DOE/ER-0487P

ENERGY MATERIALS COORDINATING COMMITTEE (EMaCC)

Fiscal Year 1989

March 1991

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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INTRODUCTION

The DOE Energy Materials Coordinating Committee (EMaCC) serves primarily to enhance coordination among the Department's materials programs and to further the 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. Four topical subcommittees are established and are continuing their own programs: Structural Ceramics, Electrochemical Technologies, Radioactive Waste Containment, and Superconductivity. In addition, the EMaCC aids in obtaining materials-related inputs for both intra- and inter-agency compilations.

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

The EMaCC reports to the Director of the Office of Energy Research in his 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 1989 and describes the materials research programs of various offices and divisions within the Department.

The Chairman of EMaCC for FY 1989 was Joseph B. Darby, Jr.; the Executive Secretary was Scott L. Richlen. The compilation of this report was assisted by Technology Assessment and Transfer, Inc.

Scott L. Richlen
Office of Industrial Technologies
Chairman of EMaCC, FY 1990

MEMBERSHIP LIST
DEPARTMENT OF ENERGY
ENERGY MATERIALS COORDINATING COMMITTEE

Organization	Representative	Phone No.
CONSERVATION AND RENEWABLE ENERGY*		
Energy Utilization Research	Stanley M. Wolf, CE-121	586-1514
	David Mello, CE-121	586-9345
Buildings and Community Systems		
Building Systems	Peter Scofield, CE-131	586-9193
Building Equipment	John Ryan, CE-132	586-9130
	Ronald Fiskum, CE-132	586-9130
	Danny C. Lim, CE-132	586-9130
Industrial Programs		
Waste Energy Reduction	Scott Richlen, CE-141	586-2078
Improved Energy Productivity	Matthew McMonigle, CE-142	586-2082
Transportation Systems		
Heat Engine Propulsion	Robert B. Schulz, CE-151	586-8051
Energy Storage and Distribution		
Electric Energy Systems	Russell Eaton, III, CE-32	586-1506
Energy Storage	Michael Gurevich, CE-32	586-6104
	Eberhart Reimers, CE-32	586-4563

*The Office of Conservation and Renewable Energy was reorganized in April 1990. The affiliations shown below were those of FY 1989. Next year's report will reflect the new office and division titles and affiliations.

MEMBERSHIP LIST (Continued)

Organization	Representative	Phone No.
Solar Heat Technologies		
Solar Thermal Technology	Frank Wilkins, CE-331	586-1684
Solar Buildings Technology	John Goldsmith, CE-332	586-8779
	David Pellish, CE-332	586-6436
Solar Electric Technologies		
Wind/Ocean Technologies	William Richards, CE-351	586-5540
Photovoltaic Technology	Morton B. Prince, CE-352	586-1725
Renewable Energy		
Biofuels and Municipal Waste	Donald Walter, CE-341	586-6104
Geothermal Technology	Raymond LaSala, CE-342	586-4198
ENERGY RESEARCH		
Basic Energy Sciences		
Materials Sciences	Iran L. Thomas, ER-132	353-3426
Metallurgy and Ceramics	Robert J. Gottschall, ER-131	353-3428
Solid State Physics and Materials Chemistry	B. Chalmers Frazer, ER-132	353-3426
Engineering and Geosciences	Oscar P. Manley, ER-15	353-5822
Advanced Energy Projects	Walter Polansky, ER-16	353-5995
Health and Environmental Research		
Physical and Technological Research	Gerald Goldstein, ER-74	353-5348

MEMBERSHIP LIST (Continued)

Organization	Representative	Phone No.
Fusion Energy		
Reactor Technologies	F. W. Wiffen, ER-533	353-4963
NUCLEAR ENERGY		
Program Support		
Safety QA and Safeguards	Benjamin C. Wei, NE-46	353-3927
Remedial Action and Waste Technology		
Waste Treatment Projects*	Henry F. Walter, NE-24	427-1622**
Uranium Enrichment		
Technology Deployment and Strategic Planning	Arnold Litman, NE-34	353-5777
Reactor Systems Development and Technology		
Defense Energy Projects and Special Applications	William Barnett, NE-522	353-3097
Advanced Reactor Programs	Andrew Van Echo, NE-542	353-3930
	J. Edward Fox, NE-531	353-3985
	Arthur S. Mehner, NE-531	353-4474
Naval Reactors	Robert H. Steele, NE-60	557-5561

*In November 1989, this program was transferred from Nuclear Energy to the new office of Environmental Restoration and Waste Management and placed in the Vitrification Projects Branch (EM-343) under the Office of Waste Operations.

**New phone number.

MEMBERSHIP LIST (Continued)

Organization	Representative	Phone No.
CIVILIAN RADIOACTIVE WASTE MANAGEMENT		
Facilities Siting Development		
Engineering Licensing	Mark Frei, RW-23	586-3217
DEFENSE PROGRAMS		
Defense Waste and Transportation Management		
High-Level Waste R&D*	Ken Chacey, DP-123	427-1621**
Weapons Research Development and Testing		
Weapons Research	A. E. Evans, DP-242.1	353-3098
	Robert A. Jones, DP-225.2	353-5492
Inertial Fusion		
Fusion Research	Carl B. Hilland, DP-232	353-3687
FOSSIL ENERGY		
Management, Planning, and Technical Coordination		
Technical Coordination	James P. Carr, FE-24	353-6519

*In November 1989, this program was transferred from Defense Programs to the new office of Environmental Restoration and Waste Management and placed in the Vitrification Projects Branch (EM-343) under the Office of Waste Operations.

**New phone number.

ORGANIZATION OF THE REPORT

The first part of the Program Descriptions consists of a funding summary for each Assistant Secretary office and the Office of Energy Research. This is followed by a summary of project titles and objectives, including the program/project manager(s) and principal investigator.

The second part of the Program Descriptions consists of more detailed project summaries with project goals and accomplishments.

The Table of Contents lists two (2) page numbers for each entry: the first page number gives the funding summary or first program description; the second page number gives the first detailed program description. The Keyword Index is referenced to the page numbers of the detailed program descriptions.

The FY 1989 Budget Summary Table for materials activities in each of the programs within the DOE is presented on page 7.

FY 1989 BUDGET SUMMARY TABLE FOR DOE MATERIALS ACTIVITIES

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

	FY 1989
Energy Conservation	$ 44,505,000
Office of Energy Utilization Research	10,419,000
Office of Buildings and Community Systems	640,000
Office of Industrial Programs	3,284,000
Office of Transportation Systems	30,162,000
Renewable Energy	$ 46,043,000
Office of Energy Storage and Distribution	18,781,000
Office of Solar Heat Technologies	4,830,000
Office of Solar Electric Technologies	20,900,000
Office of Renewable Energy Technologies	1,532,000
Office of Energy Research	$207,963,249
Office of Basic Energy Sciences	187,509,348
Office of Fusion Energy	0*
Small Business Innovation Research Program	20,453,901

*No submission was received from this office for FY 1989.

FY 1989 BUDGET SUMMARY TABLE FOR DOE MATERIALS ACTIVITIES (Continued)

	FY 1989
Office of Nuclear Energy	$142,746,000
Office of Remedial Action and Waste Technology	3,391,000
Office of Uranium Enrichment	21,660,000
Office of Civilian Reactor Development	38,865,000
Office of Space and Defense Power Systems	1,830,000
Office of Naval Reactors	77,000,000*
Office of Civilian Radioactive Waste Management	$ 13,513,000
Office of Systems Integration and Regulations	0**
Office of Civilian Radioactive Waste Management/ Yucca Mountain Project (OCRWM/YMP)	13,138,000
Sandia National Laboratories: Brittle Fracture Technology Program	375,000
Office of Defense Programs	$ 49,499,246
Office of Defense Waste Transportation Management	12,746
Office of Weapons Research, Development, and Testing	49,486,500
Office of Fossil Energy	$ 7,070,000
Office of Technical Coordination	6,970,000
Office of Coal Technology	100,000
TOTAL	**$518,102,843**

*Approximate

**No submission was received from this office for FY 1989.

PROGRAM SUMMARIES

Brief summaries of the materials research programs associated with each office and division are presented in the following text, including tables listing individual projects and the FY 1989 budgets for each. More details on the individual projects within the divisions and the specific tasks or subcontracts within the various projects are given in the paragraph descriptions.

OFFICE OF CONSERVATION AND RENEWABLE ENERGY

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

	FY 1989
1. Energy Conservation	$44,505,000
a. Office of Energy Utilization Research	$10,419,000
(1) Energy Conversion and Utilization Technologies Division	10,419,000
b. Office of Buildings and Community Systems	$ 640,000
(1) Building Systems Division	640,000
c. Office of Industrial Programs	$ 3,284,000
(1) Improved Energy Productivity Division	937,000
(2) Waste Energy Reduction Division	2,347,000
d. Office of Transportation Systems	$30,162,000
2. Renewable Energy	$46,043,000
a. Office of Energy Storage and Distribution	$18,781,000
(1) Energy Storage	4,478,000
(2) Electric Energy Systems	14,303,000

*The Office of Conservation and Renewable Energy was reorganized in April 1990. This report reflects the FY 1989 organization. Next year's EMaCC Report will use the new organizational structure.

b.	Office of Solar Heat Technologies	$ 4,830,000
	(1) Solar Buildings Technology Division	1,730,000
	(2) Solar Thermal Technology Division	3,100,000
c.	Office of Solar Electric Technologies	$20,900,000
	(1) Photovoltaic Energy Technology Division	20,900,000
d.	Office of Renewable Energy Technologies	$ 1,532,000
	(1) Geothermal Technologies Division	639,000
	(2) Biofuels and Municipal Waste Technology Division	893,000

OFFICE OF ENERGY UTILIZATION RESEARCH*

	FY 1989
Office of Energy Utilization Research - Grand Total	$10,419,000
Energy Conversion and Utilization Technologies Division**	$10,419,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$3,669,000
Solid Lubricants Deposited From the Gas Phase	75,000
Engineered Tribological Surfaces	755,000
Surface Roughness Wear Model for Ceramics	75,000
Microporous Ceramics	75,000
Chemical Vapor Deposition of Ceramic Composites	925,000
Thin-Wall Hollow Ceramic Spheres from Slurries	600,000
The Role of Inert Gas Entrapped in Rapidly Solidified Materials	365,000
Biobased Materials - Composites	130,000
Microwave-Driven Spray Drying	290,000
Additives for High-Temperature Liquid Lubricants	55,000
IAD of Tin and Cr_2O_3	100,000
Self-Lubricating Ceramic Surfaces	100,000
Surface Laser Treatment of Partially Stabilized Zirconia (PSZ)	75,000
Ultra Low Wear Materials for Energy Conservation	49,000
Materials Structures and Composition	$3,262,000
Modeling of Ordered Intermetallic Alloys	538,000
Materials-by-Design (MBD) - New Ordered Intermetallic Alloys	379,000
Polymer Decomposition Expert Systems	100,000
Thermosetting Resins with Reversible Crosslinks	165,000

*Discontinued after April 1, 1990.

**After April 1, 1990, reorganized into the Advanced Industrial Concepts Division and the Office of Advanced Transportation Materials.

