

Keywords: Atomic-level Materials Modeling, Ab-initio Electronic Structure Methods, Molecular Dynamics, Surface Science, Etching, Passivation, Tribology, Molecular Design

406. <u>Massively Parallel Simulation of Large Molecular Systems with</u> Long-Range Interactions

<u>FY 1994</u> \$200.000

DOE Contact: Alex R. Larzelere, (202) 586-1101

LLNL Contacts: Christian Mailhiot, (510) 422-4873 and James F. Belak, (510) 422-6061

Lawrence Livermore National Laboratory, Cray Research, DuPont, and Bristol-Myers Squibb are collaborating under a CRADA to develop a set of computational tools that will allow the routine study of large molecular systems (hundreds of thousands of atoms) with long-range Coulomb interactions for tens of nanoseconds. These tools will enable the study of larger length-scale and longer time-scale phenomena than is currently possible on problems of interest to the pharmaceutical and polymer industries. Because of the enormous computational resources required to study these problems, all of the software will be designed for massively parallel supercomputers. In addition to developing new parallel methods to take advantage of the emerging hardware, we will develop and implement new algorithms to treat the long range forces implicit in these systems in a computationally efficient manner. A second goal is to apply the resulting tools to address interesting scientific and materials problems in novel organic-based materials including bio-membranes, liquid crystals, optical thin films (Langmuir-Blodgett films), and the diffusion of molecules in polymers and biomembranes.

- Keywords: Atomic-level Materials Modeling, Ab-initio Electronic Structure Methods, Molecular Dynamics, Surface Science, Etching, Passivation, Tribology, Molecular Design
- 407. <u>Advanced Atomic-Level Materials Design for Massively Parallel</u> <u>Environment (High Performance Parallel Processor Computing</u> <u>Initiative: H4P)</u>

<u>FY 1994</u> \$175,000

DOE Contact: Alex R. Larzelere, (202) 586-1101 LLNL Contact: christian Mailhiot, (510) 422-5873

The objective of this Cooperative Development Project is to move massively parallel computing technology into the industrial sector rapidly by focusing Cray Research, national laboratories, and industry resources on implementing a selected set of important industrial applications written in portable MPP programming languages. Within the H4P effort, a project entitled "Advanced Materials Design for Massively Parallel Environment" teams LLNL, the Xerox Palo Alto Research Center, and Cray Research Inc. The main goal of this project is to provide U.S. industry with breakthrough capabilities in advanced atomic-level materials simulation by using innovative new MPP algorithms, methods, and computers. Moreover, many computational tasks of central importance in materials modeling and simulation have wide applicability, and their optimization will benefit other industrial areas of research outside the confines of ab-initio electronic structure calculations of materials. Another technical objective is the application of advanced ab-initio electronic structure methods, at Xerox and at LLNL, to specific physics problems of primary importance to research activities at Xerox's Electronic Materials Laboratory, including investigations of the atomic and electronic structure of amorphous silicon and defect energetics in III-V semiconductor materials. In addition, the proposed research project is to integrate LLNL's advanced ab-initio molecular dynamics simulation capabilities into UniChem, CRI's graphical interface for computational chemistry. This goal is in the interest of CRI and the DOE national laboratories.

Keywords: Atomic-level Materials Modeling, Ab-initio Electronic Structure Methods, Molecular Dynamics, Microelectronics, Optoelectronics, Molecular Design

Office of Defense Programs

408. Growth and Formation of Advanced Heterointerfaces

<u>FY 1994</u> \$500,000

DOE Contact: Iran Thomas, (301) 903-3427

LLNL Contacts: Louis J. Terminello, (510) 423-7956 and Christian Mailhiot,

(510) 422-5873

The ultimate objective of this research effort is to provide a microscopic understanding of the structural aspects of solid heterointerface growth and formation. This goal is achieved by an interdisciplinary thrust based on the most comprehensive and advanced experimental and theoretical methods currently available to the materials science community. Experimental determination of the evolution of the atomic geometry and electronic structure during the early stages of interface formation are provided by a powerful combination of holographic and synchrotron-based probes of *in situ* prepared materials. Theoretical modeling of these effects are performed with ab-initio molecular dynamics simulations in which atomic trajectories are determined from self-consistent calculations of interatomic forces including the effects of electronic charge redistribution derived from local density-functional theory. Consequently, the novel structure and chemical information obtained by interface imaging, characterization, and dynamical ab-initio modeling with our recently pioneered experimental and theoretical techniques will serve as the basis for a rational synthesis of custom heterointerfaces and thus potentially produce atomistic control of novel materials fabrication.

Keywords: Atomic-level Materials Modeling, Ab-initio Electronic Structure Methods, Molecular Dynamics, Surface and Interface Science, Photoelectron Spectroscopy, Photoelectron Diffraction, Photoelectron Holography

409.	Materials Produced with Dynamic High Pressure	<u>FY 1994</u>
	•	\$500,000
DOE	Contact: G. J. D'Alessio, (301) 903-6688	
LLN	L Contact: William Nellis, (510) 422-7200	

This project seeks to produce novel materials (crystal structures, microstructures, and properties) using high shock pressures. The terms "dynamic" and "shock" are used synonymously in this context. Tuneable shock pressure pulses are produced by the impact of a projectile launched from a small two-stage light-gas gun. Shock pressures range from 0.01-1 Mbar, temperatures range from 50 up to a few 1000°C, strain rates on loading range above 10^8 /s and quench rates on release of pressure are 10^{12} bar/s and 10^9 K/s in specimens which are recovered intact for investigation. These conditions are the physical limits in macroscopic bodies and produce novel effects, both heterogeneous and homogeneous. A gas gun 6.5 m long is used to achieve these high shock pressures. Specimens range from 1 micron to 1 mm thick and are about 10 mm in diameter. The observed material structures can be correlated with computational simulations and fast real-time measurements to

enhance understanding of the effects produced. A wide variety of materials characterization measurements are made both before and after application of high dynamic pressures. In the past year we have dynamically compacted various ceramic and magnetic powders, altered superconducting critical current densities with shock-induced defects, produced unusual glass by shocking crystalline quartz, which apparently contains small particles of Si, and performed impact experiments to help design the containment fixture for the highvelocity flywheel to be contained in the next generation supercar.

Keywords: Shock Pressures, Gas Gun, Materials Characterization, Ceramics, Magnets, Superconductors, Glass, Flywheel Containment

410. <u>Properties of Hydrogen at High Shock Pressures and Temperatures</u> 5250,000 DOE Contact: G. J. D'Alessio, (301) 903-6688 LLNL Contact: William Nellis, (510) 422-7200 and Neil Holmes, (510) 422-7213

This project measures temperatures and electrical conductivities of cryogenic liquid hydrogen and deuterium specimens shock-compressed to high pressures and temperatures with a two-stage light-gas gun. Impact velocities up to 8 km/s were used. Shock temperatures were measures optically up to 1 Mbar and 5000 K and show that hydrogen undergoes a continuous dissociative phase transition above 200 kbar. This partial dissociation absorbs energy, which causes lower temperatures and high densities in the Mbar shock pressure range than was thought previously. Thus, the equation of state of hydrogen is different than thought previously because of continuous molecular dissociation from the molecular to the atomic phase. These data and the resulting model have important implications for laser-driven implosion systems which use hydrogen. To investigate the metallization pressure of molecular hydrogen, electrical conductivities were measured in the range 1 to 2 Mbar at calculated temperatures up to 4000 K using metal electrodes. The metallization pressure is the pressure at which the molecular insulating phase transforms to the monatomic metallic phase. This phase transition also effects the equation of state. A novel technique was used to produce just enough shock heating to excite just enough electronic carriers to be able to measure the electrical conductivity of hydrogen at Mbar pressures in the short time duration of the experiment. The results are in good agreement with the theoretically predicted density-dependent energy bandgap of rotationally disordered molecular hydrogen.

Keywords: Shock Pressures, Shock Temperatures, Electrical Conductivities, Gas Gun, Hydrogen, Cryogenics, Equation of State, Dissociation, Metallization

411. Low Density Foam Shells for Cryogenic ICF Experiments

DOE Contact: G. J. D'Alessio, (301) 903-6688 LLNL Contacts: R. Cook, (510) 422-3117 and G. E. Overturf III, (510) 422-6774

This program has as its goal the development of foam shells, from 1 to 2 mm in diameter with 100 μ m foam walls whose density is 50 mg/cc and whose cell size is less than 1 μ m. These shells must also have a 5 to 10 μ m thick full density overcoat, and the outer surface finish must be better than 0.1 μ m. Foam and overcoat must be composed of atoms with Z less than 9. These foam shells will be used to provide symmetrization of liquid D_2 or DT in ICF experiments. The shells are formed using microencapsulation techniques. In one case a water-in-oil microencapsulated droplet is suspended in aqueous media, with a multi-functional polymerizable monomer (trimethylol propane trimethacrylate) incorporated in the 100 μ m thick oil phase at about 5 wt %. A second route based on resorcinolformaldehyde (R/F) foam chemistry uses an oil-in-water droplet suspended in oil since the R/F chemistry is water based.

Keywords: Polymers, Laser Fusion Targets, Low Density Foam

412. Molecular Hydrodynamics

DOE Contact: Maurice Katz, (202) 586-5799 LLNL Contacts: Clark Souers, (510) 423-4217 and James Belak, (510) 522-6061

We use molecular dynamics (MD) computer simulation methods to model the transport of shock-wave energy from intermolecular collisions into internal vibrational motion of high explosive molecules. The goal is to discover the rate of energy flow into vibrational motion and determine which vibrational modes lead to maximum energy flow and start the initiation process. The simulation code has been implemented on the emerging generation of massively parallel computers using intermolecular and intramolecular force models that realistically describe high explosive molecules. The shock wave is generated using a unique constant velocity boundary condition. The simulation is performed in the reference frame of the shock allowing arbitrarily long times to be studied with a minimum number of molecules. The simulations provide useful insight into the sequence of states through which the material transforms during shock loading. At the shock front the molecules undergo large amplitude motion into non-equilibrium structures. The calculated time for vibrational energy to reach equilibrium with translational energy (up-pumping time) is found to be quite fast, about 10 picoseconds for small molecules like nitromethane and strong shocks.

Keywords: Energetic Materials, High Explosives, Molecular Hydrodynamics, Large Scale Molecular Dynamics, Parallel Computing, Shock Physics

298

FY 1994 \$500,000

Metastable Solid-Phase High Energy Density Materials 413.

FY 1994 \$207.000

DOE Contact: Maurice Katz, (202) 586-5799 LLNL Contacts: Andrew McMahan, (510) 422-7198 and Albert Holt, (510) 423-4126

Ab-initio theoretical methods are being used to predict and characterize novel high energy density materials. The class of metastable solid phases being explored is characterized by extended and continuous networks of covalent or metallic bonds, without the weak van der Waals links of familiar chemical fuels, propellants, and explosives. Candidate materials include a phosphorus-like polymeric form of nitrogen, an aluminum-like form of boron, a distorted tetrahedrally coordinated form of carbon, as well as low-Z hydrides. These hypothetical phases are predicted to have stored energy in the range 20-34 kJ/cm^3 , which may be compared to 12 kJ/cm^3 for the HMX explosive. The new phases are predicted to be high-pressure stable, which offers in many cases a natural synthesis route. Companion proof-of-existence synthesis efforts using the laser-heated high-pressure diamond anvil cell are in progress under separate funding.