OFFICE OF ENERGY UTILIZATION RESEARCH (Continued)

	FY 1989
Materials Structures and Composition (continued)	
Biobased Materials - Packaging Plastics	140,000
Innovative Approaches to the Chemical Recycling of Plastics	435,000
Recycling of Sheet Molding Compounds	165,000
Laser Deposition of Thin Films for High Temperature Superconductors	110,000
Microwave Sintering and Joining of Advanced Ceramics (HTSC Materials, Zirconia-Toughened Alumina (ZTA) and Microwave Joining of Ceramics)	600,000
Molecular Beam Epitaxy (MBE) Synthesis of Superconducting Materials	300,000
High Strength Zirconia Fibers	60,000
Biomimetic Thin Film Ceramic Coatings	20,000
Market Impact of HTSC Technology in Selected Applications	150,000
Ceramic-Metal Joining	100,000
Materials Properties, Characterization, Behavior or Testing	$1,703,000
Friction and Wear Research and Development	423,000
Ordered Intermetallic Alloys for High Temperatures	680,000
Ordered Intermetallic Alloys for Corrosion Resistance (FeAl Development)	250,000
Characterization of SiC Whisker - $MoSi_2$ Composites for Elevated Temperature Applications	100,000
Electrochemically Conducting Polymers	250,000
Device or Component Fabrication, Behavior or Testing	$1,785,000
Development of a Wear Model for Lubricated Sliding of Ceramics	115,000
Lubrication Research and Development	760,000
Energy-Efficient Gear-Lubrication Model	50,000
Wear Mechanism Modeling	70,000

OFFICE OF ENERGY UTILIZATION RESEARCH (Continued)

	FY 1989
Device or Component Fabrication, Behavior or Testing (continued)	
Advanced Laser Fluorescence Measurements of Lubricant Film Behavior in a Diesel Engine	65,000
Effect of Cycle-to-Cycle Variations on Instantaneous Friction Torque	50,000
Novel Thin Film Acoustic Wave Sensors	290,000
Development of High-Temperature Superconducting Magnets for High-Efficiency Motors (Pulsed Laser Deposition of Conductors for HTSC Motor Solenoids and Applications for High T_c Superconducting Magnets)	75,000
Bulk Ceramic BiSrCaCuO and TlBaCaCuO Superconductors for Trapped-Flux Permanent Magnets	290,000
Electrochemical Methods for *In-Situ* Repair and Reinforcement of Metallic Coatings	20,000

OFFICE OF ENERGY UTILIZATION RESEARCH

This office supports generic research of a long-term, high-risk, high-payoff nature aimed at stimulating innovation in conservation technology. The research is both broadly based and multi-sectoral, providing a technology base and new technology options for the other conservation programs.

Energy Conversion and Utilization Technologies Division*

The mission of ECUT is to support generic, long-term, high-risk directed basic and applied research and exploratory development of new or improved concepts to produce a technology base which private industry can use in producing products that use energy more efficiently. Materials related research in the ECUT Division is found in two programs, the Materials Program** and the Tribology Program***. The Tribology Program is managed by Argonne National Laboratory (ANL) and the Materials Program out of DOE Headquarters with assistance from several National Laboratories. The goal of both projects is to develop innovative concepts to a point where they can be taken over for further development by private industry or other government programs. The materials work in the Materials Program is in the areas of intermetallic compounds, tough ceramics and composites, biodegradable plastics, recovery and reuse of plastic scrap, corrosion resistant alloys and coatings, materials processing and reliability, superconductors, and thermal insulation. Materials research in the Tribology Program is in the areas of wear of lubricated solids, the friction and wear of ceramics, and tribological surface modifications and coatings. The DOE contact is Stanley M. Wolf, (202) 586-1514 for the Materials Program and David Mello, (202) 586-9345 for the Tribology Program.

Materials Preparation, Synthesis, Deposition, Growth or Forming

1. Solid Lubricants Deposited From the Gas Phase - DOE Contact D. Mello, (202) 586-9345; Pennsylvania State University Contact E. E. Klaus, (814) 865-2574

   - Determine the kinetics of formation, the structures, and friction and wear behavior of solid lubricant films deposited on ceramic and metal surfaces from the gas phase, at high temperatures.

*After April 1, 1990, reorganized into the Advanced Industrial Concepts Division and the Office of Advanced Transportation.

**After April 1, 1990, the Advanced Industrial Materials Program.

***After April 1, 1990, the Transportation Tribology Program.

- Successful deposition of solid lubricants at temperatures up to 900°C on iron-, nickel- and copper-containing alloys was accomplished. Deposited films exhibit lubrication properties at 375°C equal to liquid lubricants at room temperature.

- Successful deposition of solid lubricants at 700°C on several ceramic substrates (Al_2O_3, SiC, etc.) with a fractional percent of metal contaminant in the surface was accomplished, with a resultant reduction in friction coefficient of 61 to 83 percent (f = 0.02 to 0.11).

2. Engineered Tribological Surfaces - DOE Contact D. Mello, (202) 586-9345; ANL Contact Fred Nichols, (312) 972-8292

   - Emphasis in FY 1989 is on the preparation of low friction surfaces for high temperature applications, by means of ion-beam-assisted deposition (IAD) of coatings.

   - An advanced ion-beam-assisted deposition system containing dual electron-beam-evaporation sources, multiple ion-beam sources, and 3-degree-of-freedom specimen manipulation was designed, and constructed, and is in operation.

   - IAD coatings of Ag on Al_2O_3 and of B_2O_2 on steel were prepared and shown to have outstanding adherence and friction and wear reduction properties.

3. Surface Roughness Wear Model for Ceramics - DOE Contact D. Mello, (202) 586-9345, SKF-MRC, Incorporated Contact John McCool, (215) 889-1300

   - Investigation of comparative tribological performance of ceramics and surface modified materials based on microgeometrical effects (effect of surface finish, material properties, and bearing pressures on wear performance in ceramics), and utilizing a microcontact model of friction and wear.

   - A PC-based computer program RUFFIAN (Rough Interface Analysis) which calculates microcontact parameters (asperity contact density, plastic contact density, real contact pressure and area, and flash temperatures (for slow sliding)) as a function of surface roughness and load has been prepared and tested, and has been transferred to interested industries.

   - An updated version of Ruffian applicable to coated surfaces is being developed.

4. Microporous Ceramics - DOE Contact Stanley M. Wolf, (202) 586-1514; LBL Contact Arlon Hunt, (415) 486-5370

   - Development and production of controlled porosity materials with tailored thermal, optical and physical characteristics.

   - Properties of finished material determined and related to preparation technique.

5. Chemical Vapor Deposition of Ceramic Composites - DOE Contact Stanley M. Wolf, (202) 586-1514; ORNL Contact Peter Angelini, (615) 574-4565; SNL-L Contact Mark Allendorf, (415) 294-2895; Thermoelectron Technologies Contact Nancy Scoville, (617) 647-1343

   - Explore novel ceramic matrix composites produced by chemical vapor deposition (CVD) of a dispersed phase and a matrix phase.

   - Develop a single step process for fabrication of ceramic composites which are stable in air at high temperatures.

6. Thin-Wall Hollow Ceramic Spheres from Slurries - DOE Contact Stanley M. Wolf, (202) 586-1514; ORNL Contact David L. McElroy, (615) 574-5976; Georgia Institute of Technology Contact J. Cochran, (404) 894-6104

   - Develop processes for economically fabricating hollow, thin wall spheres from conventional ceramic powders using dispersions.

   - Use pacifiers to reduce high temperature thermal conductivity and provide high-thermal resistance, cost-effective insulating material without ecological and health dangers.

7. The Role of Inert Gas Entrapped in Rapidly Solidified Materials - DOE Contact Stanley M. Wolf, (202) 586-1514; INEL Contact John Flinn, (208) 526-8127; SNLL Contact W. G. Wolfer, (415) 294-2307

   - Determine property modifications for rapidly solidified materials containing entrapped inert gases.

   - Determine strengthening provided by supersaturation of vacancies that are stabilized by internal oxidation.

8. Biobased Materials - Composites - DOE Contact Stanley M. Wolf, (202) 586-1514; SERI Contact Helena Chum, (303) 231-7249; University of Wisconsin Contact Ray Young, (608) 262-0873; U.S. Forest Products Laboratory Contact Roger Rowell, (608) 264-5816; University of Southern Mississippi Contact Lon Mathias, (601) 266-4868; Virginia Polytechnic Institute & State University Contact Wolfgang Glasser, (703) 231-4403

   - Develop cost-effective and environmentally compatible materials with sufficient strength and fabricability for use in the automotive industry.

   - Tailor plastic properties by design of specific chemical modifications of wood materials.

9. Microwave-Driven Spray Drying - DOE Contact Stanley M. Wolf, (202) 586-1514; LANL Contacts F. Gac, (505) 667-5126

   - Development of a generic microwave-driven spray drying process for aerosol preparation of fine, homogeneous powders.

   - Initial effort on simple metal oxide systems with work on complex metal oxide systems to follow.

10. Additives for High-Temperature Liquid Lubricants - DOE Contact D. Mello, (202) 586-9345; JPL Contact Emil Lawton, (818) 354-2982

   - Establish feasibility of chelating macrocyclic compounds as lubricant additives for the reduction of friction and wear at high temperatures.

   - Contract start delayed due to problems in negotiation of inter-agency agreement.

11. IAD of Tin and Cr_2O_3 - DOE Contact D. Mello, (202) 586-9345; NRL Contact Fred Smidt, (202) 767-4800

   - Films of TiN and Cr_2O_3 are being deposited on a high-temperature-steel substrate by ion-assisted deposition (IAD) at a variety of temperatures and ion energies, and tested for microhardness, adhesion and friction coefficient.

12. Self-Lubricating Ceramic Surfaces - DOE Contact D. Mello, (202) 586-9345; Universal Energy Systems Contact Rabi Bhattacharya, (513) 426-6900

- Establish optimum conditions for ion implantation and ion-beam mixing of suitable additives (BaF_2/CaF_2 + Ag or Sn, MoS_2, WS_2 and TaS_2) into ZrO_2 and Al_2O_3 substrates to obtain self-lubricating low friction and wear characteristics.

13. Surface Laser Treatment of Partially Stabilized Zirconia (PSZ) - DOE Contact D. Mello, (202) 586-9345; Illinois Institute or Technology Contact Victor Aronov, (312) 567-3035

- A series of specimens of PSZ with different phase compositions are subjected to laser-scanning heat treatments and then tested for wear resistance.

- This project concluding in FY 1989.

14. Ultra Low Wear Materials for Energy Conservation - DOE Contact D. Mello, (202) 586-9345; Burton Technologies, Inc., Contact R. A. Burton, (919) 839-8287

- Conduct experiments to evaluate a new, low-wear, vitreous carbon material.

Materials Structures and Composition

15. Modeling of Ordered Intermetallic Alloys - DOE Contact Stanley M. Wolf, (202) 586-1514; LANL Contact P. Jeffrey Hay, (505) 667-3663, FTS 843-3663; Yale University Contact John Hack, (203) 432-4256; Virginia Polytechnic Institute Contact Diane Farkas, (703) 961-4742

- Develop mathematical models and research software for use in the design of materials for energy technology applications.

- Modeling efforts to relate the role of boron at grain boundaries in Ni_3Al, and experimental corroboration.

16. Materials-by-Design (MBD) - New Ordered Intermetallic Alloys - DOE Contact Stanley M. Wolf, (202) 586-1514; ORNL Contacts Peter Angelini, (615) 574-4565 and D. M. Nicholson, (615) 574-5873; Imperial College (U.K.) Contact D. G. Pettifor, 011-441-589-5111, ext. 5756

- Development and use of theoretical tools to determine alloy additions which will ductilize intermetallics.

- Experimental verification of theoretical design.

17. Polymer Decomposition Expert Systems - DOE Contact Stanley M. Wolf, (202) 586-1514; ORNL Contact W. E. Thiessen, (615) 574-4973

- Develop an expert system computer program to predict potential reaction pathways for conversion of waste polymers and polymer mixtures into useful materials.

18. Thermosetting Resins with Reversible Crosslinks - DOE Contact Stanley M. Wolf, (202) 586-1514; Polytechnic of New York Contact Giuliana Tesoro, (718) 643-5244

- Determine technical feasibility of developing thermosetting resins with "reversible crosslinks."

- Produce plastics with the strengths, toughness, temperature capabilities and corrosion resistance typical of thermoset reins but which can be easily reprocessed like a thermoplastic.

19. Biobased Materials - Packaging Plastics - DOE Contact Stanley M. Wolf, (202) 586-1514; SERI Contact Helena Chum, (303) 231-7249; Michigan Biotechnology Institute Contact Ramani Narayan, (517) 349-2970

- Develop cost-effective and environmentally degradable packaging plastics which incorporate high levels of inexpensive, renewable polymers but still have the strength of synthetic thermoplastics.

20. Innovative Approaches to the Chemical Recycling of Plastics - DOE Contact Stanley M. Wolf, (202) 586-1514; SERI Contacts Helena Chum, (303) 231-7249 and Robert Evans, (303) 231-1384

- Develop cost-effective and environmentally benign processes for recovering mixed plastics from various sources (auto plastic shredder waste, carpet waste), and other source separated plastic streams.

21. Recycling of Sheet Molding Compounds - DOE Contact Stanley M. Wolf, (202) 586-1514; Stevens Institute of Technology Contact K. E. Gonsalves, (201) 420-5779

- Develop final flow sheets and assess the technical and economical feasibility of recycling thermoset composites.

- Recycling requires mechanical operations (chopping, grinding and filtration), and chemical processes (solvent extraction, hydrolysis, separation).

- Automotive sheet molding compounds (SMC) chosen for study.
- Technical collaboration with General Motors and Ashland Chemical Company established.

22. Laser Deposition of Thin Films for High Temperature Superconductors - DOE Contact Stanley M. Wolf, (202) 586-1514; ORNL Contact Peter Angelini, (615) 574-4565; NCSU Contact J. Narayan, (919) 737-7874

    - Develop laser deposition methods for films and coatings of high temperature superconductor composites, wires and tapes.
    - Study microstructures capable of high critical current density and superior mechanical properties.

23. Microwave Sintering and Joining of Advanced Ceramics (HTSC Materials, Zirconia-Toughened Alumina, ZTA and Microwave Joining of Ceramics) - DOE Contact Stanley M. Wolf, (202) 586-1514; ORNL Contacts H. E. or D. J. Kim, (615) 574-1926 (HTSC Materials) and H. D. Kimrey, (615) 576-5183 (ZTA); QuesTech, Inc., Contact D. Palaith, (703) 760-1299*

    - Evaluate the effectiveness of microwave sintering as opposed to conventional sintering techniques in both HTSC materials and in Zirconia Toughened Alumina (ZTA).
    - Explain more rapid kinetics of grain growth with microwave heating than conventional heating.
    - Demonstrate the applicability of microwave joining of ceramics to materials of industrial interest.
    - Alumina-glass-alumina and mullite-to-mullite joints were made with microwave heating.
    - Joints made with no surface preparation or interlayer—joints were stronger than base material.

*Current address: Technology Assessment and Transfer, Inc., (301) 261-8373.

24. Molecular Beam Epitaxy (MBE) Synthesis of Superconducting Materials - DOE Contact Stanley M. Wolf, (202) 586-1514; ORNL Contact Rodney McKee, (615) 574-5144

- Develop technology for growth of atomically flat, single crystal films of $YBa_2Cu_3O_7$ on practical substrates.

25. High Strength Zirconia Fibers - DOE Contact Stanley M. Wolf, (202) 586-1514; ORNL Contact Peter Angelini, (615) 574-4565; CWRU Contact A. H. Heuer, (216) 368-3868

- Provide improved oxide, single crystal reinforcement for advanced, high temperature structural composites.

- Determined that 4.5 m/o Y_2O_3 partially stabilized ZrO_2 single crystals have flow stresses in excess of 700 MPa at 1400°C and solid solution strengthened ZrO_2, fully stabilized, single crystals, show a maximum in yield stress at 21 m/o Y_2O_3 1400°C.

26. Biomimetic Thin Film Ceramic Coatings - DOE Contact Stanley M. Wolf, (202) 586-1514; PNL Contact Gary McVay, (509) 375-3762

- Develop energy conserving, novel processing methods (mimicking natural or biological processes) for the nucleation and growth of ceramic oxide thin films on metal, ceramic, and polymer surfaces from aqueous solutions.

27. Market Impact of HTSC Technology in Selected Applications - DOE Contact Stanley M. Wolf, (202) 586-1514; ANL Contact E. J. Daniels, (708) 972-5279

- Market survey of the potential for energy conservation through use of HTSC technology in four applications: magnetic separation, motors, heat pumps, and transportation.

- Energy savings estimated at one-half to one quad per year.

28. Ceramic-Metal Joining - DOE Contact Stanley M. Wolf, (202) 586-1514; ORNL Contact Peter Angelini, (615) 574-4565

- Develop new high temperature, high strength, oxidation resistant alloys for brazing of structural ceramics.

- Correlate braze alloy thermodynamic properties, joint microstructures and joint properties.

Materials Properties, Characterization, Behavior or Testing

29. Friction and Wear Research and Development - DOE Contact D. Mello, (202) 586-9345; ORNL Contact Peter Blau, (615) 574-1514

- Measurements of the wear and friction coefficients for elevated temperature, unlubricated sliding of alumina/silicon-carbide-whisker composites and zirconia-toughened alumina-matrix composites.

- Measurement of effect of lubricating layers on wear in SiC/Al_2O_3 composites.

- Investigation of nickel aluminides for tribological applications.

- Development of a "friction microprobe" for the measurement of friction coefficients of individual micrometer-sized constituent phases on the bearing surfaces of engineering materials.

- Investigation of SiC/Si_3N_4 composite for high-temperature tribological applications.

30. Ordered Intermetallic Alloys for High Temperatures - DOE Contact Stanley M. Wolf, (202) 586-1514; ORNL Contacts Peter Angelini, (615) 574-4565 and C. T. Liu, (615) 574-4459

- Develop low-density, high strength ordered intermetallic alloys for high-temperature structural use in advanced energy conversion systems and heat engines.

- Use macroalloying and microalloying processes to improve metallurgical and mechanical properties of intermetallic alloys based on NiAl and Ti_5Si_3.

- More than 100 percent increases in high temperature strength and room temperature ductility have been achieved through alloy additions.

- With industrial input, identified a need for a high-yield, creep resistant, castable alloy which has been developed by addition of molybdenum and reduction of boron to 50 ppm.

31. Ordered Intermetallic Alloys for Corrosion Resistance (FeAl Development) - DOE Contact Stanley M. Wolf, (202) 586-1514; ORNL Contacts Peter Angelini, (615) 574-4565 and C. T. Liu, (615) 574-4459

- Identify an FeAl composition with the best combination of room temperature ductility and corrosion resistance in oxidizing molten nitrate sale environments.

- Minor alloying additions to FeAl led to room temperature tensile ductility greater than 10 percent, (a five-fold increase over pure binary aluminide).

- FeAl compositions with excellent corrosion resistance in molten nitrate salts were also identified.

32. Characterization of SiC Whisker - $MoSi_2$ Composites for Elevated Temperature Applications - DOE Contact Stanley M. Wolf, (202) 586-1514; LANL Contact J. J. Petrovic, (505) 667-0125

- Develop SiC whisker-$MoSi_2$ matrix composites for elevated temperature structural applications in oxidizing environments.

- Solid solution alloying of the composite matrix yielded strengths at 1500° that were 8-10 times higher than pure $MoSi_2$, with retention of ductility and oxidation resistance.

33. Electrochemically Conducting Polymers - DOE Contact Stanley M. Wolf, (202) 586-1514; LANL Contact S. Gottesfeld, (505) 667-0853

- Develop electrochemical techniques for the synthesis and analysis of conducting polymers.

Device or Component Fabrication, Behavior or Testing

34. Development of a Wear Model for Lubricated Sliding of Ceramics - DOE Contact D. Mello, (202) 586-9345; Georgia Institute of Technology Contact Ward Winer, (404) 894-3270

- Investigation of the effect of lubricant compositions on the wear of several advanced ceramics (PSZ, SiN, SiC, and Sialon) at temperatures up to 150°C.

- Development of a wear model based on ceramic-lubricant/additive interactions.

35. Lubrication Research and Development - DOE Contact D. Mello, (202) 586-9345; NIST-Gaithersburg Contact Stephen Hsu, (301) 975-6119

- Development of test methods for evaluating performance of ceramic coatings for engine applications.

- Measurement and analysis of the effect of advanced ceramics (e.g., SiC, SiN, PSZ) substrates on the properties (volatility, thermal, and oxidation stability) of lubricants.

- Investigation of the effect of new additive chemistries on the performance of lubricants at high temperatures (200-600°C).

36. Energy-Efficient Gear-Lubrication Model - DOE Contact D. Mello, (202) 586-9345; Northwestern University Contact Herbert Cheng, (312) 491-7062

- A model to predict gear friction and power losses in spur gears has been developed and is being experimentally validated.

- A dynamic time-dependent model for predicting wear in spur gears, for partial-elasto-hydrodynamic contacts, has been developed and will be validated.

37. Wear Mechanism Modeling - DOE Contact D. Mello, (202) 586-9345; Cambridge University Contact M. F. Ashby, 0-223-33-2-2622

- Uses normalized coordinates to correlate an extremely large and varied database on friction and wear, for steel-on-steel. This is to be extended to other wear pairs.

- A consistent technique for calculating both bulk and flash temperature due to frictional heating is being developed.

38. Advanced Laser Fluorescence Measurements of Lubricant Film Behavior in a Diesel Engine - DOE Contact D. Mello, (202) 586-9345; MIT Contact John Heywood, (617) 253-2243

- *In situ* measurement of oil film thickness between the cylinder liner and the piston rings in an operating, experimental diesel engine.

- Development of a model for lubricant behavior for a variety of engine materials and operational conditions.

39. Effect of Cycle-to-Cycle Variations on Instantaneous Friction Torque - DOE Contact D. Mello, (202) 586-9345; Wayne State University Contact Naeim Henein, (313) 577-3887

- Work being conducted in parallel with research program sponsored by the NSF to develop and evaluate methodology for measurement of Instantaneous Friction Torque (IFT) in an operating engine.

- Project will measure and develop methods for correcting for the effect of cycle-to-cycle torsional vibrations on the accuracy of the measured IFT.

40. Novel Thin Film Acoustic Wave Sensors - DOE Contact Stanley M. Wolf, (202) 586-1514; SNLA Contact A. C. Frye, (505) 844-0787

- Develop a new class of chemical sensors for process monitors that will improve process energy efficiency.

- Use of sol-gel chemistry and surface modification techniques to develop oxide coatings with controlled pore sizes and tailored chemical properties.

- Obtain films with chemical selectivity based on both molecular size and chemical interactions.

41. Development of High-Temperature Superconducting Magnets for High-Efficiency Motors (Pulsed Laser Deposition of Conductors for HTSC Motor Solenoids and Applications for High T_c Superconducting Magnets) - DOE Contact Stanley M. Wolf, (202) 586-1514; ORNL Contacts Peter Angelini, (615) 574-4565, D. H. Lowndes, (615) 574-6306 and R. Feenstra, (615) 574-4341

- Develop pulsed laser deposition methods which will continuously deposit HTSC films on practical substrates.

- Pulsed laser deposition conditions have been found that result in high J_c (>1 MA/cm^2), high T_c (~92°K) $YBa_2Cu_3O_{7-x}$ films formed on single crystal substrates.

- Identify applications for HTSC magnets for motors, heat pumps, etc., and develop general design requirements for magnets in these applications.

42. Bulk Ceramic BiSrCaCuO and TlBaCaCuO Superconductors for Trapped-Flux Permanent Magnets - DOE Contact Stanley M. Wolf, (202) 586-1514; PNL Contact Larry R. Pederson, (509) 375-2731; Boeing Aerospace Contact Thomas Luhman, (206) 234-2683

- Design and demonstrate a trapped-flux permanent magnetic device using bulk, polycrystalline superconducting ceramics in the BiSrCaCuO and/or TlBaCaCuO systems that have critical current densities of at least $10^5 A/cm^2$ at 77°K.