Keywords: Energetic Materials, High Energy Density Materials, Atomic-level Materials Modeling, Ab-initio Electronic Structure Methods

414.	Sub-Picosecond Laser Induced Damage	<u>FY 1994</u>	
DOE	Contact: G. J. D'Alessio, (301) 903-6688	\$100,000	

T LLNL Contacts: Mike Perry, (510) 442-4915 and Mike Feit, (510) 442-4128

We are carrying out extensive experimental and theoretical investigations of laser induced damage in dielectrics caused by intense laser pulses at 1053 and 526 nm wavelength to determine intrinsic limits for optical materials. A chirped pulse amplification solid state laser allows us to vary the pulselength continuously from 275 fs to 1 ns. This capability enables fundamental studies of damage as a function of continuously varying pulsewidth. We observe a new physical regime for the shorter (less than 10 ps) pulses exemplified by changes in the dependence of damage threshold on pulse duration and the observed damage morphology. The damage threshold also becomes more sharply defined. This behavior is due to the fact that electrons, produced initially by multiphoton absorption, can absorb energy faster than they can transfer energy to the lattice. This short pulse regime is ultimately simpler to understand than the messier long pulse case. In addition to dielectrics, we are investigating laser-tissue interaction of short pulse lasers. We intend to demonstrate that the advantage of short pulses for surgery lies in low collateral damage and greatly reduced sensitivity to tissue type.

Keywords: Laser Damage, Dielectrics, Breakdown, Multiphoton Absorption

415. <u>Novel High Energy Density Materials:</u> Synthesis by Megabar Hot <u>Pressing</u>

FY 1994 \$328,000

DOE Contact: Maurice Katz, (202) 586-5799 LLNL Contacts: H. Lorenzana, (510) 422-8982 and A. K. McMahan, (510) 422-7198

The goal of this proposal is to demonstrate proof-of-principle synthesis of one or more of a new class of energetic materials derived metastably from first and second row elements. Growing theoretical evidence, for example, predicts that nitrogen can be stablized under ambient conditions in a three-dimensional continuously bonded configuration characterized by a stored energy density per unit volume more than three times that of typical chemical explosives. Such a material would offer important new opportunities as an explosive as well as an environmentally transparent, solid fuel or monopropellant since its only reaction by-product would be innocuous N2 gas. The recently developed laser-heated diamond-anvil-cell offers the most promising synthesis route for proof-of-existence demonstration of these novel high-pressure phases, given the technique's diagnostic versatility and controlled access to extremes of pressure and temperature.

Keywords: Novel Energetic Materials, Synthetic Fuels, Properties and Composition, Clean Energy Storage, Advanced Propulsion Fuels, High Pressures and High Temperatures, Hot Pressing

416. AFM Investigations of Crystal Growth

<u>FY 1994</u> \$210,000

DOE Contact: G. J. D'Alessio, (301) 903-6688 LLNL Contact: J. J. DeYoreo, (510) 423-4240

The nanometer-scale morphology of crystalline surfaces exerts a strong control on materials properties and performance. While many researchers have studied vapor deposited metal and semiconductor surfaces grown far from equilibrium, few studies have given attention to the morphology of crystal surfaces grown from melts or solutions near equilibrium despite the fact that most bulk crystals are grown in this regime. Understanding the mechanisms of growth and the origin of defects in such crystals can impact materials performance in a number of fields including optics, electronics and structural biology. We are using atomic force microscopy (AFM) to investigate the growth of single crystal surfaces from solution in order to determine the mechanisms of step advancement, the importance of surface diffusion, the effect of impurities and the origin of defects.

In 1994 we performed both *ex situ* and *in situ* AFM measurements on two systems, the ionic crystal HK_2PO_4 (KDP), the canonical solution grown crystal, and the protein crystal Canavalin, a prototypical macromolecular biological crystal. Our results have provided

insight into the mechanisms of growth and defect incorporation in these systems. In 1995 we will continue with these systems and begin to investigate antibody and virus crystals.

Keywords: Morphology, Crystal Surfaces, Atomic Force Microscopy

417. <u>Plutonium Process Technology Development</u>

<u>FY 1994</u> \$6,000,000

DOE Contact: Andre Cygleman, (202) 586-8814 LLNL Contact: Mark C. Bronson, (510) 422-3061

The scope of this activity is the development and demonstration of plutonium chemical processes for the recovery, purification, and conversion of actinide (plutonium, americium, and uranium) bearing materials. This was being carried out in support of the Reconfiguration Program and the Environmental Restoration/Waste Minimization Program. Currently this effort is supporting the Nuclear Material Disposition Program. Development emphasis is on waste minimization, worker dose reduction, and minimizing construction costs.

During FY94, 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, mediated electrochemical dissolution, molten salt oxidation, UV/H_2O_2 photolysis, ceramic waste forms, and treatment of Idaho National Engineering Laboratory (INEL) calcine waste.

Keywords: Pyrochemical, Plutonium Processing, Waste Treatment, Plutonium Recovery, Plutonium Immobilization

Los Alamos National Laboratory

Materials Preparation, Synthesis, Deposition, Growth or Forming

418. <u>Actinide Processing Development</u>

<u>FY 1994</u> \$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,

302

420.

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

419. <u>Plutonium Oxide Reduction</u>

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

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 25μ m down to the 1μ m range, depending on the process. Composite foams are being produced with submicron cell sizes while maintaining structural properties.

Keywords: Foams, Polyolefins, Polyurethanes, Silicones, Polyesters

421. <u>Physical Vapor Deposition and Surface Analysis</u>

Low Density Microcellular Plastic Foams

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

Office of Defense Programs

<u>FY 1994</u> \$150,000

> <u>FY 1994</u> \$200,000

<u>FY 1994</u> \$300,000

<u>FY 1994</u> \$150,000

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

422. <u>Chemical Vapor Deposition (CVD) Coatings</u>

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 μ m 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)

423. Polymers and Adhesives

<u>FY 1994</u> \$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

424. <u>Tritiated Materials</u>

<u>FY 1994</u> \$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

 425.
 Salt Fabrication
 FY 1994

 5800,000
 \$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

426. Slip Casting of Ceramics

<u>FY 1994</u> \$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
- 427. Plasma-Flame Spraving Technology

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, ²³⁸U, MoSi₂ and ZrO₂. 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
- 428. Rapid Solidification Technology

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

305

<u>FY 1994</u> \$300,000

FY 1994 \$500,000

429. Bulk Ceramic Processing

<u>FY 1994</u> \$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

430. Synthesis of Ceramic Coatings

<u>FY 1994</u> \$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

431. Actinide Surface Properties

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**

432.	Neutron Diffraction of Pu and Pu Alloys and Other Actinides	FY 1994
	•	\$237,000
DOE	Contact: G. J. D'Alessio, (301) 903-6688	-
LANI	L (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

433.	Surface, Material and Analytical Studies	FY 1994
		\$300,000
DOE	Contact: G. J. D'Alessio, (301) 903-6688	
LANI	(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-

307

FY 1994 \$700.000 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

434.	Mechanical Properties of Plutonium and Its Alloys	<u>Y 1994</u>
	\$	450,000
DOE	Contact: G. J. D'Alessio, (301) 903-6688	
LANI	L (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

435.	Phase Transformations in Pu and Pu Allovs	<u>FY 1994</u>
		\$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	9

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

436. <u>Plutonium Shock Deformation</u>

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

<u>FY 1994</u> \$350,000 437. <u>Non-Destructive Evaluation</u>

<u>FY 1994</u> \$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

438. <u>Powder Characterization</u>

<u>FY 1994</u> \$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

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439. Shock Deformation in Actinide Materials	<u>FY 1994</u> \$300,000
DOE Contact: G. J. D'Alessio, (301) 903-6688 LANL (Contract No. W-7405-ENG-36) Contact: R. L. Gutierrez, (505) 665-39	19
Measurement of shock-wave profiles in uranium, plutonium, and pluton Use of soft-shock recovery test to examine the microstructural changes occurs shock deformation. Measurement of spall strength in actinide materials and ex of fracture surfaces.	ium alloys. ing during camination
Keywords: Actinides, Shock Deformation, Microstructure, Spall Strength	
440. Dynamic Mechanical Properties of Weapons Materials	<u>FY 1994</u> \$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 materia nuclear weapons. Development of plastic constitutive relations.	ls used for
Keywords: Dynamic, Strength, Fracture, Microstructure	

Device or Component Fabrication, Behavior or Testing

441. <u>Target Fabrication</u>

<u>FY 1994</u> \$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

442. Filament Winder

<u>FY 1994</u> \$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

443.	High Energy Density Welding in Hazardous Environments	51	<u>FY 1994</u>
			\$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

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444.	<u>Uranium</u>	Scrap Conversion and Recover	ery	. • .		•	•		<u>FY 1994</u>
		-	· ·			•.	1	•,	\$1,500,000
DOE O	Contact:	G. J. D'Alessio. (301) 903-668	38						

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

445. <u>Electronically Correlated Materials at Ambient</u> and Extreme Conditions

<u>FY 1994</u> \$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

446.	Organometallic Chemical Vapor Deposition	<u>FY 1994</u>
		\$248,000
DOE	Contact: M. J. Katz, (202) 586-5799	-
LAN	L (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

447.	Polymer Sorbents for Hazardous Metal Uptake	<u>FY 1994</u>
		\$164,000
DOE	Contact: M. J. Katz, (202) 586-5799	
LAN	L (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

448.	Microscopic Materials Modeling: Textures and Dynamics	<u>FY 1994</u>
		\$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

449. Surface Modification of Materials	<u>FY 1994</u>
	\$315,000
DOE Contact: M. J. Katz, (202) 586-5799	
LANL (Contract No. W-7405-ENG-36) Contact: M. Nastasi, (505) 667-700)7

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

450. Integration of Fundamental Knowledge in Plasticity and <u>Textures to Provide Technical Tools for Microscopic</u> <u>Applications</u>

FY 1994 \$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

451.	High Resolution Electron Microscopy of Materials	<u>FY 1994</u>
DOE	Contact: M. J. Katz, (202) 586-5799	\$350,000
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

452. <u>Nano-Fabrication</u>

<u>FY 1994</u> \$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 nanofabrication 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

453.	Thin Film Micro-Electrochemical Sensor Development	<u>FY 1994</u>
	-	\$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

454. <u>Liquid Crystal Thermosets</u>

<u>FY 1994</u> \$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

455.	Neutron and Resonant X-ray Scattering by Materials	<u>FY 1994</u> \$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.

FY 1994 \$360,000

Keywords: Neutron Scattering, X-ray Scattering, Actinides, Ferromagnets

456.	Structural and Electronic Competitions in Low-Dimensional
	Materials

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

457. <u>Fundamental Aspects of Photoelectron Spectroscopy in</u> <u>Highly Correlated Electronic Systems</u>

<u>FY 1994</u> \$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

458. <u>Development of High Strength High Conductivity Materials for</u> <u>High Magnetic Field Devices</u>

<u>FY 1994</u> \$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
459. Low Temperature STM for Structural and Spectroscopic Studies of High Temperature Superconductors and Other Electronic Materials

FY 1994 \$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

FY 1994 460. Materials with Fine Microstructures

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

461. Ion Beam Materials Research

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

FY 1994 \$330,000

\$365,000

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

462.	Texture Studies of Highly Deformed Composite Materials	<u>FY 1994</u>
	· · · · · · · · · · · · · · · · · · ·	\$192,000
DOE	Contact: M. J. Katz, (202) 586-5799	
LANI	(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

463.	Pressure Dependency	of the Structure	of High Explosives:	Nitromethane

FY 1994 \$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

Office of Defense Programs

464. Neutron Reflection Studies of Thin Film and Multilayer Structures

FY 1994 \$300,000

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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

465. Neutron Reflectivity Studies of In Situ Corrosion of Metal Surfaces

<u>FY 1994</u> \$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

466.The Dynamics of Amorphous MaterialsFY 1994\$330,000\$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

467. Advanced Material Science Algorithms for Supercomputer Architectures

FY 1994 \$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

468.	Metal Vapor Synthesis in Organometallic Chemistry		
		\$235,000	
DOE	Contact: M. J. Katz, (202) 586-5799		
LANI	(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

469. Separation Chemistry of Toxic Metals

<u>FY 1994</u> \$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

470.	Polymers for Integrated Optical Interconnects	<u>FY 1994</u>
		\$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

471. <u>High Temperature Materials Synthesis Without Heat: Oxide Layer</u> <u>Growth on Electronic Materials Using High Kinetic Energy</u> <u>Atomic Species</u>

<u>FY 1994</u> \$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

472.	Dynamic Deformation of Advanced Materials	<u>FY 1994</u>
		\$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

473. Strain Measurements in Individual Phases of Multi-Phase MaterialsFY 1994\$130,000\$130,000

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 MoSi₂.

Keywords: Neutron Diffraction, Aluminum/Titanium Carbide Composites, Molybdenum Disilicide Composites

474. Artificially Structured Nonlinear Optic and Electro-Optic Materials

<u>FY 1994</u> \$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

475.	Structural Phase Transitions in Non-Stoichiometric Oxides	<u>FY 1994</u>
		\$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

476. Strongly Correlated Electronic Materials

<u>FY 1994</u> \$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

 477. <u>Plasma Immersion Ion Implantation for Semiconductor Film Growth</u> \$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

478. <u>Analysis of Structure and Orientation of Adsorbed Polymer in</u> Solution Subject to Dynamic Shear Stress

<u>FY 1994</u> \$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

479.	Development of Pair Distribution Function Analysis of Mesostructural		
	Details i	n Single Crystal Perovskites and Nanocrystalline Materials	<u>FY 1994</u>
			\$170,000
DOE	Contact:	M. J. Katz, (202) 586-5799	-
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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

480. <u>Neutron Scattering as a Probe of the Structure of Liquid Crystal</u> <u>Polymer-Reinforced Composite Materials</u> \$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

481. <u>Strain Measurements in Individual Phases of Multi-Phased</u> <u>Materials During Thermomechanical Loading: LANSCE Neutron</u> <u>Scattering Experiment Support</u>

<u>FY 1994</u> \$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 MoSi₂.

Keywords: Neutron Diffraction, Metal Matrix Composites, Ceramic Matrix Composites

482. <u>A New Approach to Texture Measurements: ODF Determination by</u> <u>Rietveld Refinement</u>

<u>FY 1994</u> \$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

483.	Applications of Fullerenes in Nuclear Technology	<u>FY 1994</u>
		\$360,000
DOE	Contact: M. J. Katz, (202) 586-5799	
LAN	L (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

484. <u>Ceramic Oxide Foams for Separation</u>

FY 1994 \$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

485. <u>Materials Modeling Project</u>

<u>FY 1994</u> \$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

486. <u>Synthesis and Optical Characterization of Novel Fullerene-Based Composites</u> <u>FY 1994</u> \$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

Office of Defense Programs

Technology Transfer Initiative

487. <u>A Pilot Program: Chemical Vapor Deposition of Diamond in a</u> <u>Fluidized-Bed for Cutting Tool and Tribological Applications</u>

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.

<u>FY 1994</u> \$250,000

FY 1994

\$632,000

Keywords: Diamond Coatings, Chemical Vapor Deposition, Cutting Tools, Tribology

488. Advanced Beryllium Processing

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

489.	Automated Pulsed Laser Deposition System	<u>FY 1994</u>
		\$130,000
DOE	Contact: W. P. Chernock (202) 586-7590	
LANI	L (Contract No. W-7405-ENG-36) Contact: Ross Muenchausen, (505)	665-4949

A program to design an automated pulsed laser deposition system to deposit hightemperature superconducting thin films.

Keywords: Pulsed-Laser-Deposition, High-Temperature Superconducting Films

490. Plasma Source Ion Implantation for the Automotive Industry

<u>FY 1994</u> \$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

491.	Processing Modeling and Control for U.S. Steel Industry	<u>FY 1994</u>
		\$1,195,000
DOE	Contact: W. P. Chernock (202) 586-7590	
LANI	C (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.

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Keywords: Steel, Electric-Arc-Furnace, Scrap Steels

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	<u>FY 1994</u>
Office of Fossil Energy - Grand Total	\$8,628,000
Office of Advanced Research	\$8,628,000
Fossil Energy AR&TD Materials Program	\$8,628,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	\$4,305,000
Coating Process Development for Cr-Nb Alloys	90,000
Procurement of Advanced Austenitic and Aluminide Alloys	30,000
Development of Iron Aluminides	293,000
Microalloved Iron Aluminides	280,000
Low-Aluminum Content Iron-Aluminum Allovs	270.000
Technology Transfer - Iron Aluminides	0
Development of a Modified 310 Stainless Steel	120,000
Technology Transfer - Advanced Austenitics	0
Influence of Processing on Microstructure and Properties of	
Aluminides	175,000
Investigation of Electrospark Deposited Coatings for	
Protection of Materials in Sulfidizing Atmospheres	50,000
Technology Transfer - Electrospark-Deposited Coatings for	
Protection of Materials in Sulfidizing Atmospheres	80,000
Engineering-Scale Development of the Vapor-Liquid-Solid	
(VLS) Process for the Production of Silicon Carbide	
Fibrils	197,000
Ceramic Composite Processing Equipment	30,000
Fabrication of Fiber-Reinforced Composites by Chemical	150.000
Vapor Infiltration and Deposition (CVID)	150,000
Development of Oxidation/Corrosion-Resistant Composite	150.000
Materials and Interfaces	150,000
for Ceremic Compositor	50.000
Transport Properties of Ceramic Composites	1/0 000
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I	FY 1994
Office of Advanced Research (continued)	
Fossil Energy AR&TD Materials Program (continued)	
Materials Preparation, Synthesis, Deposition, Growth	
or Forming (continued)	
Modeling of Fibrous Preforms for CVD Infiltration	55,000
Corrosion Protection of SiC-Based Ceramics with CVD	.,
Mullite Coatings	100,000
Feasibility of Synthesizing Oxide Films on Ceramic and	·
Metal Substrates	100,000
Oxide Coating Development	75,000
High-Temperature Heat Exchanger and Hot-Gas Filter Development	: 250,000
Ceramic Coating Evaluation	50,000
Low-Temperature Fabrication of Transparent Silicon Nitride	180,000
Microwave-Assisted Chemical Vapor Infiltration	50,000
Development of Microwave-Heated Diesel Particulate Filters	75,000
Carbon Fiber Composite Molecular Sieves	310,000
Activation of Carbon Fiber Composite Molecular Sieves	75,000
Production of Aluminum Reduction Electrodes from Solvent-Extract	ed
Coal-Derived Carbon Feedstocks	15,000
Exploration of Coal-Based Pitch Precursors for Ultra-High Thermal	
Conductivity Graphite Fibers	30,000
Development of Carbon-Carbon Composites from Solvent-Extracted	
Pitch	25,000
Conversion of Pitches and Cokes from Solvent-Extracted Materials	40,000
Carbon Products Consortium	175,000
Economic Analysis of West Virginia University Solvent Extraction	
Process	50,000
Development of Precursors for Production of Graphites and Carbon	<
Products	65,000
Solvent Extraction of Coal	300,000
Radio-wave Nano-Phase Silicon Nitride and Silicon Carbide	100 000
Processes	100,000

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Office of Advanced Research (continued)

Fossil Energy AR&TD Materials Program (continued)

Materials Properties, Behavior, Characterization or Testing	
Investigation of the Weldability of Polycrystalline Iron	
Aluminides	75,000
Stress-Assisted Corrosion of Iron Aluminides	50,000
Fireside Corrosion Tests of Candidate Advanced Austenitic Allo	vs.
Coatings, and Claddings	80,000
Joining Techniques for Advanced Austenitic Allovs	65,000
Fatigue and Fracture Behavior of Cr-Nb Alloys	50,000
Corrosion and Mechanical Properties of Alloys in FBC and	
Mixed-Gas Environments	310,000
Mechanically Reliable Coatings and Scales for High-Temperature	e
Corrosion Resistance	100,000
Environmental Effects on Iron Aluminides	225,000
Investigation of Moisture-Induced Embrittlement of Iron	-
Aluminides	60,000
Corrosion Protection of Ultrahigh Temperature Intermetallic	·
Alloys	220,000
Oxide Dispersion Strengthened (ODS) Iron Aluminide	
Equipment	50,000
Oxide Dispersion Strengthened (ODS) Iron Aluminides	75,000
Materials Support for HITAF	175,000
Support Services for Ceramic Fiber-Ceramic Matrix Composites	50,000
Development of Nondestructive Evaluation Methods and Effects	,
of Flaws on the Fracture Behavior of Structural Ceramics	310,000
Fracture Behavior of Advanced Ceramic Hot-Gas Filters	114,000
Ceramic Catalyst Materials	225,000

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Office of Defense Programs

OFFICE OF FOSSIL ENERGY

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	<u>FY 1994</u>
Office of Advanced Research (continued)	
Fossil Energy AR&TD Materials Program (continued)	
Device or Component Fabrication, Behavior or Testing	\$1,650,000
Materials and Components in Fossil Energy Applications	
(Newsletter)	60,000
Fabrication of Full-Scale Fiber-Reinforced Hot-Gas Filters by	
Chemical Vapor Deposition	115,000
Development of Ceramic Membranes for Gas Separation	400,000
Investigation of the Mechanical Properties and Performance of	
Ceramic Composite Components	100,000
Stability of Solid Oxide Fuel Cell Materials	250,000
Mixed Oxygen Ion/Electron-Conducting Ceramics for Oxygen	
Separation and Fuel Cells	225,000
Proton-Conducting Cerate Ceramics	225,000
Technology Transfer - Iron Aluminide Filters	50,000
Thermal and Mechanical Analysis of a Ceramic Tubesheet	40,000
Thermal and Mechanical Analysis of a Ceramic Tubesheet	10,000
Technology Transfer - Ceramic Joining	175,000
Instrumentation and Facilities	\$ 439,000
Management of the Fossil Energy AR&TD Materials Program	400,000
General Technology Transfer Activities	35,000
Gordon Research Conference Support	4,000

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The Office of Fossil Energy responsibilities include management of the Department's fossil fuels (coal, oil and natural gas) research and development program. This research is generally directed by the Office of Coal Technology (OCT), the Office of Gas and Petroleum Technology, and the Office of Advanced Research and Special Technologies in support of the National Energy Strategy Goals for Increasing Energy Efficiency, Securing Future Energy Supplies, Respecting the Environment, and Fortifying our Foundations. Three specific fossil energy goals are currently being pursued:

- The first is to secure liquids supply and substitution. This goal targets the enhanced production of domestic petroleum and natural gas, the development of advanced, cost-competitive alternative fuels technology, and the development of coal-based, end-use technology to substitute for oil in applications traditionally fueled by liquid and gaseous fuel forms.
- The second is to develop power generation options with environmentally superior, high-efficiency technologies for the utility, industrial, and commercial sectors. This goal targets the development of super-clean, high-efficiency power generation technologies.
- The third is to pursue a global technology strategy to support the increased competitiveness of the U.S. in fossil fuel technologies, to maintain world leadership in our fossil fuel technology base, and provide expanded markets for U.S. fuels and technology. This crosscutting goal is supported by the activities in the above two technology goals.

Office of Advanced Research

Fossil Energy AR&TD Materials Program

Fossil Energy (FE) materials-related research is conducted under an Advanced Research and Technology Development (AR&TD) Materials subactivity and is an integral part of the R&D conducted by the Office of Advanced Research and Special Technologies. The AR&TD Materials program includes cross-cutting research to obtain a fundamental understanding of materials and how they perform in fossil-based process environments and the development of new classes of generic materials that will allow the development of new fossil energy systems or major improvements in existing systems. The present program is focused on ceramics (composite structural ceramics, catalyst supports, solid state electrolytes, membranes, and ceramic filters), new alloys (aluminides, advanced austenitic steels, and coatings and claddings), corrosion research, and technology development and transfer. The AR&TD research is carried through development and technology transfer to industry. Special emphasis is being given to technology transfer to ensure that the materials will be available for subsequent fossil commercial applications. This also enhances U.S. technological competitiveness not only in the fossil area but in the materials industry in general and other technology application areas as well. The research is conducted in industry, universities, not-for-profit agencies, and national laboratories. This widespread participation also helps maintain the U.S. materials technology capabilities.