43. Electrochemical Methods for *In-Situ* Repair and Reinforcement of Metallic Coatings - DOE Contact Stanley M. Wolf, (202) 586-1514; ORNL Contact Peter Angelini, (615) 574-4565; University of Florida Contact Ellis D. Verink, (904) 392-8163

- Assess the feasibility of anodizing diffused aluminum coatings on ferrous alloy substrates (immersed in molten nitrite/nitrate baths at temperatures in the range of 600°C).
- Determine whether the aluminum oxide produced by this anodizing could repair and/or reinforce diffused aluminum coatings by sealing off surface imperfections.
- Indications are that new aluminum oxide forms in imperfections in the coating, and on the surface at large.

OFFICE OF BUILDINGS AND COMMUNITY SYSTEMS

	FY 1989
Office of Buildings and Community Systems - Grand Total	$640,000
Building Systems Division	$640,000
Materials Properties, Behavior, Characterization or Testing	$640,000
Unguarded Thin Heater Tester	150,000
Variable R/Switchable Surface Analysis	30,000
Energy Savings with Advanced Building Materials	100,000
Recommended R-Levels - ZIP Program	30,000
CFC Foam Characterization	70,000
Foam Insulation Research	85,000
Development of Non-CFC Foam Insulations	75,000
Evacuated Powder Panel Insulation	100,000

OFFICE OF BUILDINGS AND COMMUNITY SYSTEMS

The Office of Buildings and Community Systems works to increase the energy efficiency of the buildings sector through performance of R&D on building systems, building equipment, and community energy systems. In addition, the Office carries out the statutory requirements of appliance standards and labeling, building energy performance standards, and residential conservation service, and Federal energy management program. 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;
- improve the energy efficiency of advanced electric heat pump and refrigeration systems, and of light systems; and
- develop new planning techniques and systems that will decrease the energy consumption of communities.

<u>Building Systems Division</u>

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 develop and improve existing insulating materials; to develop and verify analytical models that are useful to building designers and researchers for predicting the thermal performance characteristics of materials; to develop methods for measuring the thermal performance characteristics; and to 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

44. Unguarded Thin Heater Tester - DOE Contact Peter Scofield, (202) 586-9193; ORNL Contact David McElroy, (615) 574-5976

    - Study of transient and steady-state properties of insulation materials including mineral fiberboard and powdered insulations.

45. Variable R/Switchable Surface Analysis - DOE Contact Peter Scofield, (202) 586-9193; ORNL Contact David McElroy, (615) 574-5976

    - Assessment of the energy conserving potential by the use of active thermal insulation systems and switchable surface emittances.

46. Energy Savings with Advanced Building Materials - DOE Contact Peter Scofield, (202) 586-9193; LBL Contact Ron Kammerud, (415) 486-6620

    - Assess the energy savings potential in commercial buildings of high R-value and variable R-value insulations, selective surface coatings and switchable emittance films.

47. Recommended R-Levels - ZIP Program - DOE Contact Peter Scofield, (202) 586-9193; NIST Contact Steve Petersen, (301) 975-6136

    - Provide recommendations for insulation levels in residences for each Zip Code area in the USA.

    - Upgrade the ZIP computer program that was used to calculate the recommended insulation levels.

48. CFC Foam Characterization - DOE Contact Peter Scofield, (202) 586-9193; NIST Contact H. Fanney, (301) 975-5864

    - This work evaluates the relationship between thermal conductivity, temperature and time for existing CFC blown foam insulation materials.

49. Foam Insulation Research - DOE Contact Peter Scofield, (202) 586-9193; MIT Contact Dr. Leon Glicksman, (617) 253-2233

- Investigation of new concepts which reduce overall thermal conductivity of common foam insulations.

- Develop foam thermal conductivity aging models.

50. Development of Non-CFC Foam Insulations - DOE Contact Peter Scofield, (202) 586-9193; ORNL Contact David McElroy, (615) 574-5976

- Develop and evaluate with foam insulation industry and EPA new foam insulations that are blown with non-CFC gasses.

- Determine thermal properties and aging characteristics with laboratory testing.

- Determine mechanical properties with application field testing.

51. Evacuated Powder Panel Insulation - DOE Contact Peter Scofield, (202) 586-9193; ORNL Contact David McElroy, (615) 574-5976

- Develop super insulation concept using a soft vacuum in a layer of powder encased in flexible films.

OFFICE OF INDUSTRIAL PROGRAMS

	FY 1989
Office of Industrial Programs - Grand Total	$3,284,000
Improved Energy Productivity Division	$ 937,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 197,000
Composite Cathode Materiel Development	185,000
Cerox Inert Anode Material	12,000
Materials Properties, Behavior, Characterization or Testing	$ 740,000
Expand and Control Inert Electrode Cell Operating Conditions	740,000
Waste Energy Reduction Division	$2,347,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	
Microwave Sintering of β-Alumina for Use in the Sodium Heat Engine	0
Materials Properties, Behavior, Characterization or Testing	$1,249,000
Advanced Heat Exchanger Material Technology Development	770,000
Assessment of Strength Limiting Flaws in Ceramic Heat Exchanger Components	300,000
National Laboratory Support to Assessment of Strength Limiting Flaws in Ceramic Heat Exchanger Components	120,000
Ceramic Fiber Residue Measurement	59,000

OFFICE OF INDUSTRIAL PROGRAMS (Continued)

	FY 1989
Device or Component Fabrication, Behavior or Testing	$1,098,000
Ceramic Composite Heat Exchanger for the Chemical Industry	923,000
HiPHES System Design Study for Energy Production from Hazardous Wastes	0
HiPHES System Design for an Advanced Reformer	0
Ceramic Components for Stationary Gas Turbines in Cogeneration Service	175,000

OFFICE OF INDUSTRIAL PROGRAMS

This office supports cost-shared research and development for industrial energy conservation technologies that offer large potential for saving scarce fuels. It also encourages the private sector to implement and deploy such technologies as they are developed. Materials research is done in support of the technologies under development, to develop materials with lower embodied energy and to provide materials for use in equipment/systems which can improve energy efficiency.

Improved Energy Productivity Division

This division conducts research and creates new energy conserving processes for ore reduction, metals production, and basic shape processing; sensing and control instrumentation; separation processes; and new coatings.

Materials Preparation, Synthesis, Deposition, Growth or Forming

52. Composite Cathode Material Development - DOE Contact M. J. McMonigle, 3202) 586-2082; Great Lakes Contact L. A. Joo, (615) 543-3111

    - Testing of TiB_2-graphite samples to determine optimum composition and factors influencing useful life.

53. Cerox Inert Anode Material - DOE Contact M. J. McMonigle, (202) 586-2082; EL TECH Contact Tom Gilligan, (216) 357-4066

    - Evaluation of operating conditions that affect the formation, characteristics and stability of a CeO_2 coating that forms in-situ from molten cryolite on an oxygen evolving electrode.

Materials Properties, Behavior, Characterization or Testing

54. Expand and Control Inert Electrode Cell Operating Conditions - DOE Contact 5. J. McMonigle, (202) 586-2087; PNL Contact Larry Morgan, (509) 375-3874

    - Development of cermets for inert anodes.

• Waste Energy Reduction Division

Waste Energy Reduction is concerned with the efficient conversion of fuel to a more useful energy form and with the utilization of energy embodied in waste products—solids, liquids, and gases. This division conducts research to develop advanced waste energy recovery technologies for the industrial sector.

Materials Preparation, Synthesis, Deposition, Growth or Forming

55. Microwave Sintering of β-Alumina for Use in the Sodium Heat Engine - DOE Contact J. Eustis, (202) 586-2098; ORNL Contact W. Snyder, (615) 574-2178

- Development of higher toughness β-Alumina through use of microwave sintering.

Materials Properties, Behavior, Characterization or Testing

56. Advanced Heat Exchanger Material Technology Development - DOE Contact S. Richlen, (202) 586-2078; ORNL Contact M. Karnitz, (615) 574-5150

- Development of improved materials and fabrication processes for advanced ceramic heat exchangers.
- Expanding the material data base for advanced ceramic heat exchangers.
- Evaluation of the effect of corrosive waste stream constituents on candidate ceramic materials.
- Development of advanced wet forming techniques for monolithic ceramic components.

57. Assessment of Strength Limiting Flaws in Ceramic Heat Exchanger Components - DOE Contact S. Richlen, (202) 586-2078; Babcock & Wilcox Contact J. Bower, (804) 522-5742

- Evaluation of the effect of operating environments on flaw populations of ceramic heat exchanger components using advanced NDE methods.

58. National Laboratory Support to Assessment of Strength Limiting Flaws in Ceramic Heat Exchanger Components - DOE Contact S. Richlen, (202) 586-2078; Idaho National Laboratory Contact W. Reuter, (208) 526-1708

- Development of advanced NDE, test methods, and other key technologies to support Babcock & Wilcox studies of strength limiting flaws in ceramics.

59. Ceramic Fiber Residue Measurement - DOE Contact S. Richlen, (202) 586-2078; ORNL Contact M. Karnitz, (615) 574-5150

- Determination if health hazards could be caused by the handling, processing, or machining of continuous ceramic fiber components.

Device or Component Fabrication, Behavior or Testing

60. Ceramic Composite Heat Exchanger for the Chemical Industry - DOE Contact S. Richlen, (202) 586-2078; Babcock & Wilcox Contact D. Hindman, (804) 522-5825

- Design and field test of heat exchanger for the chemical industry.

- Evaluation of composite systems in industry environment.

61. HiPHES System Design Study for Energy Production from Hazardous Wastes - DOE Contact S. Richlen, (202) 586-2078; Solar Turbines Incorporated Contact M. Ward, (619) 544-2553

- Development of preliminary design for high pressure heat exchange systems (HiPHES) to produce heated pressurized air to a turbine.

- Identification of critical material and design problems.

62. HiPHES System Design Study for an Advanced Reformer - DOE Contact S. Richlen, (202) 586-2078; Stone & Webster Engineering Corp. Contact P. Koppel, (617) 589-5293

- Development of preliminary design for high pressure heat exchange system (HiPHES) for an advanced convective reformer.

- Identification of critical material and design problems.

63. Ceramic Components for Stationary Gas Turbines in Cogeneration Service - DOE Contact W. Parks, (202) 586-2093; Battelle Contact D. Anson, (614) 424-5823

- Develop ceramic composite components for stationary gas turbines used in cogeneration systems.