The acronym PYF indicates that the work in the designated year was supported by prior-year funds.

Materials Preparation, Synthesis, Deposition, Growth or Forming

492. Coating Process Development for Cr-Nb Allovs

<u>FY 1994</u> \$90,000

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

493.	Procurement of Advanced Austenitic and Aluminide Allovs	<u>FY 1994</u>
		\$30,000
DOE	Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (615) 576-0735	
Oak I	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

494. Development of Iron Aluminides

<u>FY 1994</u> \$295,000

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

495.Ultrahigh Temperature Intermetallic AlloysFY 1994
\$280,000DOE Contacts:J. P. Carr, (301) 903-6519 and E. E. Hoffman, (615) 576-0735

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

496. Microalloyed Iron Aluminides

FY 1994 \$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

497. Low-Aluminum Content Iron-Aluminum Alloys

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, lowdensity 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

498. <u>Technology Transfer - Iron Aluminides</u>

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

A Cooperative Research and Development Agreement (CRADA) has been established with ABB Combustion Engineering for the development of corrosion-resistant surface protection for fossil power systems.

Keywords: Alloys, Iron-Aluminum, Corrosion, Technology Transfer

499. <u>Development of a Modified 310 Stainless Steel</u>

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 task is to evaluate structural alloys for improved performance of high-temperature components in advanced combined-cycle and coal-combustion systems.

Keywords: Materials, Mechanical Properties, Austenitics, Hot-Gas

500. Technology Transfer - Advanced Austenitics

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

A Cooperative Research and Development Agreement (CRADA) has been established with ABB Combustion Engineering for the development of advanced austenitic alloys for fossil power systems.

Keywords: Alloys, Austenitics, Technology Transfer

FY 1994 \$120,000

FY 1994

\$0

<u>FY 1994</u> \$0

501. <u>Influence of Processing on Microstructure and Properties</u> of Aluminides

<u>FY 1994</u> \$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

 502.
 Investigation of Electrospark Deposited Coatings

 for Protection of Materials in Sulfidizing Atmospheres
 FY

FY 1994 \$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 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

 503.
 Technology Transfer - Electrospark Deposited Coatings for

 Protection of Materials in Sulfidizing Atmospheres
 FY

<u>FY 1994</u> \$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 Westinghouse Hanford Company Contact: R. N. Johnson, (509) 376-3582

The purpose of this task is to transfer to industry the electrospark deposition coating process technology for the application of corrosion-, erosion-, and wear-resistant coatings to candidate superheater alloys.

Keywords: Coatings, Materials, Deposition

504. <u>Engineering-Scale Development of the Vapor-Liquid-Solid (VLS)</u> Process for the Production of Silicon Carbide Fibrils

<u>FY 1994</u> \$197,000

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: William Hollar, (716) 278-2097

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

505.Ceramic Composite Processing EquipmentFY 1994\$30,000DOE Contacts:J. P. Carr, (301) 903-6519 and E. E. Hoffman, (615) 576-0735Oak 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

506.	Fabrication of Fiber-Reinforced Composites by Chemical Vapor	
	Infiltration and Deposition (CVID)	<u>FY 1994</u>
		\$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 the development of a process for the fabrication of fiberreinforced 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

507. <u>Development of Oxidation/Corrosion-Resistant Composite Materials</u> and Interfaces

<u>FY 1994</u> \$150,000

FY 1994

\$50,000

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

Fiber-reinforced SiC-matrix composites have been observed to fail in fossil energy applications for two reasons. First, the mechanical properties of composites deteriorate under stressed oxidation because oxidants such as steam penetrate cracks formed in the SiC matrix and react with the carbon or boron nitride interface. The mechanical properties of composites may degrade because of corrosion due to sodium species typically present in fossil systems. Therefore, the purposes of this task are to first, develop fiber-matrix interfaces that are resistant to oxidation and yet optimize the mechanical behavior of composites, and second, to develop protective overcoats or oxide matrices that are resistant to oxidation and corrosion.

Keywords: Composites, Ceramics, Fiber-Reinforced, Interfaces

508. <u>Optimization of the Chemical Vapor Infiltration Technique for</u> <u>Ceramic Composites</u>

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

This project is focussed on an optimization of the forced chemical vapor infiltration (CVI) technique for fabrication of ceramic matrix composites (CMCs) using process models. In particular, a process model developed at the Georgia Tech Research Institute shall be thoroughly investigated. Experimental verification of the process model shall be conducted in light of microstructural characterization using both destructive and nondestructive evaluation techniques. An optimized process for manufacturing CMCs shall be demonstrated. Moreover, mechanistic understanding regarding the effects of processing parameters on microstructural features, and fatigue and fracture behavior of CMCs shall be provided.

Keywords: Composites, Fiber-Reinforced, Ceramics

509. Transport Properties of Ceramic Composites

<u>FY 1994</u> \$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

510. Modeling of Fibrous Preforms for CVD Infiltration

FY 1994 \$55,000

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

511. <u>Corrosion Protection of SiC-Based Ceramics with CVD Mullite</u> <u>Coatings</u>

<u>FY 1994</u> \$100,000

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 Boston University Contact: Vinod Sarin, (617) 353-6451

This project involves the growth of dense mullite coatings on SiC-based substrates by chemical vapor deposition. SiC and SiC-based composites have been identified as the leading candidate materials for stringent elevated temperature applications. At moderate temperatures and pressures, the formation of a thin self-healing layer of SiO₂ is effective in preventing catastrophic oxidation by minimizing the diffusion of O₂ to the substrate. The presence of impurities can increase the rate of passive oxidation by modifying the transport rate of oxygen through the protective scale, can cause active oxidation via formation of SiO which accelerates the degradation process, or can produce compositions such as Na_2SO_3 which chemically attack the ceramic via rapid corrosion. There is therefore a critical need to develop adherent oxidation/corrosion-resistant, and thermal-shock-resistant coatings that can withstand such harsh environments. Mullite has been identified as an excellent candidate material due to its desirable properties of toughness, corrosion resistance, and a good coefficient of thermal expansion match with SiC.

Keywords: Ceramics, Coatings

512. <u>Feasibility of Synthesizing Oxide Films on Ceramic and</u> Metal Substrates

<u>FY 1994</u> \$100,000

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 Lawrence Berkeley Laboratory Contact: Ian Brown, (510) 486-4174

The objective of this project is the study of the feasibility of synthesizing metal oxide ceramic films on ceramic and metal substrates. This feasibility will be demonstrated by use of plasma-based deposition and ion mixing techniques. The films shall be characterized for properties such as composition, structure, hardness, high temperature oxidation resistance, adhesion to the substrate, and stability to high temperature cycling. The value of intermediate transition or buffer layers, composed of materials with suitably matched thermal expansion characteristics and atomically graded interfaces, as a technique for improving the high temperature survivability of the films, shall be explored. Samples shall be formed on substrates of various shapes and sizes, including perhaps on the inside and outside of pipes, as well as on small flat coupons. The issue of deposition onto and atomic mixing into substrates which are insulating shall be addressed experimentally. The work is divided into two parts: (1) Al_2O_3 films on alumina-forming alloy substrates, and (2) oxides on SiC.

Keywords: Ceramics, Films, Oxides

513. Oxide Coating Development

FY 1994 \$75,000

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

Monolithic SiC heat exchangers and fiber-reinforced SiC-matrix composite heat exchangers and filters are susceptible to corrosion by alkali metals at elevated temperatures. Protective coatings are currently being developed to isolate the SiC materials from the corrodants. Unfortunately, these coatings typically crack and spall when applied to SiC substrates. The purpose of this task is to determine the feasibility of using a compliant material between the protective coating and the substrate. The low-modulus compliant layer could absorb stresses and eliminate cracking and spalling of the protective coatings.

Keywords: Ceramics, Oxides, Coatings

514.	High-Temperature Heat Exchanger and Hot-Gas Filter Development	<u>FY 1994</u>
		\$250,000
DOE	Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (615) 576-0735	
Oak F	Ridge National Laboratory Contact: N. C. Cole, (615) 574-4824	
Penns	ylvania State University Contact: R. E. Tressler, (814) 865-7961	

This project has two principal parts: (1) screening analysis of candidate ceramic hotgas filter materials, and (2) development of ceramic heat exchanger materials with chromium surface treatments for corrosion resistance. A flow-through screening test will be developed to test ceramic hot-gas filter elements in simulated coal combustion environments. Corrosion-resistant heat exchanger tubes will be fabricated by incorporating chromium in the surface layers.

Keywords: Ceramics, Corrosion

515. <u>Ceramic Coating Evaluation</u>

FY 1994 \$50,000

DOE Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (615) 576-0735 Oak Ridge National Laboratory Contacts: P. F. Tortorelli, (615) 574-5119

The purpose of this work is to generate the information needed for the development of improved (slow growing, adherent, sound) protective oxide coatings and scales The specific objectives are to (1) systematically investigate the relationships among substrate composition and surface oxide structure, adherence, soundness, and micromechanical properties, (2) use such information to predict scale and coating failures, and (3) identify and evaluate compositions and synthesis routes for producing materials with damage-tolerant scales and coatings.

Keywords: Coatings, Corrosion

516.Low-Temperature Fabrication of Transparent Silicon NitrideFY 1994\$180,000DOE Contacts:J. P. Carr, (301) 903-6519 and E. E. Hoffman, (615) 576-0735Oak Ridge National Laboratory Contact:N. C. Cole, (615) 574-4824National 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

517.Microwave-Assisted Chemical Vapor InfiltrationFY 1994\$50,000

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 research effort is to explore the feasibility of using microwave heating to enhance the chemical vapor infiltration (CVI) process developed under the Fossil Energy Materials Program (FEMP) sponsorship. The goal is to achieve faster deposition rates, greater control over deposition conditions and resulting microstructures, and perhaps lower temperature infiltration.

Keywords: Ceramics, Microwave Processing

518. <u>Development of Microwave-Heated Diesel Particulate Filters</u>

<u>FY 1994</u> \$75,000

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 research is to help develop microwave-heated diesel engine particulate filter/burner devices. The goal is to develop materials that will perform both as filter and heater in such a device. A Cooperative Research and Development Agreement (CRADA) between Martin Marietta Energy Systems (MMES) and the Cummins Engine Company is in place that supports this work, CRADA No. ORNL93-0172. The Department of Energy (DOE) CRADA monies come from both the Fossil Energy AR&TD Materials Program and the Energy Efficiency and Renewable Energy - Office of Transportation Technologies (EE-OTT), Heavy Duty Transport Program.

The project will develop a ceramic composite structure of SiC-coated ceramic fiber that can be used as a diesel engine particulate filter. For commercial usage a particulate filter must: (1) filter carbon particles from high temperature diesel exhaust gas at an acceptable (low) backpressure; (2) survive thousands of thermal transients caused by regeneration (cleaning) of the filter by oxidizing the collected carbon; (3) be durable and reliable over the life of the filter, which is in excess of 300,000 miles (10,000 hours of operation); and, (4) provide a low overall operating cost which is competitive with other filtering techniques.

Keywords: Ceramics, Microwave Processing

519. <u>Carbon Fiber Composite Molecular Sieves</u>

<u>FY 1994</u> \$310,000

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

520. Activation of Carbon Fiber Composite Molecular Sieves

<u>FY 1994</u> \$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 University of Kentucky Contact: Frank Derbyshire, (606) 257-0305

A novel monolithic adsorbent carbon, manufactured from carbon fibers, has been invented jointly by researchers at ORNL and 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

 521.
 Production of Aluminum Reduction Electrodes from Solvent-Extracted

 Coal-Derived Carbon Feedstocks
 FY 1994

 \$15,000

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 Alcoa Aluminum Company Contact: Dave Belitskus, (412) 337-4812

This research is directed toward the objective of producing aluminum reduction electrodes from solvent-extracted coal-derived carbon feedstocks obtained from West Virginia University (WVU) and Koppers Industries, Inc.

Keywords: Carbon, Feedstocks, Coal-Derived

522. Exploration of Coal-Based Pitch Precursors for Ultra-High Thermal Conductivity Graphite Fibers FY 1994 \$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 Amoco Performance Products, Inc. Contact: G. V. Deshpande

The preparation of high-performance carbon (graphite) fibers requires a mesophase pitch precursor. Traditionally, in the USA, this has been derived from a petroleum precursor. Overseas suppliers have, however, developed high- performance fibers from coal derived precursors. Amoco Performance Products' goal is to explore coal-based pitch precursors' utility for use in ultra-high thermal conductivity graphite fibers.

Keywords: Carbon, Fibers, Graphite, Precursors

523. <u>Development of Carbon-Carbon Composites from Solvent-Extracted</u> <u>Pitch</u>

FY 1994 \$25.000

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 Fiber Materials, Inc. Contact: Cliff Baker, (207) 282-5911

The manufacture of carbon-carbon composites for use in the aerospace industry has been heavily reliant on petroleum and coal tar pitches as matrix precursors. It is of great importance to strategic materials production for the Department of Defense that a stable, long-lived source of pitch be developed. Consequently, Fiber Materials, Inc. (FMI) will work with staff members at the Oak Ridge National Laboratory (ORNL) and at West Virginia University (WVU) to develop carbon-carbon composite materials from pitches derived from coal via a solvent extraction process. The objectives of this project shall be twofold. First, FMI shall use solvent extracted pitch to develop carbon-carbon composites with similar or improved properties over those currently manufactured from Allied 15V coal tar or Ashland A-240 petroleum pitches. Second, FMI shall develop improved, lower-cost composites from improved solvent extracted pitches supplied by WVU.

Keywords: Carbon, Composites, Pitch

524.Conversion of Pitches and Cokes from Solvent-Extracted MaterialsFY 1994\$40,000

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 Koppers Industries, Inc. Contact: R. McHenry, (412) 826-3989

The closure of by-product coke ovens has caused the domestic production of coal tar pitch to decline at 3 percent to 4 percent per annum during the mid-1990s. This reduction has directly affected Koppers' capability to produce required quantities of quality binder and impregnating pitches used in the aluminum and commercial carbon and graphite industries. Moreover, the other major constituent of carbon anodes and graphites is a coke, usually produced from petroleum pitch precursors, 50 percent of which are imported. The objectives of this research are to develop dependable domestic coal-based raw materials for the production of: binder pitches for aluminum cell anodes and graphite products and graphite products; impregnating pitches for commercial carbon and graphite products and specialty materials; oils for wood treatment and carbon black production; chemicals for phthalic anhydride and other products; and metallurgical and foundry grade cokes.

Keywords: Coke, Pitch, Conversion

525. Carbon Products Consortium

<u>FY 1994</u> \$175,000

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

Hydrogen and Methane gas recovery technologies are required to (1) allow the upgrading of heavy hydrocarbons to transport fuels, thus reducing the amount of carbon rejected during crude oil refining, and (2) to improve the yield and process economics of natural gas wells. The purpose of this work is to develop carbon fiber composite molecular sieves (CFCMS) from porous carbon fiber composites (CFC) manufactured from solvent extracted coal tar pitch derived carbon fibers. The work will be performed in collaboration with other members of the Cooperative Research Partnership on Carbon Products and the Non Fuel Uses of Coal.

Keywords: Consortium, Carbon Products

526. <u>Economic Analysis of West Virginia University Solvent</u> <u>Extraction Process</u>

FY 1994 \$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 Pittsburgh Energy Technology Center Contact: M. A. Nowak, (412) 892-6020

This project will analyze the West Virginia University solvent extraction process for producing pitch from coal. The aim of the project is to determine the economic viability of the process when scaled to commercial size.

Keywords: Solvent Extraction

527. <u>Development of Precursors for Production of Graphites and</u> <u>Carbon Products</u>

<u>FY 1994</u> \$65,000

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 UCAR Carbon Company Contact: Irv Lewis, (216) 676-2203

The manufacture of graphite utilizes cokes and pitches derived from petroleum refining by-products and by-product coke ovens. These include isotropic and anisotropic cokes, binder, and impregnant pitches. Assuring feedstock quality is of great importance to the graphite industry. Therefore, a stable long-lived source of feedstock pitch (and hence coke) would be of considerable benefit to the industry. Consequently, UCAR Carbon Company Inc. shall work with staff members at the Oak Ridge National Laboratory (ORNL) and at the West Virginia University to develop suitable precursor pitches, binders, impregnants, and cokes for the production of graphites and other carbon products.

Keywords: Carbon Products, Precursors, Graphites

528. Solvent Extraction of Coal

<u>FY 1994</u> \$300,000

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 West Virginia University Contact: Al Stiller, John Zondlo

This project is to develop a process for the solvent extraction of coal to produce an extract suitable for the production of a variety of carbon products, such as coke, graphite, carbon anodes, and carbon fibers. The process uses N-methyl pyrolodone as the extraction medium and is based on a West Virginia University patent.

Keywords: Solvent Extraction

529. <u>Radio-Wave Nano-Phase Silicon Carbide and Silicon Nitride</u> <u>Processes</u>

<u>FY 1994</u> \$100,000

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: R. J. Buss, (505) 844-3504

This program examines the use of radio-frequency plasma discharges as a synthetic route to nanometer-size silicon carbide and silicon nitride particles.

Keywords: Nanophase, Silicon Nitride, Silicon Carbide

Materials Properties, Behavior, Characterization or Testing

530. Investigation of the Weldability of Polycrystalline Iron Aluminides F

<u>FY 1994</u> \$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

531. Stress-Assisted Corrosion of Iron Aluminides

<u>FY 1994</u> \$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 University of Tennessee Contact: R. A. Buchanan, (615) 974-4858

The objective of this project is to investigate (1) evaluation of the effects of surface conditions on the corrosion and embrittlement of Fe-Al alloys, and (2) corrosion fatigue properties of Fe-Al alloys.

Keywords: Alloys, Aluminides, Corrosion, Stress

532.	Fireside Corrosion Tests of Candidate Advanced Austenitic Alloys,	
	Coatings, and Claddings	<u>FY 1994</u>
		\$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 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

533. Joining Techniques for Advanced Austenitic Alloys

FY 1994 \$65,000

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: 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

534. Fatigue and Fracture Behavior of Cr-Nb Alloys

FY 1994 \$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 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 will be required to characterize the fracture behavior of these structural alloys. Mechanical tests shall be performed to determine the fatigue and fracture behavior of Cr_2Nb -based alloys. The microstructure of the alloys shall be characterized and correlated with the mechanical properties.

Keywords: Fracture, Fatigue, Alloys
535. <u>Corrosion and Mechanical Properties of Alloys in FBC and</u> <u>Mixed-Gas Environments</u>

<u>FY 1994</u> \$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 chromiaand 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

536. <u>Mechanically Reliable Coatings and Scales for High-Temperature</u> <u>Corrosion Resistance</u>

<u>FY 1994</u> \$100,000

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

This project involves the development of mechanically reliable coatings and scales for high-temperature corrosion resistance. ANL shall systematically generate the knowledge required to establish a scientific basis for design and synthesis of improved (slow growing, adherent, sound) protective oxide coatings and scales on high temperature materials, without compromising the requisite bulk material properties. In addition, ANL shall provide information on the performance of advanced candidate materials from the standpoint of corrosion resistance and residual mechanical properties, after exposure in simulated combustion environments typical of indirectly-fired gas turbines. The work shall emphasize corrosion evaluation of materials in air, salt, and coal/ash environments at temperatures between 1000° and 1400°C, and measurement of residual toughness properties of the materials after corrosion.

Keywords: Corrosion, Coatings, Scales

537. Environmental Effects on Iron Aluminides

<u>FY 1994</u> \$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

538. Investigation of Moisture-Induced Embrittlement of Iron Aluminides 538. Investigation of Moisture-Induced Embrittlement of Iron Aluminides 538. FY 1994 \$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

539. Corrosion Protection of Ultrahigh Temperature Intermetallic Alloys 539. Corrosion Protection of Ultrahigh Temperature Intermetallic Alloys 539. FY 1994 \$220,000 539. 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, corrosionresistant 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

540. Oxide Dispersion Strengthened (ODS) Iron Aluminide Equipment FY 1994 \$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

This task provides funds for the procurement of major equipment items necessary for AR&TD Materials Program activities.

Keywords: Equipment

541.Oxide Dispersion Strengthened (ODS) Iron AluminidesFY 1994\$75,000DOE Contacts:J. P. Carr, (301) 903-6519 and E. E. Hoffman, (615) 576-0735Oak Ridge National Laboratory Contact:N. C. Cole, (615) 574-4824

The purpose of this task is to develop fabrication procedures for making oxide dispersion-strengthened (ODS) iron-aluminum alloys based on Fe₃Al. The suitability of the procedures is measured in terms of the high temperature oxidation resistance and creep strength of the ODS alloys compared with Fe₃Al alloys fabricated by conventional ingot and powder processes.

<u>FY 1994</u> \$175,000

Keywords: Aluminides

542. Materials Support for HITAF

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 involves the measurement of selected mechanical and physical properties of structural ceramics which are proposed for use in the construction of the High Temperature Advanced Furnace (HITAF) air heater design being developed under the Combustion 2000 program for PETC/DOE. The purpose of the research is to evaluate candidate structural ceramics for this application by studying the fast fracture and fatigue (both dynamic and interrupted static) properties at temperatures from 1100 to 1400 °C in air, their corrosion behavior, property uniformity of components and long term degradation of ceramic properties due to exposure in prototype HITAF systems.

Keywords: Furnace, Materials, HITAF

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543. <u>Support Services for Ceramic Fiber-Ceramic Matrix Composites</u> 543. <u>Support Services for Ceramic Fiber-Ceramic Matrix Composites</u> 543. <u>FY 1994</u> 550,000 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

Oak Ridge National Laboratory Contact: N. C. Cole, (615) 574-4824 University of North Dakota Energy and Environmental Research Center (UNDEERC)

Contact: J. P. Hurley, (701) 777-5159

This task will review and, if appropriate, propose modifications to plans, materials, and tests planned by researchers on the AR&TD Materials Program in work to test materials for coal-fueled energy systems. The changes shall be suggested in order to make the corrosion experiments more reflective of the actual conditions that will be encountered by the materials in the energy systems. UNDEERC shall accomplish this task by reviewing the major advanced energy system projects being funded by the DOE, and by working with the company's technical monitor and staff to prepare a summary of the expected corrosion problems. Both gasification and combustion systems will be included. Ceramic materials in two subsystems will be the focus of this work: (1) hot gas cleanup systems and (2) high-temperature heat exchangers. UNDEERC shall review and suggest improvements to materials testing procedures that are used to determine material behavior when used in hot-gas cleanup or heat exchanger applications. A limited amount of computer modeling and laboratory experimentation shall be a part of this effort.

Keywords: Composites, Ceramics, Fibers

 544.
 Development of Nondestructive Evaluation Methods and Effects

 of Flaws on the Fracture Behavior of Structural Ceramics
 FY 1994

 \$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

545. Fracture Behavior of Advanced Ceramic Hot-Gas Filters

<u>FY 1994</u> \$114,000

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 the fracture behavior of ceramic hot-gas filters. ANL shall evaluate mechanical/physical properties and microstructure, identify critical flaws and failure modes, and correlate mechanical/physical properties with microstructure and critical flaws to provide much needed information for selection of materials and optimization of fabrication procedures for hot- gas ceramic filter modules. As part of the information base, requirements for strength and fracture toughness of the filter material shall be established from stress and fracture mechanics analyses of typical filters subjected to loadings expected during operation and pulse-cleaning cycles.