OFFICE OF TRANSPORTATION SYSTEMS

	FY 1989
Office of Transportation Systems - Grand Total	$30,162,000
Materials Preparation, Synthesis, Deposition, Growth or Fo	$ 8,712,000
Silicon Carbide Powder Synthesis (WBS No. 1112)	15,000
Turbomilling of SiC (WBS No. 1116)	172,000
TiB_2 Whiskers (WBS No. 1117)	0
Powder Characterization (WBS No. 1118)	110,000
Sintered Silicon Nitride (WBS No. 1121)	200,000
Si_3N_4 Powder Synthesis (WBS No. 1123)	0
Microwave Sintering (WBS No. 1124)	300,000
Advanced Processing (WBS No. 1141)	2,701,000
Improved Processing (WBS No. 1142)	355,000
Advanced Processing (WBS No. 1143)	2,701,000
Processing Science for Reliable Structured Ceramics Based on Silicon Nitride (WBS No. 1144)	166,000
Dispersion Toughened Si_3N_4 (WBS No. 1221)	480,000
Dispersion Toughened Si_3N_4 (WBS No. 1223)	160,000
Composite Development (WBS No. 1224)	421,000
Advanced Composites (WBS No. 1225)	127,000
Dispersion Toughened Oxide Composites (WBS No. 1231)	360,000
Transformation Toughened Ceramics Processing (WBS No. 1232)	0
Development of Toughened Ceramics (WBS No. 1237)	167,000
Low Expansion Ceramics (WBS No. 1242)	277,000
Materials Properties, Behavior, Characterization or Testing	$ 7,620,000
Ceramic Component Design Technology	100,000
Microstructural Modeling of Cracks (WBS No. 2111)	86,000
Adherence of Coatings (WBS No. 2212)	22,000
Dynamic Interfaces (WBS No. 2221)	188,000
Advanced Statistic Calculations (WBS No. 2313)	191,000
Microstructural Analysis (WBS No. 3111)	50,000
Physical Properties (WBS No. 3112)	99,000

OFFICE OF TRANSPORTATION SYSTEMS

	FY 1989
Materials Properties, Behavior, Characterization or Testing (continued)	
Microstructural Characterization of Silicon Carbide and Silicon Nitride Ceramics for Advanced Heat Engines (WBS No. 3114)	200,000
Project Data Base (WBS No. 3117)	100,000
Characterization of Transformation-Toughened Ceramics (WBS No. 3211)	100,000
Fracture Behavior of Toughened Ceramics (WBS No. 3213)	220,000
Cyclic Fatigue of Toughened Ceramics (WBS No. 3214)	220,000
Tensile Stress Rupture Development (WBS No. 3215)	315,000
Rotor Materials Data Base (WBS No. 3216)	300,000
Toughened Ceramics Life Prediction (WBS No. 3217)	324,000
Life Prediction Methodology (WBS No. 3222)	586,000
Life Prediction Methodology (WBS No. 3223)	1,621,000
Ceramic Durability Evaluation AGT	80,000
Environmental Effects in Toughened Ceramics (WBS No. 3314)	690,000
LHR Diesel Coupon Tests (WBS No. 3315)	150,000
High Temperature Tensile Testing (WBS No. 3412)	225,000
Standard Tensile Test Development (WBS No. 3413)	220,000
Fracture Toughness Determination of Thin Coatings (WBS No. 3414)	69,000
Non-Destructive Evaluation (WBS No. 3511)	435,000
NDE of Advanced Ceramics by Synchrotron Computed Tomography (WBS No. 3513)	0
Ceramic Component NDE Technology	100,000
Computed Tomography (WBS No. 3515)	110,000
Nuclear Magnetic Resonance Imaging (WBS No. 3516)	216,000
Powder Characterization (WBS No. 3517)	360,000
Spectroscopic Characterization (WBS No. 3518)	81,000
Surface Adsorption (WBS No. 3519)	81,000
Thermodynamics of Surfaces (WBS No. 3520)	81,000

OFFICE OF TRANSPORTATION SYSTEMS

	FY 1989
Technology Transfer and Management Coordination	$ 1,409,000
Management and Coordination (WBS No. 111)	900,000
International Exchange Agreement (IEA) Annex II Management and Support (WBS No. 4115)	379,000
Standard Reference Materials (WBS No. 4116)	130,000
Device or Component Fabrication, Behavior or Testing	$ 12,421,000
Advanced Coating Technology (WBS No. 1311)	175,000
Advanced Coating Technology AGT (WBS No. 1312)	512,000
Wear Resistant Coatings (WBS No. 1331)	270,000
Wear Resistant Coatings (WBS No. 1332)	264,000
Active Metal Brazing PSZ-Iron (WBS No. 1411)	220,000
Metal-Ceramic Joints AGT (WBS No. 1412)	205,000
Metal-Ceramic Joints AGT (WBS No. 1413)	0
Ceramic-Ceramic Joints AGT (WBS No. 1421)	325,000
Thick Thermal Barrier Coatings	25,000
Thick Thermal Barrier Coatings	175,000
Sliding Seal Materials for Diesel	0
High Temperature Solid Lubricant Coatings	50,000
Advanced Turbine Technology Applications Project (ATTAP, AGT-5)	5,100,000
Advanced Turbine Technology Applications Project (ATTAP, AGT-101)	5,100,000

OFFICE OF TRANSPORTATION SYSTEMS

The Office of Transportation Systems has established a number of programs to conserve energy used for transportation and to shift transportation energy demand to non-petroleum fuels.

The Heat Engine Propulsion program is underway to provide industry with proof-of-concepts for advanced gas turbine and Stirling engine technologies that demonstrate improvements in fuel efficiency and to develop technology for heavy-duty diesel operation under uncooled minimum friction conditions, including waste heat utilization.

The Advanced Materials Development program's objective is to establish an industrial technology base capable of providing reliable and cost-effective structural ceramics for application to advanced heat engines. Project management responsibility for the Heat Engine Highway Vehicle Systems project (gas turbine diesel and Stirling engines) has been delegated to the NASA Lewis Research Center. Project management of the Ceramic Technology for Advanced Heat Engines project (Advanced Materials Development program) has been assigned to the Oak Ridge National Laboratory (ORNL).

The success of these advanced heat engine systems depends strongly on the development of new or improved materials. Ceramic materials are needed for the hot-flow-path components of the advanced gas turbine and the minimum friction adiabatic (uncooled) diesel engines, to meet operating temperature and manufacturing cost requirements. The Stirling engine requires low-cost iron-based alloys capable of operating at high temperatures while exposed to high-pressure hydrogen. Material technology development programs are underway for each of these heat engine systems. The generic ceramic technology program consists of three general topics: materials and processing; data base and life prediction; and design methodology. To support the advanced material work conducted under this and other research programs, a High Temperature Materials Laboratory (HTML) has been constructed at ORNL.

Key elements of each program are organized and described briefly in the following. Robert B. Schulz is the DOE contact, (202) 586-8051, for overall coordination in the following Office of Transportation Systems material projects.

Materials Preparation, Synthesis, Deposition, Growth or Forming

64. Silicon Carbide Powder Synthesis (WBS No. 1112) - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact E. L. Long, Jr., (615) 574-5172; Carborundum Contact Harry A. Lawler, (716) 278-6345

   - Develop a volume scalable process to produce high purity, high surface area, sinterable silicon carbide powder.

65. Turbomilling of SiC (WBS No. 1116) - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact T. N. Tiegs, (615) 574-5173; Southern Illinois University Contact Dale E. Wittmer, (618) 536-2396

   - Design and fabricate prototype turbomilling units and investigate the turbomilling process as a means of improved processing for SiC whisker-ceramic matrix composites.

66. TiB_2 Whiskers (WBS No. 1117) - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact R. L. Beatty, (615) 574-4536; Keramont Contact J. C. Withers, (602) 746-9442

   - Produce TiB_2 whiskers, TiB_2-coated alpha-SiC whiskers, consolidate SiC matrix composites, and test in air above 1200°C.

67. Powder Characterization (WBS No. 1118) - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact D. Ray Johnson, (615) 576-6832; National Institute for Standards and Technology (NIST) Contact S. Malghan, (301) 975-2000

   - Develop a fundamental understanding of surface chemical changes which take place when silicon nitride powder is attrition-milled in an aqueous environment.

68. Sintered Silicon Nitride (WBS No. 1121) - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact D. Ray Johnson, (615) 576-6832; AMTL Contact G. E. Gazza, (617) 923-5408

   - Determine optimum sintering aid and time-temperature-pressure for sintered Si_3N_4 containing yttria/silica and small additions of MO_2C.

   - Includes technical support for sintering of silicon nitride (AMTL) via on-site personnel assignments to conduct high nitrogen pressure sintering experiments.

69. Si$_3$N$_4$ Powder Synthesis (WBS No. 1123) - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact E. L. Long, Jr., (615) 574-5172; Ford Contact Gary M. Crosbie, (313) 574-1208

- Develop improved, sinterable, high-purity, and low-cost silicon nitride powder, involving a low temperature reaction of silicon tetrachloride with liquid ammonia to form a diimide silicon nitride precursor.

- To achieve major improvements in the quantitative understanding of how to produce sinterable Si_3N_4 powders having highly controlled particle size, shape, surface area, impurity content, and phase content.

70. Microwave Sintering (WBS No. 1124) - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contacts D. Ray Johnson, (615) 576-6832 and T. N. Tiegs, (615) 574-5173

- 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.

71. Advanced Processing (WBS No. 1141) - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact R. L. Beatty, (615) 574-4536; Norton Contact D. M. Tracey, (508) 393-5811

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

72. Improved Processing (WBS No. 1142) - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contacts D. Ray Johnson, (615) 576-6832 and R. L. Beatty, (615) 574-4536

- Determine and develop the reliability of selected advanced ceramic processing methods.

73. Advanced Processing (WBS No. 1143) - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact R. L. Beatty, (615) 574-4536; GTE Laboratories Contact L. J. Bowen, (617) 466-2536

- Develop the powder, process improvements, and controls needed to enable the reproducible fabrication of silicon nitride ceramics which demonstrate program goals for strength and Weibull modulus.

74. Processing Science for Reliable Structural Ceramics Based on Silicon Nitride (WBS No. 1144) - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact R. L. Beatty, (615) 574-4536; University of California Contact Fred F. Lange

- Obtain a basic understanding of relevant problems associated with forming powder compacts from slurries which will densify to produce reliable structural ceramics.

75. Dispersion Toughened Si_3N_4 (WBS No. 1221) - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact T. N. Tiegs, (615) 574-5173; Garrett Ceramic Components Division Contact H. C. Yeh, (213) 618-7449

- Develop high toughness, high strength, refractory ceramic matrix composites which are amenable to low-cost, near-net-shape forming for application as structural components in automotive engines.

- Maximize the toughness in a high strength, high temperature SiC whisker/Si_3N_4 matrix material system that can be formed to shape by slip casting and densified by a method amenable to complex shape mass production.

76. Dispersion Toughened Si_3N_4 (WBS No. 1223) - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact M. A. Janney, (615) 574-4281; GTE Contact S. T. Buljan, (617) 890-8460

- Develop silicon nitride composites of enhanced fracture toughness and strength, utilizing particulate and whisker dispersoids, for AGT applications.

- Evaluate UBE, Toyo Soda Si_3N_4, and American Matrix, Tokai, and Tateho SiC whiskers as alternative precursor materials for composite preparation.

- Optimize the process for near-net-shape part fabrication through optimization of binders and the compounding step of the process, injection molding, and densification parameters.

77. Composite Development (WBS No. 1224) - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact D. Ray Johnson, (615) 576-6832; Norton Contact N. D. Corbin, (508) 393-6600

- Develop fully dense Si_3N_4 matrix SiC whisker composites utilizing the ASEA HIP (hot isostatic pressure) process.
- Tailor the whisker/matrix interface and determine the optimum whisker morphology for fracture toughness improvements for candidate Si_3N_4 matrix SiC whisker composites developed in Phase I.

78. Advanced Composites (WBS No. 1225) - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact D. Ray Johnson, (615) 576-6832; University of Michigan Contact T. Y. Tien, (313) 764-9449

- Obtain dense silicon nitride composites containing silicon carbide whiskers by liquid phase sintering.

79. Dispersion Toughened Oxide Composites (WBS No. 1231) - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contacts D. Ray Johnson, (615) 576-6832 and T. N. Tiegs, (615) 574-5173

- Development and characterization of SiC whisker-reinforced oxide composites for improved mechanical performance.

80. Transformation Toughened Ceramics Processing (WBS No. 1232) - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact P. F. Beçher, (615) 574-5157; Norton Contact Giulio A. Rossi, (508) 393-5829

- Develop zirconia toughened ceramics that exhibit high toughness and high strength at temperatures up to 1000°C and can be fabricated by pressureless sintering to full density.
- Optimize the properties of two classes of transformation-toughened ceramics, Y-TZP (Y_2O_3) stabilized tetragonal zirconia polycrystals and Ce-ZTA (CeO_2-ZrO_2 toughened Al_2O_3), studied in Phase I.