Keywords: Ceramics, Flaws, Fracture, Failure

546. <u>Ceramic Catalyst Materials</u>

<u>FY 1994</u> \$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

547. <u>Materials and Components in Fossil Energy Applications (Newsletter)</u> FY

FY 1994 \$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 Battelle-Columbus Laboratories Contact: I. G. Wright, (614) 424-4377

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

548. <u>Fabrication of Full-Scale Fiber-Reinforced Hot-Gas Filters by</u> <u>Chemical Vapor Deposition</u>

<u>FY 1994</u> \$115,000

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 3M Company Contact: M. A. Leitheiser, (612) 733-9394

The purpose of this project is to scale-up the chemical vapor infiltration and deposition (CVID) process developed at Oak Ridge National Laboratory for fabricating ceramic fiber-ceramic matrix composites. The goal is to use the scaled-up CVID process to produce composite filters that have the requisite strength and toughness, but which also have sufficient porosity to be permeable to gas streams and the appropriate size and distribution of porosity to be an effective filter. A practical process for fabricating porous ceramic fiber-ceramic matrix candle filters (full-size) with increased surface area will be developed.

Keywords: Ceramics, Composites, Filters

549. Development of Ceramic Membranes for Gas Separation

<u>FY 1994</u> \$400,000

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 Oak Ridge K-25 Site Contact: D. E. Fain, (615) 574-9932

The purpose of this activity is to fabricate inorganic membranes for the separation of gases at high temperatures and/or in hostile environments, typically encountered in fossil energy conversion processes such as coal gasification. This work is performed in conjunction with a separate research activity that is concerned with the development and testing of the ceramic membranes.

Keywords: Ceramics, Membranes, Filters, Separation

550.Investigation of the Mechanical Properties and Performance of
Ceramic Composite ComponentsFY 1994
\$100,000

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 Virginia Polytechnic Institute Contact: K. L. Reifsnider, (703) 231-5259

The purpose of this project is to develop a test system and test methods to obtain information on the properties and performance of ceramic composite materials. The work involves a comprehensive mechanical characterization of composite engineering components such as tubes, plates, shells, and beams subjected to static and cyclic multiaxial loading at elevated temperatures for extended time periods.

Keywords: Ceramics, Composites, Mechanical Properties, Testing

551.	Stability of Solid Oxide Fuel Cell (SOFC) Materials	<u>FY 1994</u>
		\$250,000
DOE	Contacts: J. P. Carr, (301) 903-6519 and E. E. Hoffman, (615) 576-0735	
Oak H	Ridge National Laboratory Contact: N. C. Cole, (615) 574-4824	
Pacific	c Northwest Laboratory Contact: L. R. Pederson, (509) 375-2579	

The purpose of this task is to evaluate the chemical and physical stability of fuel cell materials and interfaces under conditions relevant to an operating SOFC and to identify features in SOFC operation that would limit system performance.

Keywords: Fuel Cells, SOFC

552. <u>Mixed Oxygen Ion/Electr on-Conducting Ceramics for Oxygen</u> Separation and Fuel Cells

<u>FY 1994</u> \$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 Pacific Northwest Laboratory Contact: L. R. Pederson, (509) 375-2579

The purpose of this task is to develop ceramic compositions and physical forms that will provide the highest possible oxygen separation efficiencies from air at the lowest cost.

Keywords: Fuel Cells, Electrochemical, Electrolytes

553. Proton-Conducting Cerate Ceramics

<u>FY 1994</u> \$225,000

<u>FY 1994</u> \$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 Pacific Northwest Laboratory Contact: L. R. Pederson, (509) 375-2579

The purpose of this task is to develop cerate perovskites for use as hydrogen separation membranes, as hydrogen sensors, in membrane reactors, and in gas cleanup.

Keywords: Fuel Cells, Electrochemical, Electrolytes

554. Technology Transfer - Iron Aluminide Filters

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 Oak Ridge K-25 Site Contact: D. E. Fain, (615) 574-9932

The purpose of this activity is to establish a Cooperative Research and Development Agreement (CRADA) with an industrial partner for the development of iron aluminide filters.

Keywords: Filters, Aluminides

555. Thermal and Mechanical Analysis of a Ceramic Tubesheet

FY 1994 \$40,000

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 Mallett Technology Contact: R. H. Mallett, (919) 406-1500

A transport combustor is being commissioned at the Southern Services facility in Wilsonville, Alabama, to provide a gaseous product for the assessment of hot-gas filtering systems. These hot-gas filtration systems will include granular-bed and barrier filter concepts. Filters will be evaluated for carbonizer and gasifier gaseous products. In addition, a pressurized fluidized-bed combustor (PFBC) will be installed to burn the carbonizer product, and a hot gas filter will be installed in the PFBC gas stream. Compositions of the gas streams will range from oxidizing to reducing, and the partial pressures of oxygen and sulfur will vary substantially. Temperatures of the gas streams will range from 840 to 980°C (or higher). One of the barrier filters under consideration incorporates a ceramic tubesheet to support the candle filters. This system, to be designed and built by Industrial Filter & Pump Manufacturing Company (IF&PM) is unique and may offer distinct advantages over metal/ceramic systems that have been tested extensively in other EPRI/DOE projects. To gain an insight that could prove to be useful in the scaleup of a commercial-size, all-ceramic system, work will be undertaken to develop a design methodology applicable to the thermal-mechanical analysis of the all-ceramic system.

Keywords: Ceramics, Tubesheet

556.	Thermal and Mechanical Analysis of a Ceramic Tubesheet	<u>FY 1994</u>
		\$10,000
DOF	Contacts: J. P. Carr. (301) 903-6519 and F. F. Hoffman. (615) 576-0735	·

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 purpose of this task is to perform thermal and mechanical analyses of critical regions in a ceramic tubesheet support for barrier filters in a hot gas cleanup vessel designed for use in gasifier, carbonizer, and pressurized fluidized bed combustion gas streams.

Keywords: Ceramics, Tubesheet

557. <u>Technology Transfer - Ceramic Joining</u>

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: Ceramics, Joining, Technology Transfer

Instrumentation and Facilities

558. <u>Management of the Fossil Energy AR&TD Materials Program</u> FY 1994

<u>F1 1994</u> \$400,000

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 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

<u>FY 1994</u> \$175,000

559. General Technology Transfer Activities

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 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

560. Gordon Research Conference Support

FY 1994 \$4,000

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 task provides funds to support the annual Gordon Research Conference.

Keywords: Technology Transfer

FY 1994 \$35,000

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KEYWORD INDEX

A

Ab-initio Electronic Structure Methods (293-296), (299) AC Application (99) AC Losses (97) Acid (94) Acoustic Manipulation (159) Acoustic Sensors (146) Actinides (162), (307), (310), (316) Adherence (64), (65) Adhesive Bonding (69) Adhesives (25), (259), (265), (304) Adsorbing Materials (102) Adsorption Refrigeration (102) Advanced Batteries (80) Advanced Heat Engines (62) Advanced Materials (27) Advanced Metal Forming (69) Advanced Propulsion Fuels (300) Aerogels (30), (291) Aging (244) AGT (62) Alcohol Fuels (86) All-Optical Switching (291) Allov Development (172), (305) Alloys (35), (241), (242), (249), (251-253), (255), (272), (273), (307), (308), (337-339), (352), (353) Alternative Final Waste Form (205), (206), (208) Alternative Fuels (86) Alumina (50), (56), (59), (220), (221) Aluminides (337), (338), (340), (352), (355), (356), (361) Aluminizing (337) Aluminum Titanate (51) Aluminum/Titanium Carbide Composites (324) Amorphous Materials (89) Amphiboles (154) Analysis (238), (245), (262), (263), (266-268) Aquifer (101) Arc (212)

Ash (200) Atomic Force Microscopy (167), (283), (301) Atomic-level Materials Modeling (293-296), (299) Austenitics (337), (339), (353) Automotive Catalysts (33)

В

Basalt (203) Batteries (74), (78), (79), (83), (84) Behavior (289) Bench-Scale (200), (207), (210) Beryllium (176) Beryllium Alloy Processing (330) Beryllium Processing (330) Beryllium-Yttrium Hydride (221) Biaxial Stress (144) **Bifunctional Air Electrodes (85)** Binary Alloys (142) Binder (61) **Biobased Materials (38)** Biodegradable (26) **Biomechanics** (286) Biometric (247) Biomimetic (37) Bipolar (288) Bismuth (97) Bitter Magnets (169) Blue-Emitting Devices (169) Bonding (244), (249), (259), (282), (309) Borosilicate Glass (199), (202) Brazing (66), (249) Breakdown (299) Brittle Failure (156) Buckyballs (158) Bulk Characterization (93)

С

C-O-H Fluids (155) CAP (257) Capacitive Deionization (287) Capacitors (31) Carbon (274), (348), (349) Carbon Fibers (347), (348) Carbon Products (350), (351) Carbon-Carbon (218) Carbon-Fiber Composite (176) Carbonate Minerals (152) Carbonation (93) Casting (292) Catalyst Performance (86) Catalysts (86), (149), (274), (358) Cathodes (77) Cation Diffusion (150) Cement (93), (199), (201) Cementation (156) Centrifugal Atomization (330) Centrifugal Forces (142) Centrifugal Furnace (209) Ceramic Coatings (37), (306), (314) Ceramic Composites (22), (23), (36), (327) Ceramic Fibers (28) Ceramic Nitrides (323) Ceramic Oxides (323) Ceramic Powder (309) Ceramic Precursors (161) Ceramics (27), (29), (31), (34), (158), (161), (163), (172), (173), (175-178), (200), (208), (220), (239), (240), (241), (246-249), (264), (269-271), (293), (297), (305), (306), (341-347), (357-360), (362), (363) CFC (15) Characterization (211), (289) Chelates (322) Chemical (266-268) Chemical Analysis (55) Chemical Reaction (286) Chemical Sensors (315) Chemical Vapor Deposition (32), (63), (89), (90), (161), (303), (312), (330) Chemical Vapor Infiltration (31), (36), (39)

Chemometric (245), (266) Chlorinated Hydrocarbons (315) Chromium-Niobium (338), (356) Chromizing (337) Cine Radiography (309) Claddings (27), (29) Clean Energy Storage (300) Cleaning (242-244) CM (313) **CMZP** (51) Coal-Derived (348) Coatings (28), (29), (39), (63-65), (75), (89), (90), (239), (243), (251), (253), (264), (273), (276), (283), (303), (305), (337), (340), (344), (345), (346), (354)Cogeneration (24) **Coils (99)** Coke (350) Cold Pressing (306) Combustion Chemical Vapor Deposition (28) Compatibility (172), (175), (176), (178) Complex Alloys (281) Complex Compound (102) Component Designs (71-73) Component Test (72) Components (52), (53), (359) Composite Conductors (99) Composites (23), (25), (28), (31), (32), (34), (38), (39), (49), (50), (72), (73), (92), (101), (159), (161), (173), (174), (218), (243), (258), (259), (275), (304), (305),(308), (311), (314), (323), (341-343), (347-349), (357), (359), (360)Composition (211) Compound (267) Computational Model (133) Computed Microtomography (153) Computed Tomography (60) Computer Simulation (290), (291) Concentrated Sunlight (27) Condensed Matter (313) Conductive Materials (317) Conduit (179) Consolidation of Powder (216) Consortium (350) Constitutive Model (130), (150) Consumable Arc Melt (217)

Contact (139) Continuous Fiber (22) Control (136) Convection (142) Conversion (350) Cooperative/Antagonistic Binding Sites (322) Coordination (62) Copolymer (259) **Copper (178)** Corrosion (21), (54), (63), (74), (92), (102), (243), (251), (264), (303), (320), (337-339), (345), (346), (352-356) Corrosion Resistance (64) Cost Effective Ceramics (47), (48), (50), (52), (53), (66-69) Cost Reduction (279) Coupled Processes (151) **CRADA (275)** Creep (54), (56-59), (128) Creep Rupture (354) Cryogenics (297) Crystal (284) Crystal Growth (140) Crystal Silicon (91) Crystal Surfaces (301) Crystallization (278) Crystallographic Slip (130) Cutting Tools (330) CVD (64), (247), (272) Cyclic Fatigue (56)