81. Development of Toughened Ceramics (WBS No. 1237) - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact D. Ray Johnson, (615) 576-6832; Ceramatec Contact R. A. Cutler, (801) 486-5071

- Develop layered ceramic composites which incorporate zirconia as a second phase to achieve improved strength and toughness at temperatures of up to 1000°C.
- Study processing methods for fabricating these layered composites via sintering.
- Increase the use temperature of three-layer composites by substituting HfO_2 for ZrO_2.
- Develop aqueous and nonaqueous slip casing techniques for three-layer composites in order to obtain better layer uniformity and to maximize residual compressive stress by optimizing the outer layer thickness.
- Superimpose temperature stresses on transformation-induced stresses in three-layer composites.
- Demonstrate improved thermal shock resistance and damage resistance in optimized composites.

82. Low Expansion Ceramics (WBS No. 1242) - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact D. Ray Johnson, (615) 576-6832; Virginia Polytechnic Institute and State University Contact J. J. Brown, Jr., (703) 961-6777

- Develop an economic, isotropic, ultra-low thermal expansion ceramic material having stable properties above 1200°C.
- Continue investigation of two promising materials, a zircon (NZP) composition and a beta-eucryptite composition

Materials Properties, Behavior, Characterization or Testing

83. Ceramic Component Design Technology - DOE Contact Saunders B. Kramer, (202) 586-8012; NASA Contact John Gyekenyesi, (216) 433-3210

- Develop probabilistic computer codes for ceramic component design.

84. Microstructural Modeling of Cracks (WBS No. 2111) - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact D. R. Johnson, (615) 576-6832; University of Tennessee Contact J. A. M. Boulet, (615) 974-2171

- Develop mathematical procedures by which existing design methodology for brittle fracture could accurately account for the influence of non-planar crack faces on fracture of cracks with realistic geometry under arbitrary stress states.

85. Adherence of Coatings (WBS No. 2212) - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact C. J. McHargue, (615) 574-4344

- Financial support is provided for a graduate research assistant to conduct studies on adherence of coatings deposited on substrates subjected to ion beam mixing.

86. Dynamic Interfaces (WBS No. 2221) - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact E. L. Long, Jr., (615) 574-5172; Battelle Contact K. F. Dufrane, (614) 424-4618

- Develop an understanding of the friction and wear processes of ceramic interfaces based on experimental data.

- Address the performance of advanced toughened monolithic ceramics, thermal-spray coatings, surface modifications, and high temperature lubricants.

87. Advanced Statistic Calculations (WBS No. 2313) - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact M. K. Ferber, (615) 576-0818; GE Contact C. A. Johnson, (518) 387-6421

- To advance the current understanding of fracture statistics in the following areas: optimum testing plans and data analysis techniques, consequences of time-dependent crack growth on the evolution of initial flaw distributions, and confidence and tolerance bounds on predictions that use the Weibull distribution and function.

88. Microstructural Analysis (WBS No. 3111) - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact D. Ray Johnson, (615) 576-6832; National Institute for Standards and Technology (NIST) Contact S. M. Wiederhorn, (301) 975-2000

- Identify the mechanisms of failure in structural ceramics subjected to mechanical loads in various test temperatures and environments.

89. Physical Properties (WBS No. 3112) - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contacts D. Ray Johnson, (615) 576-6832 and D. L. McElroy, (615) 574-5976

- Develop an improved understanding of the factors which determine the thermal conductiveness of structural ceramics at high temperatures.

90. Microstructural Characterization of Silicon Carbide and Silicon Nitride Ceramics for Advanced Heat Engines (WBS No. 3114) - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contacts D. Ray Johnson, (615) 576-6832 and T. A. Nolan, (615) 574-0811

- Determine the microstructure of monolithic and composite ceramics and relate that microstructure to mechanical properties and material performance.
- Materials of interest are silicon carbides and silicon nitrides developed by U. S. manufacturers as part of this program and ATTAP.
- Relate microstructural observations to available mechanical test data.

91. Project Data Base (WBS No. 3117) - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contacts D. Ray Johnson, (615) 576-6832 and B. P. Keyes, (615) 574-5113

- Develop and maintain a comprehensive computer data base containing mechanical property data for ceramic materials generated in the overall program effort.

92. Characterization of Transformation-Toughened Ceramics (WBS No. 3211) - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact D. Ray Johnson, (615) 576-6832; AMTL Contact J. J. Swab, (617) 923-5410

- Define the extent and magnitude of potential losses in strength and toughness after long exposures to elevated temperatures tetragonal zirconia polycrystal materials (TZP) and toughened composite ceramics.

93. Fracture Behavior of Toughened Ceramics (WBS No. 3213) - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contacts D. Ray Johnson, (615) 576-6832 and P. F. Becher, (615) 574-5157

- Examine toughening and delayed failure properties of transformation-toughened and whisker-reinforced materials.

94. Cyclic Fatigue of Toughened Ceramics (WBS No. 3214) - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contacts D. Ray Johnson, (615) 576-6832 and K. C. Liu, (615) 574-5116

- Develop and demonstrate the capability of performing uniaxial tension-tension dynamic fatigue testing of structural ceramics at elevated temperatures.

- Establish a data base for design and analysis applications.

95. Tensile Stress Rupture Development (WBS No. 3215) - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contacts D. Ray Johnson, (615) 576-6832 and K. C. Liu, (615) 574-5116

- Develop the test capability for performing uniaxial tensile stress-rupture tests on candidate structural ceramics.

96. Rotor Materials Data Base (WBS No. 3216) - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contacts D. Ray Johnson, (615) 576-6832 and M. K. Ferber, (615) 576-0818

- To systematically study the tensile strength of a silicon nitride and a silicon carbide ceramic as a function of temperature and time in an air environment.

97. Toughened Ceramics Life Prediction (WBS No. 3217) - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact D. Ray Johnson, (615) 576-6832; NASA-Lewis Research Center Contact Stanley. R. Levine, (216) 433-3276

- Determine the behavior of toughened ceramics, especially SiC whisker-toughened Si_3N_4, as a function of time and temperature as the basis for developing a life prediction methodology.

98. Life Prediction Methodology (WBS No. 3222) - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact C. R. Brinkman, (615) 574-5106; Allison Gas Turbine Division Contact D. L. Vaccari, (317) 230-4313

- Develop and demonstrate the necessary nondestructive examination (NDE) technology, materials data base, and design methodology for predicting the useful life of structural ceramic components of advanced heat engines.

99. Life Prediction Methodology (WBS No. 3223) - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact C. R. Brinkman, (615) 574-5106; Garrett Auxiliary Power Division Contact John Cuccio, (602) 220-3600

- Develop the methodology required to adequately predict the useful life of ceramic components used in advanced heat engines.

100. Ceramic Durability Evaluation AGT - DOE Contact Sauders B. Kramer, (202) 586-8012; NASA Contact Sunil Dutta, (216) 433-3282; Garrett Turbine Engine Contact L. Lindberg, (602) 231-4001

- Assess the capability of ceramic materials to perform satisfactorily at temperatures and exposure times defined for automotive turbine engines.

101. Environmental Effects in Toughened Ceramics (WBS No. 3314) - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact V. J. Tennery, (615) 574-5123; University of Dayton Contact N. L. Hecht, (513) 229-4341

- Develop 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.

102. LHR Diesel Coupon Tests (WBS No. 3315) - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contacts D. Ray Johnson, (615) 576-6832 and C. R. Brinkman, (615) 574-5106

- Subject a number of candidate advanced ceramic materials and metal-ceramic joints to diesel "adiabatic" engine environments where the effects of a number of variables (e.g., temperature, fuel type, and engine operating conditions) can be determined.

103. High Temperature Tensile Testing (WBS No. 3412) - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact D. Ray Johnson, (615) 576-6832; North Carolina A&T State University Contact V. S. Avva, (919) 334-7620

- Test and evaluate advanced ceramic materials at temperatures up to 1500°C in uniaxial tension.

104. Standard Tensile Test Development (WBS No. 3413) - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact D. Ray Johnson, (615) 576-6832; National Institute of Standards and Technology (NIST) Contact S. M. Wiederhorn, (301) 921-2901

- Develop 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.

105. Fracture Toughness Determination of Thin Coatings (WBS No. 3414) - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact W. C. Oliver, (615) 576-7245; Vanderbilt Contact James J. Wert, (615) 322-7311

- Develop the scientific base and technology required to obtain the fracture toughness of a material from ultra-low load indentation experiments using the mechanical properties microprobe (MPM).

106. Non-Destructive Evaluation (WBS No. 3511) - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contacts D. Ray Johnson, (615) 576-6832 and D. J. McGuire, (615) 574-4835

- Develop nondestructive evaluation (NDE) techniques for quantitative determination of conditions in ceramics that affect the structural performance using high-frequency ultrasonics and radiography.

107. NDE of Advanced Ceramics by Synchrotron Computer Tomography (WBS No. 3513) - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact D. Ray Johnson, (615) 576-6832; Radiation Science Contact Allen S. Krieger, (508) 494-0335

- Obtain computed tomography (CT) scans of ceramic specimens with resolution an order of magnitude finer than that which can be achieved with electron impact X-ray tubes or radioactive sources using synchrotron radiation.

108. Ceramic Component NDE Technology - DOE Contact Saunders B. Kramer, (202) 586-8012; NASA Contact Alex Vary, (216) 433-6019

- Identify and develop NDE techniques for ceramic heat engine components.

109. Computed Tomography (WBS No. 3515) - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact D. Ray Johnson, (615) 576-6832; Argonne National Lab Contact W. A. Ellingson, (312) 972-5068

- Develop techniques for reliable use of polychromatic X-ray computed tomography to characterize structural ceramics relative to density distributions, presence of voids, inclusions, and cracks.

- Develop calibration methods for CT scanners for ceramic materials.

110. Nuclear Magnetic Resonance Imaging (WBS No. 3516) - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact D. Ray Johnson, (615) 576-6832; Argonne National Lab Contact W. A. Ellingson, (312) 972-5068

- Establish the feasibility of using NMR imaging systems to map organic B/P distributions in injection-molded green ceramics.

- Examine potential for NMR spectroscopy to determine if there are any chemical variations within and/or between batches of organic binder which impact process reliability.

- Determine the sensitivity of NMR imaging methods to injection molding process variables as manifested in distribution of the organic.

111. Powder Characterization (WBS No. 3517) - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contacts D. Ray Johnson, (615) 576-6832 and O. O. Omatete, (615) 576-7199

- Identification, characterization, and modification of those aspects of the chemistry and physics of a ceramic powder and of the powder/solvent interface that control processing;
- Development of standard methods of analysis for achieving the above;
- Development of procedures for writing specifications for ceramic powders that include any of the methods of analysis developed during this project.

112. Spectroscopic Characterization (WBS No. 3518) - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact M. A. Janney, (615) 574-4281; University of Wisconsin Contact M. A. Anderson, (608) 202-2470

- Develop an understanding of the critical characterization parameters for powders to be used as the starting materials for high-performance ceramics.
- Perform a thorough spectroscopic analysis and characterization of selected ceramic powders and/or whiskers in non-aqueous suspension.

113. Surface Adsorption (WBS No. 3519) - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact M. A. Janney, (615) 574-4281; Rutgers University Contact D. J. Shanefield, (201) 932-2226

- Develop an understanding of the critical characterization parameters for powders to be used as the starting materials for high-performance ceramics.
- Conduct a study of the basic mechanisms of adsorption from non-aqueous solvents onto ceramic surfaces, and the modification of those surfaces to make them uniformly processable.

114. Thermodynamics of Surfaces (WBS No. 3520) - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact M. A. Janney, (615) 574-4281; Pennsylvania State University Contact J. H. Adair, (814) 863-0857

- Develop an understanding of the critical characterization parameters for powders to be used as the starting materials for high-performance ceramics.
- Determine the thermodynamic nature of the ceramic powder surface in non-aqueous powder suspension.

Technology Transfer and Management Coordination

115. Management and Coordination (WBS No. 111) - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact D. Ray Johnson, (615) 576-6832

- 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.

116. International Exchange Agreement (IEA) Annex II Management and Support (WBS No. 4115) - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contacts D. Ray Johnson, (615) 576-6832 and Victor J. Tennery, (615) 547-5123

- Assist and encourage international cooperation in the development of voluntary standard methods for determining mechanical, physical, and structural properties of advanced ceramic materials.

117. Standard Reference Materials (WBS No. 4116) - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact D. Ray Johnson, (615) 576-6832; National Institute of Standards and Technology (NIST) Contact A. L. Dragoo, (301) 975-5785

- Develop standard reference material from the ceramic powder chosen by the U.S. consulting committee for the IEA agreement.

- Critical assessment and modeling of ceramic powder characterization methodology toward the establishment of an international basis for standard materials and methods for the evaluation of powders prior to processing.

Device or Component Fabrication, Behavior or Testing

118. Advanced Coating Technology (WBS No. 1311) - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contacts D. Ray Johnson, (615) 576-6832 and D. P. Stinton, (615) 574-4556

- Develop an adherent coating that will prevent sodium corrosion of silicon nitride, silicon carbide, or other ceramics used as components in gas turbine engines.

119. Advanced Coating Technology AGT (WBS No. 1312) - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact D. Ray Johnson, (615) 576-6832; GTE Contact Han Kim, (617) 466-2742

- Develop oxidation-resistant, high toughness, adherent coatings to reduce contact stress in silicon-based ceramic substrates, namely reaction bonded Si_3N_4, sintered SiC, and Hiped Si_3N_4 for use in an advanced gas turbine engine. Multiple/graded coatings will be applied by computer controlled CVD process.

120. Wear Resistant Coatings (WBS No. 1331) - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact D. P. Stinton, (615) 574-4556, Caterpillar Contact C. D. Weiss, (309) 578-8672

- Develop wear-resistant coatings for application to metallic components of low-heat-loss diesel engines, specifically piston rings and cylinder liners.

121. Wear Resistant Coatings (WBS No. 1332) - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact D. P. Stinton, (615) 574-4556; Cummins Contact Malcolm Naylor, (812) 377-7713

- Develop wear-resistant coatings for application to metallic components of low-heat-loss diesel engines, specifically piston rings and cylinder liners.

122. Active Metal Brazing PSZ-Iron (WBS No. 1411) - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contacts D. Ray Johnson, (615) 576-6832 and M. L. Santella, (615) 574-4805

- Develop strong reliable joints containing ceramic components for applications in advanced heat engines.

123. Metal-Ceramic Joints AGT (WBS No. 1412) - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact M. L. Santella, (615) 574-4805; GTE Contact E. M. Dunn, (617) 466-2312

- Demonstrate analytical tools for use in designing ceramic-to-metal joints including the strain response of joints as a function of the mechanical and physical properties of the ceramic and metal, the materials used in producing the joint, the geometry of the joint, externally imposed stresses both mechanical and thermal in nature, temperature, and the effects on joints exposed for long times at high temperature in an oxidizing (heat engine) atmosphere.

124. Metal-Ceramic Joints AGT (WBS No. 1413) - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact M. L. Santella, (615) 574-4805; Battelle Contact A. T. Hopper, (614) 424-4567

- Develop analytical tools necessary to design reliable high strength ceramic oxide-to-ceramic oxide and ceramic oxide-to-metal joints.

125. Ceramic-Ceramic Joints AGT (WBS No. 1421) - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact M. L. Santella, (615) 574-4805; Norton Contact G. A. Rossi, (508) 393-5829

- Develop techniques for producing reliable ceramic-ceramic joints and analytical modeling to predict the performance of the joints under a variety of environmental and mechanical loading conditions including high temperature, oxidizing atmospheres.

126. Thick Thermal Barrier Coatings - DOE Contact John W. Fairbanks, (202) 586-8066; NASA Contact M. Murray Bailey, (216) 433-3416; Cummins Contact Thomas M. Yonushonis, (812) 377-7078

- Develop a thermal barrier coating with enhanced durability for application in advanced diesel engines.

127. Thick Thermal Barrier Coatings - DOE Contact John W. Fairbanks, (202) 586-8066; NASA Contact M. Murray Bailey, (816) 433-3416; Caterpillar Contact H. J. Larson, (309) 578-6549

- Develop a thermal barrier coating with enhanced durability for application in advanced diesel engines.

128. Sliding Seal Materials for Diesel - DOE Contact John W. Fairbanks, (202) 586-8066; NASA Contact Richard Barrows, (216) 433-3388; Southwest Research Institute Contact Shannon Vinyard, (512) 684-5111

- Refine the information base on carbide seal/ceramic cylinder liner combinations for use in the high performance near-adiabatic diesel engine. Completed in 1989.

129. High Temperature Solid Lubricant Coatings - DOE Contact John W. Fairbanks, (202) 586-8066; NASA Contact Hal Sliney, (216) 433-6055; Case Western Reserve University Contact Joseph Prahl, (216) 368-2000

- Develop and evaluate high temperature wear resistant coating systems for use in the range of 500°C in diesel engines.

130. Advanced Turbine Technology Applications Project - DOE Contact Saunders B. Kramer, (202) 586-8012; NASA Contact Paul Kerwin, (216) 433-3409; General Motors, Allison Gas Turbine Division, Contact Phil Haley, (317) 230-2272

- Develop an advanced ceramic component technology base applicable to a competitive automotive gas turbine.

131. Advanced Turbine Technology Applications Project - DOE Contact Saunders B. Kramer, (202) 586-8012; NASA Contact Thomas N. Strom, (216) 433-3408; Garrett Turbine Engine Contact Jim Kidwell, (602) 220-3463

- Develop an advanced ceramic component technology base applicable to a competitive automotive gas turbine.

OFFICE OF ENERGY STORAGE AND DISTRIBUTION

	FY 1989
Office of Energy Storage and Distribution - Grand Total	$18,781,000
Energy Storage	$ 4,478,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 137,000
Corrosion-Resistant Coatings for High-Temperature, High-Sulfur Activity Applications	137,000
Materials Properties, Behavior, Characterization or Testing	$ 924,000
Materials Durability in the Zinc/Bromine System	104,000
Solid-Electrolyte Cell Research	150,000
Zinc Electrode Morphology in Acid Electrolytes	100,000
Zinc/Air Battery Development for Electric Vehicles	119,000
Dendritic Zinc Deposition in Flow Batteries	0
Fast Ion Conduction and Corrosion Processes in Lithium Glasses	50,000
Polymeric Electrolytes for Ambient-Temperature Lithium Batteries	46,000
Exploratory Cell Research and Study of Fundamental Processes in Solid State Electrochemical Cells	0
Corrosion, Passivity, and Breakdown of Alloys Used in High-Energy-Density Batteries	0
Advanced Chemistry and Materials for Fuel Cells	150,000
Electrocatalysts for Oxygen Reduction and Generation	205,000
Materials Structure and Composition	$ 641,000
Molten Salt Cell Research	350,000
New Alkali-Based Battery Materials	205,000
Spectroscopic Studies of Passive Films on Alkali and Alkaline Earth Metals in Nonaqueous Solvents	86,000
Raman Spectroscopy of Electrode Surface in Ambient-Temperature Lithium Secondary Battery	0

OFFICE OF ENERGY STORAGE AND DISTRIBUTION (Continued)

	FY 1989
Device or Component Fabrication, Behavior or Testing	$ 2,776,000
Proton-Exchange-Membrane Fuel Cells for Vehicles	1,350,000
Incorporation of Phase-Change Materials in Building Materials	148,000
Component Stress During Freeze/Thaw Cycling of Sodium/Sulfur Cell	210,000
β-Alumina Electrolyte Degradation	52,000
Aluminum/Air Technology Development	580,000
Research on Slurry Zinc/Air Battery	0
Aluminum Anode Research	0
Solid Polymer Electrolytes for Rechargeable Batteries	97,000
Advanced Membrane Development for the Zinc/Bromine System	140,000
Improved Chromium Platings for Sodium/Sulfur Cell Containers	69,000
Dispersed Phase-Change Material Evaluation	20,000
Phase-Change Materials Wallboard Fabrication and Testing	60,000
Effects of Dopants on Solid-State Phase-Change Materials	50,000
Electric Energy Systems	$14,303,000
Materials Properties, Behavior, Characterization or Testing	$11,744,000
High-Temperature Superconducting Materials Pilot Centers	6,000,000
Microfilamentary Superconducting Composite	170,000
Practical Superconductor Development for Electric Power Applications	1,359,000
Practical Conductor Development for Electric Power Systems	1,150,000
Thin Films Superconductors for Electric Power Systems	830,000
High-Temperature Superconductor Materials and Power Device Development	1,000,000
Fabrication Development of High-Temperature Superconductor for Electric Utility Applications	575,000
Development of Practical Conductors Utilizing High-Temperature Oxides	560,000
Evaluation of Polymers for Electric Insulation	100,000

OFFICE OF ENERGY STORAGE AND DISTRIBUTION (Continued)

		FY 1989
Device or Component Fabrication, Behavior or Testing	$	2,559,000
Films Processing Methods and Device Technology Development		800,000
Device Technology Development/System Study for HTS Equipment		300,000
Prototype Testing of Dynamic Insulation Using Sol-Gel Zinc Oxide		0
Interfacial Aging Phenomena in Power Cable Insulation Systems		50,000
Conducting Polymer Research for Electric Power Equipment Applications		9,000
Fuel Cells for Transportation - Fuel Cell Testing		170,000
Fuel Cells for Transportation - Electrode Optimization		240,000
Fuel Cells for Transportation - Non-Pt Electrocatalysts		110,000
Fuel Cells for Transportation - State of Water and Water Transport in Proton Exchange Membranes		110,000
Fuel Cells for Transportation - CO Tolerance		120,000
Fuel Cells for Transportation - Industrial Contract International Fuel Cells Inc.		650,000

OFFICE OF ENERGY STORAGE AND DISTRIBUTION

The mission of the Office of Energy Storage and Distribution is to lead a national research and development program focused on translating technical and scientific breakthroughs into options for electric energy delivery and control systems and for energy conversion. The Office manages programs in electric energy systems and energy storage and is responsible for the formulation and execution of appropriate national policies and the verification of program balance and priorities among the technologies.

Energy Storage

The Energy Storage Program supports research and development of advanced energy storage and electrochemical conversion systems that will facilitate the substitution of nuclear and renewable energy sources for oil and gas 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 three subprograms: Electrochemical Energy Storage, Battery Development, and Thermal Energy Storage.

Materials Preparation, Synthesis, Growth or Forming

132. Corrosion-Resistant Coatings for High-Temperature, High-Sulfur Activity Applications - DOE Contact A. Landgrebe, (202) 586-1483; Illinois Institute of Technology Contact J. R. Selman, (312) 567-3037

    - Explore electrodeposition and chemical vapor deposition techniques used to prepare corrosion-resistant coatings for high-temperature batteries.

Materials Properties, Behavior, Characterization or Testing

133. Materials Durability in the Zinc/Bromine System - DOE Contact A. Landgrebe, (202) 586-1483; Sandia National Laboratory Contact C. Arnold, (505) 844-8728

    - Improve the chemical durability and evaluate the extent of degradation for several potential battery flow frame materials.