D

Damage (143) Database (55), (68) DC (212) Debris (206) Defect Structure (150) Deformation (151) Deformation Bonding (285) Dendrites (140) Depleted Uranium (292) Deposition (340)

Design Codes (54) Diamond (160), (247) **Diamond Coatings (330)** Diamond Powders (158) Diamond-like Carbon (160) Dielectric (145), (241), (258), (299) Diesel (62) **Diesel Combustion (59)** Diffraction (263), (267), (268), (328) Diffusion (151), (152) Diffusion Mechanism (150) Diffusivity (155) Direct Oxide Reduction (302) Disordered Media (142) **Dissociation** (297) **Ditopical Receptors (322)** Dopant Diffusion (290) Dopants (279) Drill Cores (153) Drilling (93) Ductility (302) Durability (94) Dynamic Stress Testing (85) Dynamics (284), (310)

Ε

ECM (257) Elastic (145) Elasticity (147) Electric Vehicles (74), (79), (83), (84) Electric-Arc-Furnace (331) Electrical Conductivities (297) Electrical Properties (172), (173), (177), (178) Electrical Resistivity (302) Electrically Conducting Polymers (31) Electro-Optic Materials (324) Electrocatalysts (81), (82) Electrochemical (75), (77), (79), (152), (361) Electrochromic Windows (170) Electrodeposition (90), (97)

Electrodes (78), (80), (83), (84) Electroluminescence (291) Electroluminescent Polymers (322) Electrolytes (79), (361) Electrolytic Cell Development (288) Electron Beam Processing (162) Electronic (246), (258), (260-262), (264), (271), (275) Electronic Correlations (317), (325) Electronic Materials (158), (318) Electronic Structure (281), (282) Electrooptic (260), (270), (271) Electrooxidation (81) Electrorefining (162), (302) Embrittlement (264), (355) Emitters (221) Encapsulation (102), (200), (255), (257), (328) Energetic Materials (298), (299) Energetic Metastable Materials (293) Energy Storage Devices (165) Engines (57), (59), (63-65) Enriched Uranium (292), (311) **Environmental Effects (59)** Environmentally Benign High Explosive Waste Destruction (288) Equation of State (297) Equipment (341), (356) Erosion (176) Etching (286), (293-295) **EXAFS (78)** Excimer Laser Ablation (280) Experimental Rock Deformation (156) Experiments (130) Explosive Front Propagation Mechanisms (319) Explosives (284), (308) Extrusion (217)

F

Fabrication (72), (92), (94), (244) Failure (243), (264), (272), (358) Failure Analysis (57), (58), (131), (147) Failure Mechanism (54)

Failure Testing (57), (58) Fastcast (251), (252) Fatigue (59), (128), (353) Fault Current Limiter (100) Feedstocks (348) Feldspar (152) Ferric Hyrdoxides (155) Ferric Oxides (155) Ferroelectric (241), (248), (270), (271) Ferromagnets (316) Ferrous Metals (224) Fertilizer (26) Fiber Architecture (22) Fiber Optic Beam Delivery (311) Fiber-Reinforced (341-343) Fibers (218), (341), (349), (357) Field Tests (94) Field-Scale (208) Filament Winding (311) Filaments (30) Film (241), (247), (248), (270-272), (276), (345) Filters (274), (359-361) Final Form (207), (208), (210) Final Waste Form (199), (200), (203) Flat Plan Displays (291) Flaws (358) Flow Induced Deformation (326) Fluid Flow (151) Fluidized-Bed Combustion (354) Fluids (138) Flux Flow (143) Flux Pinning (97) Flywheel Containment (297) Foam (244), (256), (258), (274), (302) Foam Insulation (15) Foil (244) Forming (61) Fouling Coefficient (92) Four-Wave Mixing (146) Fracture (54), (59), (128), (131), (132), (137), (143), (147), (175), (269), (272), (310), (353), (358) Fracture Evolution (150)

423

Fracture Mechanics (129) Fracture Toughness (57) Frank-Read Dislocations (313) Friction (64), (65) FSU (253) Fuel Cells (81), (82), (360), (361) Full-Scale (207) Fullerene Composites (329) Fullerenes (27), (158), (160), (161), (168), (257), (291), (328) Furnace (357) Fusion (280) Fusion Welds (281)

G

Gallium Nitride (169) Galvanic Cells (78) Galvanostatic Charge/Discharge (79) Garnets (150) Gas Gun (297) Gas Separation (31) Gas Turbines (24), (71), (72) Gas-Phase Chemistry (32) Gas-Transfer (244), (257) Gasification (354) Gel Casting (49) Generator (100) Geologic Repository (224) Germanium (280) Ginzburg-Landau Phenomenological Models (321) Glass (149), (200), (201), (204), (246), (269), (297) Glass Waste (225) Gold Sulfides (154) Grain Boundary (130) Graphite (212), (220), (349), (351) Green State (60) Grout (200)

Η

Hall-Heroult Cell (39) Halogen Gases (315) Hard Structure Munitions (282) Hazardous Environments (311) Heat Exchangers (23) Heat Pipes (222) Heat Storage (101) Heat Transfer (15), (92) Heavy Electron Systems (312) Heavy Metal Ligands (329) Heisenberg Model (313) Heteroepitaxy (287) High Efficiency Energy Conversion (167) High Energy Density Materials (299) High Explosives (298) High Pressure (138), (293) High Pressures and High Temperatures (300) High Resolution Electron Microscopy (315) High Temperature (129), (130), (138), (209) High Temperature Microstructure (35) High Temperature Properties (56), (57), (59) High Temperature Service (57), (218), (305) High Temperature Superconducting Materials (321) High Temperature Superconductors (139), (287), (327) High-Strain Rate Deformation (323) High-Temperature Electronic Materials (325) High-Temperature Superconducting Films (330) History Dependent Damage (129) HITAF (357) . Hot Carrier Solar Cells (167) Hot Pressing (300) Hot-Gas (339) HR Coatings (278) HVOF Sprays (141) Hydrides (293), (304), (307) Hydrogen (297) Hydrogen Effects (307) Hydrothermal Stability (93) Hydroxide Sludge (205)

I

ICF (244), (279), (284) IEA (62), (63) Image Enhancement (309) Imperfections (135) In Drum Melting (205) Incoloy (179) Induction Heat Treating (242) Industrial Waste Heat Recovery (21) Inertial Fusion (291), (310) Infrared Spectroscopy (149) Inhomogeneities (135) Instrumentation or Technique Development (54) Insulating Layers (323) Insulation (15) Insulation Sheathing (15) Insulators/Thermal (218) Integrated Contractors (304) Integrated Optical Interconnects (322) Intelligent Neural Net Controllers (242) Intercalation Electrodes (77) Interfaces (157), (282), (308), (342) Interior Processing of Materials (159) Intermetallic Coatings (314) Intermetallics (28), (34), (162), (305), (323), (338) Inventories (311) Ion Beam Characterization (319) Ion Beam/Laser Mixing (314) Ion Beams (160), (164) Ion Exchange (199) Ion Implantation (80), (164), (290), (314), (331) Ion Plating (303) Ion Source (164) Ion Transport (76) Iron Aluminide (33) Iron Aluminides (29) Iron-Aluminum (339) Irradiated Microstructures (166) Irradiation Effects (172-178) Irrigation (26)

J

:

Joining (66), (176), (241), (242), (244), (249-251), (255), (272), (274), (352), (353), (363) Josephson Junctions (287), (313) Joule Heated Glass Melter (210)

Κ

KDP (278), (284) KE Atomic Heating (323) Kinetic-Gas Theory (74)

L

Lactic Acid (26) Lactide Plastic (26) Laminated Metal Composites (285) Lanthanides (321) Large Scale Molecular Dynamics (298) Laser (250), (251), (284) Laser Damage (283), (284), (286), (299) Laser Fusion Targets (279), (280), (298) Laser Welding (311) Laser-Assisted Deposition Processes (329) Lead (201), (206) Li Batteries (75), (76), (78), (85) Life Prediction (54), (57), (58) Light and Electron Optical Analysis (33) Liquid Crystals (168), (316) Liquid Metal Processing (253) Lithium (172), (288) Lithium Ceramics (175), (176) Lithography (261) London Phenomenological Models (321) Long Length Wire (99) Low Activation Materials (291) Low Conductivity Gases (15) Low Density Foam (298) Low Heat Rejection Diesel Engines (72), (73)
Low Pressure Plasma (305) Low Resistivity (139) Low Temperature Scanning (318) Low-Dimensional Electronic Materials (316) Low-Level Mixed Waste (207), (208), (210) Low-Level Waste (201)

Μ

Machining (66-69), (292), (304) Macrocrystallization of Metals (78) Macroencapsulation (201) Magnesium Alloys (61) Magnet Materials (178), (179) Magnetic Coil Designs (317) Magnetic Dynamics (321) Magnetic Field Processing (30), (35) Magnetic Fields (142) Magnetic Fusion (290) Magnetic NDE Techniques (144) Magnetic Properties of Thin Films (320) Magnets (297) Management (62), (363) Manufacturing (279), (292) Material Degradation (93) Materials (339), (340), (357), (359) Materials at the Atomic Level (315) Materials Characterization (242), (244), (297) Materials Program (363) Materials Properties (289) Materials Science (145), (313) Materials Under Extreme Conditions (312) MAWS (209), (211) MDA (257) Me Phase Boundary Tuning (316) Mechanical Alloying (216) Mechanical Miniaturization (159) Mechanical Properties (35), (38), (55), (57), (62), (63), (339), (346), (360) Melter (212)Melting (241), (243), (251-255), (273) Membrane (247), (255), (360)

Keyword Index

Meniscus Coater (278) Mesostructural Nanocrystals (327) Metal Carbide Thin Films (312) Metal Complexes (313) Metal Ion Chelating Agents (329) Metal Matrix Composites (29), (69), (327) Metal Powder (309) Metal Thin Films (312) Metal Transport (154) Metal Vapor Synthesis (321) Metal-Air Batteries (85) Metallic Glasses (321) Metallization (27), (297) Metals (65), (66), (241-244), (246), (249-255), (264), (266), (272-274), (305) Metals: Ferrous (128), (132) Methanol Oxidation (82) Micas (154) Micro-mechanical Modeling (28) Microalloy (338) Microelectronics (295) Micromechanical (130) Micromechanical Fracture Models (329) Microporous (240), (255), (256), (258), (259), (274) Microscopy (262), (267), (268) Microstructure (55), (97), (152), (241), (248-250), (252-255), (262), (263), (267), (268), (273), (305), (307), (308), (310), (318), (340) Microstructure and Solar Cells (91) Microwave Joining (35) Microwave Processing (30), (31), (35), (36), (39), (253), (346), (347) Microwave Sintering (47), (163), (306) Microwave Solidification (205) Minerals (101), (151) Mixed Waste (313) Mixed-Gas (355), (356) Mixtures (138) Modeling (32), (64), (173-175), (242), (244), (246), (247), (249-252), (255), (257), (260), (261), (265), (272), (273), (275), (276), (314), (343)Moderators (221) Moisture (355) Molecular Design (293-295) Molecular Dynamics (293-296), (315) Molecular Hydrodynamics (298)

429

Molten Salt Extraction (302) Molybdenum Disilicide (315) Molybdenum Disilicide Composites (324) Molybdenum-Niobium (221) Morphology (301) Motor (100) Mulch (26) Mullite (64) Multicomponent Diffusion (156) Multilayer Capacitors (39) Multilayer Fabrication (170) Multilayer Technology (277) Multiphase Alloys (318) Multiphoton Absorption (299)

Ν

Na/polymer Cells (77) Na/S Batteries (75) Nano-fabrication (315) Nano-Lithography (286) Nano-Stethoscope (286) Nanocrystals (291) Nanomachining (315) Nanoparticles (158) Nanophase (70), (351) Nanostructures (159) Natural Gas Adsorbent Materials (86) $Nb_{3}Sn$ (178) NDE (60), (134), (286) Net Shape (243), (251), (254), (304) Neutron Diffraction (324), (327) Neutron Embrittlement (144) Neutron Reflectometry (320), (326) Neutron Scattering (316) Nickel Aluminide (34) Nickel Aluminides (33), (38) NIF (279) Niobium (220), (222) Nitrate Salts (206) Nitration (306)

Nitride (248), (254), (293) Nitromethane (319) NMR (81), (275) Noble Metal (217) Nondestructive Evaluation (49), (58), (60), (61), (68), (71), (91), (140), (146), (303), (309), (358) Noninvasive Diagnostics (163) Nonlinear (150), (260) Nonlinear Crystals (278) Nonlinear Optic (165), (324) Novel Energetic Materials (300) Novel Materials Applications (293) Nuclear Applications (311) Nuclear Magnetic Resonance (61) Nuclear Waste (328) NZP (51)

10 C 10

0

Optical (246), (260), (264), (271) **Optical Coatings (286)** Optical Devices (160) Optical Fibers (135), (165), (177) **Optical Finishing (279) Optical Gratings (286) Optical Properties (177)** Optical Sensing (132) Optical Switch (165) Optimization (133) **Opto-electronic Switches (168)** Optoelectronics (291), (295) Ordered Alloys (34) Organic Interfaces (37) Organic Polymers (35) Organics (244), (255-261), (265), (274-276) Orientation Distribution Function (328) Oxidation (26), (58), (64) Oxides (293), (345)

Ρ

Packaging (239), (241-243), (246), (258), (261), (272), (273) Parallel Computing (298) Particle Size (309) Particle/Plasma Interaction (131) Passivation (293-295) Patterning (160) Performance Criteria (211) Permeability (93), (101), (151) Petroleum (149) Phase Change Materials (86), (101), (102) Phase Development (97) Phase Diagrams (302) Phase Stability (281) Phase Transformation (93), (134), (281) Phosphate (208) Photo-initiated Electron Transfer (168) Photocatalyst (26) Photodiodes (329) Photoelectron Diffraction (296) Photoelectron Holography (296) Photoelectron Spectroscopy (296) Photoemission Spectroscopy (317) Photonics (291) Photovoltaic Devices (329) Photovoltaics (168) Physical Properties (33) Physical Vapor Deposition (90), (303), (314) Physical/Mechanical Properties (49-51) Piezoelectric (145), (270) Pinning (143) Pitch (349), (350) Plasma (146), (207-210), (212), (239), (275), (276), (280), (331) Plasma Chemistry (329) Plasma Diagnostics (138) Plasma Ion Implantation (326) Plasma Polymer (280) Plasma Processing (131), (133), (138) Plasma-Enhanced CVD (74) Plasma-Facing Components, (176) Plasma-Flame Spraying (305)

Plasma-Sprayed (239) Plastic Anisotropy (314) Plastic Deformation (128), (151), (156), (314) Plastics (304) Plastics Recycling (37) Plutonics (160) Plutonium (292), (302), (328) Plutonium Alloys (302), (308) Plutonium Immobilization (301) Plutonium Processing (301) Plutonium Recovery (301) Polarized Neutron Diffusion in Multilayers (320) Polycrystal Plasticity (314) Polyesters (302) Polyethylene (205), (208) Polymer Composites (94), (327) Polymer Electrolytes (75), (76) Polymer Extrusion (206) Polymer Macroencapsulation (206) Polymer Microencapsulation (206) Polymer Molecules (326) Polymer Solidification (205) Polymer Sorbents (313) Polymeric Electrolytes (74-76), (79) Polymers (30), (39), (92), (94), (199), (200), (255-262), (265), (274-276), (279), (280), (291), (298), (304) Polyolefins (302) Polyurethanes (302) Pore Structure (153) Poroelasticity (151) 1.17 1.18 1.18 1.2 Porosity (252), (263) Porosity Structure (155) • · Porous Carbons (165) Porous Materials (153) Porous Silicon (291) Powder (249) Powder Characterization (46), (47), (62), (63) Powder Consolidation (318) Powder Diffraction Analysis (327) Powder Processing (46), (49) Powder Synthesis (47), (216) Precursors (349), (351)

Keyword Index

Preforms (36) Pressure Dependencies (319) **Process Characterization (242)** Process Control (47), (49), (52), (53), (199) Processing (38), (47), (49), (311), (340) Properties and Composition (300) Propylene Glycol (26) Protected Volumes (239) **Proton Adsorption (155)** Proton Exchange Membranes (82) Pulse Propagation (135) Pulsed-Laser-Deposition (330) Pumpable Slurries (93) **PV-Powered Windows (170)** Pyrochemical (301) Pyrolysis (25), (37) Pyroxenes (150)

Q

QEXAFS (281) Quantum Wells (164) Quartz (152)

R

Radiation Damage (166), (290), (291) Radioactive Materials (302), (304), (307), (308) Radioactive Waste (313) Radioactive Waste Host (199), (202) Radiography (60), (309) Rapid Prototyping (69) Rapid Solidification (35), (305) Reactive Metal Infiltration (29) Real-Time Radiography (309) Rechargeable Batteries (77), (80) Reconfiguration (268) Recovery (311) Reference Material (46), (63) Reflective Films (15)

Reflectivity (259) Refractory Metals (219) Refractory Oxides (315) Resonant Ultrasound Spectroscopy (325) Retarders (93) Rig and Engine Testing (71) Rock Permeability (155) Rocks (152) Romp (256) Roofs (15)

S

Salt Solutions (142) Scale-Resistant (92) Scales (354-356) Scanning Electron Microscopy (55) Scanning Tunneling Microscope (318) Scattering (140), (275) Scrap Steels (331) Secure Containers (239) Semiconductor Processing (290) Semiconductors (89-91), (139), (216), (267), (276), (326) Sensors (253) Separation (162), (256), (360) **SERDP (288)** Shape Memory Alloys (34) Shear Strain Localization (150) Shock Deformation (310) Shock Physics (298) Shock Pressures (297) Shock Temperatures (297) Shock-Wave Deformation (323) Short Range Order (281) Si Light Emission (286) SiAlON (50), (52), (54), (57) Sieves (347), (348) Silica (321) Silica Aerogels (321) Silica Foams (329) Silica Sol-Gels (329)

Silicate Liquids (149) Silicate Melts (156) Silicate Minerals (149), (150) Silicon (239), (240) Silicon Carbide (35), (49), (50), (54-56), (63), (66), (71), (173), (174), (351) Silicon Carbide Whisker Reinforced Aluminum (319) Silicon Carbide/Silicon Nitride Interfaces (315) Silicon Nitride (46-50), (52), (54-61), (63), (66-69), (71), (351) Silicon Oxide (25) Silicones (302) Sintering (36), (48), (306) Small-Angle Neutron Scattering (327) Smart Windows (170) SOFC (360) Soil Washing (204) Sol Gel (30), (329), (241), (248), (270), (271), (306) Sol Gel Coatings (278) Sol-Gel Electrolytes (76) Sol-Gel Processing (39) Solar Cells (90), (91), (168) Solar Furnaces (27) Solar Processing (27) Solder (242), (250), (272), (273) Solid Electrolyte Batteries (170) Solid State Batteries (170) Solid-State Cells (74) Solid-State Electrodes (84) Solidification (142), (206), (208) Solubility (152), (155) Solution Calorimetry (154) Solvent Extraction (350), (351) Space Reactors (219-222) Spall Strength (310) Speciation (149) Spectroscopy (79), (81), (238), (245), (266-268) Sputtering (75), (303) Sputtering and Solar Cells (89), (90) **SRBSN (48)** Stability (99), (201), (302) Starch (26) Statistics (54) Steels (172-175), (178), (274), (331)

Strain (134), (284) Strength (93), (305), (308), (310) Stress (134), (352) Stress Analysis (145) Stress Corrosion Cracking (166) Stress Induced Grain Growth (286) Structural and Sheet Applications (61) Structural Ceramics (21), (24), (51), (53-55), (57), (59), (60), (62-68), (71-73) Structural Phase Transitions (325) Structure (23), (246), (269) Sulfur (199) Sulfur Oxides (315) Super Critical (249) Superalloys (162) Superconducting Powder (309) Superconductors (134), (140), (143), (158), (169), (178), (287), (297) Superlattice Materials (324) Surety (239), (240) Surface (251), (268), (272), (273), (308) Surface Activation (25) Surface Analytical Analysis (33) Surface and Interface Science (296) Surface Area (309) Surface Characterization and Treatment (66-69), (91), (305), (307) Surface Coatings (141) Surface Complexation (154), (157) Surface Morphology (145) Surface Properties (281) Surface Reactivity (155) Surface Science (293-295) Surface Structure (155) Surface Treatment (164) Surface Waves (153) Synchrotron Radiation (153), (281) Synchrotron X-ray Absorption Spectroscopy (157) Synthesis (249) Synthetic Fuels (300) Synthetic Pad Polishing (279)

T

Target Fabrication (310) Technology Transfer (339), (363), (364) Temperatures (293) Tensile Testing (56), (57), (59) Test Procedures (16), (53), (59), (63) Testing (225), (360) Texture Measurement (328) Textures (313), (314) Thallium (97) Thallium Conductor (99) Thermal Barrier Coatings (72), (73) Thermal Conductivity (65) Thermal Diffusion (156) Thermal Expansion (302) Thermal Fatigue (176) Thermal Insulation (30) Thermal Modeling (80) Thermal Resistance (16) Thermal Shock (305) Thermionic (220-222) Thermochemistry (154) Thermodynamics (302) All the second Thermoelectric Cells (219) Thermoelectric Devices (164) Thermoelectrics (216, (286) Thermomechanical Testing (38) Thermophotovoltaics (167) Thermophysical Properties (29), (138) Thermoplastic (200), (208) Thermoset Plastic (206) Thick Film (97) Thin Films (277), (286) Thin-Film Batteries (84) Time-Dependent (56), (57), (59) Tires (25) Titanium Dioxide (26) Tomography (32), (309) Tool Hardening (331) Toughened Ceramics (50), (56) Toughening (28)

Keyword Index

TR-XRD (281) Transformation (93), (307), (308) Transformation Toughened Ceramics (305) Transformation-Toughened (59) Transition Metals (149) Transmission Cable (100) Transport Current (97) Treatment (69) Tri-Layers (287) Tribology (219), (293-295), (330) Tritiated Materials (304) Tritium (304) Tritium Release (175), (176) Tubesheet (362) Tungsten (220), (222) Tungsten Wire Reinforced Copper (319) Turbine Blades (162) Two Phase Deformation (319)

· . .

U

Ultra-low Expansion (51) Ultracapacitors (70) Ultrasonic Microscopy (309) Ultrasonic Sensing (132) Ultrasonic Wave Propagation (153) Ultrasonics (60) Uranium (311), (328) Uranium Alloy (292) Uranium Carbide (222) Uranium Dioxide (220) Uranium Scrap (311)

.

V

Vacuum (15) Vanadium (172-176), (178) Variable Frequency (39) Varistor (269), (271) Vibration Dynamics (321) Viscoplasticity (130) Vitrification (201), (204), (205), (209), (210), (212) Vortex Motion (143)

W

Waste (25), (202) Waste Acceptance Specifications (202) Waste Canisters (225) Waste Conversion (25) Waste Form (202), (211) Waste Minimization (292) Waste Packages (224) Waste Recovery (25) Waste Streams (37) Waste Treatment (301) Weapons Design (304) · · · · · Weapons Engineering (304) Wear (53), (64), (65) Weibull (54) Welding (132), (136), (172), (241), (244), (250), (251), (255), (274), (352), (353) Well Completions (93) Whiskers (22), (341) Wood (25) e General de la composition de la

X

X-ray (32), (252), (253), (262), (263), (266), (273) X-ray Absorption (82) X-ray Diffraction (309) X-ray Laser Heating Experiments (293) X-ray Scattering (316) XeF (286)

Y

Yttria (220)

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