134. Solid-Electrolyte Cell Research - DOE Contact A. Landgrebe, (202) 586-1483; Argonne National Laboratory Contact C. Christianson, (312) 972-7563

    - Develop mechanically stable materials for providing hermetic glass-to-header seals in sodium/sulfur batteries.

135. Zinc Electrode Morphology in Acid Electrolytes - DOE Contact A. Landgrebe, (202) 586-1483; Brookhaven National Laboratory Contact J. McBreen, (516) 282-4513

- Study zinc electrode morphology in acidic zinc chloride and zinc bromine electrolytes.

136. Zinc/Air Battery Development for Electric Vehicles - DOE Contact A. Landgrebe, (202) 586-1483; Metal Air Technology Systems International Contact R. Putt, (415) 654-1960

- Develop a process for pre-plating copper substrate on a reticulated electrode structure to yield to yield a dense, uniform, and continuous zinc deposit.

137. Dendritic Zinc Deposition in Flow Batteries - DOE Contact A. Landgrebe, (202) 586-1483; Illinois Institute of Technology Contact J. R. Selman, (312) 567-3037

- Determine the effects of current modulation on hydrogen evolution during zinc deposition from acidic solutions.

138. Fast Ion Conduction and Corrosion Processes in Lithium Glasses - DOE Contact A. Landgrebe, (202) 586-1483; MIT Contact H. Tuller, (617) 253-6890

- Investigate the role of calcium oxide in stabilizing against lithium attack in ion-conduction glasses.

139. Polymeric Electrolytes for Ambient-Temperature Lithium Batteries - DOE Contact A. Landgrebe, (202) 586-1483; University of Pennsylvania Contact G. Farrington, (215) 898-6642

- Determine the hydration/dehydration characteristics of polymeric electrolytes for lithium batteries.

140. Exploratory Cell Research and Study of Fundamental Processes in Solid State Electrochemical Cells - DOE Contact A. Landgrebe, (202) 586-1483; University of Minnesota Contact W. Smyrl, (612) 625-0717

- Investigate mechanisms occurring at the electrode/electrolyte interface of novel electrochemical cells containing thin-film polymer electrolytes.

141. Corrosion, Passivity, and Breakdown of Alloys Used in High-Energy-Density Batteries - DOE Contact A. Landgrebe, (202) 586-1483; Johns Hopkins University Contact J. Kruger, (301) 338-8937

- Investigate the corrosion resistance of commercial cell container materials in water-containing organic electrolytes by electrochemical and ellipsometric techniques.

142. Advanced Chemistry and Materials for Fuel Cells - DOE Contact A. Landgrebe, (202) 586-1483; Brookhaven National Laboratory Contact J. McBreen, (516) 282-4513

- Investigate oxygen reduction in new acidic electrolytes and evaluate new fuel cell electrocatalysts.

143. Electrocatalysts for Oxygen Reduction and Generation - DOE Contact A. Landgrebe, (202) 586-1483; Case Western Reserve University Contact E. Yeager, (216) 386-3626

- Develop highly active and stable electrocatalysts by examining the factors controlling O_2 reduction and generation on various electrocatalysts.

Materials Structure and Composition

144. Molten Salt Cell Research - DOE Contact A. Landgrebe, (202) 586-1483; Argonne National Laboratory Contact C. Christianson, (312) 972-7563

- Develop separator/electrolyte systems that are stable at high Li activities by investigating the use of high temperature immobilized electrolyte materials.

145. New Alkali-Based Battery Materials - DOE Contact A. Landgrebe, (202) 586-1483; Stanford University Contact R. Huggins, (415) 723-4110

- Investigate several alloy compositions to act as fast, reversible sodium-conducting electrodes in sodium metal chloride batteries.

146. Spectroscopic Studies of Passive Films on Alkali and Alkaline Earth Metals in Nonaqueous Solvents - DOE Contact A. Landgrebe, (202) 586-1483; Case Western Reserve University Contact D. G. Scherson, (216) 368-5186

- Develop insight into the physicochemical properties of films, thus gaining an understanding of passive phenomena in rechargeable lithium batteries.

147. Raman Spectroscopy of Electrode Surface in Ambient-Temperature Lithium Secondary Battery - DOE Contact A. Landgrebe, (202) 586-1483; Jackson State University Contact H. Tachikawa, (601) 968-2171

- Characterize the surface of lithium anodes in non-aqueous solutions by *in situ* Raman spectroscopy.

Device or Component Fabrication, Behavior or Testing

148. Proton-Exchange-Membrane Fuel Cells for Vehicles - DOE Contact A. Landgrebe, (202) 586-1483; Los Alamos National Laboratory Contact S. Gottesfeld, (505) 667-0853

- Develop better gas diffusion electrodes, measure and model mass transport properties of membranes, determine optimal performance characteristics of fuel cells.

149. Incorporation of Phase-Change Materials in Building Materials - DOE Contact E. Reimers, (202) 586-2826; University of Dayton Research Institute Contact I. Salyer, (513) 229-2113

- Develop inexpensive, inert, and effective materials that melt and freeze sharply for use in thermal storage building interior and wallboard systems.

150. Component Stress During Freeze/Thaw Cycling of Sodium/Sulfur Cell - DOE Contact A. Landgrebe, (202) 586-1483; Sandia National Laboratory Contact J. Braithwaite, (505) 844-7749

- Develop a mathematical model to provide a methodology for improving the freeze/thaw durability of sodium/sulfur cells.

151. β-Alumina Electrolyte Degradation - DOE Contact A. Landgrebe, (202) 586-1483; Sandia National Laboratory Contact E. Beauchamp, (505) 844-6039

- Study mechanisms that lead to the failure of β-alumina electrolyte in sodium/sulfur battery cells.

152. Aluminum/Air Technology Development - DOE Contact A. Landgrebe, (202) 586-1483; Eltech Research Corporation Contact E. Rudd, (216) 357-4073

- Optimize materials and design of aluminum/air batteries to increase life, reduce cost, and improve reliability.

153. Research on Slurry Zinc/Air Battery - DOE Contact A. Landgrebe, (202) 586-1483; Pinnacle Research Institute Contact H. S. Alcazar, (408) 252-1360

- Develop and generate dendritic zinc slurry and demonstrate its use in a zinc/air cell.

154. Aluminum Anode Research - DOE Contact A. Landgrebe, (202) 586-1483; SRI International Contact D. MacDonald, (415) 859-3195

- Develop improved aluminum alloys for aluminum/air batteries by investigating solution-phase inhibitors for controlling corrosion.

155. Solid Polymer Electrolytes for Rechargeable Batteries - DOE Contact A. Landgrebe, (202) 586-1483; SRI International Contact D. MacDonald, (415) 859-3195

- Develop high-conductivity polymeric electrolytes for rechargeable lithium battery cells.

156. Advanced Membrane Development for the Zinc/Bromine System - DOE Contract A. Landgrebe, (202) 586-1483; Sandia National Laboratory Contact C. Arnold, (505) 844-8728

- Evaluate chemical pretreatment techniques for use on polyethylene separators in zinc/bromine batteries.

157. Improved Chromium Platings for Sodium/Sulfur Cell Containers - DOE Contact A. Landgrebe, (202) 586-1483; Sandia National Laboratory Contact W. D. Bonivert, (415) 294-2987

- Develop techniques to electroplate high-quality chromium coatings onto carbon and stainless steel containers used in sodium/sulfur batteries.

158. Dispersed Phase-Change Material Evaluation - DOE Contact E. Reimers, (202) 586-4563; A.D. Solomon Contact A. Solomon, 1-972-57-699698 (Israel)

- Develop a mathematical model and computer program able to predict the thermal response of phase-change materials used in building materials.

159. Phase-Change Materials Wallboard Fabrication and Testing - DOE Contact E. Reimers, (202) 586-4563; Martin Marietta Energy Systems Contact J. Tomlinson, (615) 574-0768

- Fabricate facility for preparing full-size samples of phase-change materials and for conducting thermal performance tests.

160. Effects of Dopants on Solid-State Phase-Change Materials - DOE Contact E. Reimers, (202) 586-4563; University of Nevada - Reno Contact D. Chandra, (816) 276-1283

- Develop temperature-adjusted, organic, solid-state phase-change materials that exhibit a heat of transition near room temperature.

Electric Energy Systems

The Electric Energy Systems Program supports research and development directed toward solving mid- to long-term problems in electric energy transmission and distribution and promotes the development and integration of new materials, advanced controls, and new design concepts into the utility network. The program supports research activities in the following areas: Electric Field Effects, Reliability, and Electric Systems and Materials Research.

Materials Properties, Behavior, Characterization or Testing

161. High-Temperature Superconducting Materials Pilot Centers - DOE Contact R. Eaton, (202) 586-1506; Oak Ridge National Laboratory Contact A. C. Schaffhauser, (615) 574-4826; Argonne National Laboratory Contact E. Kaufmann, (312) 972-3606; Los Alamos National Laboratory Contact R. Quinn, (505) 665-3030

- Perform materials research in cooperation with private industry to maintain U.S. leadership in the development of high-temperature superconducting materials.

162. Microfilamentary Superconducting Composite - DOE Contact R. Eaton, (202) 586-1506; Ames Laboratory Contact D. K. Finnemore, (515) 294-3312

- Develop a material processing technique to make stabilized microfilamentary superconducting wires suitable for magnets that operate at 35K.

163. Practical Superconductor Development for Electric Power Applications - DOE Contact R. Eaton, (202) 586-1506; Argonne National Laboratory Contact R. Weeks, (312) 972-4930

- Improve the current-carrying capacity, flexibility, chemical stability, and other properties of high-temperature superconducting (HTS) wires and tapes.

164. Practical Conductor Development for Electric Power Systems - DOE Contact R. Eaton, (202) 586-1506; Brookhaven National Laboratory Contact D. Welch, (516) 282-3517

- Investigate various methods for fabricating composite conductors containing high-T_c oxides, and characterize composite conductors with respect to their superconducting properties.

165. Thin Films Superconductors for Electric Power Systems - DOE Contact R. Eaton, (202) 586-1506; Solar Energy Research Institute Contact R. McConnell, (303) 231-1019

- Characterize the properties of fabricated thin film high temperature superconductors with sufficient current-carrying capability and stability in configurations suitable for use in electric power system devices.

166. High-Temperature Superconductor Materials and Power Device Development - DOE Contact R. Eaton, (202) 586-1506; Sandia National Laboratory Contact D. Schueler, (505) 844-1068

- Develop high temperature ceramic conductors with increased superconductor critical current density.

167. Fabrication Development of High-Temperature Superconductor for Electric Utility Applications - DOE Contact R. Eaton, (202) 586-1506; Los Alamos National Laboratory Contact G. Maestas, (505) 667-3973

- Develop a bulk high current conductor with a current capability of 100A in 1 mm^2 in a field of 2 Tesla at a temperature above 35K.

168. Development of Practical Conductors Utilizing High-Temperature Oxides - DOE Contract R. Eaton, (202) 586-1506; Oak Ridge National Laboratory Contact A. Schaffhauser, (615) 574-4826

- Reduce or eliminate grain boundary resistance in polycrystalline high-T_c oxide superconductors to produce high current-carrying conductors.

169. Evaluation of Polymers for Electric Insulation - DOE Contact R. Eaton, (202) 586-1506; Oak Ridge National Laboratory Contact H. McCoy, (615) 574-5115

- Characterize the mechanical, electrical, and thermal properties of polymers suitable for use in dielectric materials.

Device or Component Fabrication, Behavior or Testing

170. Films Processing Methods and Device Technology Development - DOE Contact R. Eaton, (202) 586-1506; Lawrence Berkeley Laboratory Contact N. E. Phillips, (415) 486-4896

- Provide a basis for the fabrication of practical conductors by investigating methods for producing thin films of high-T_c superconductors.

171. Device Technology Development/System Study for HTS Equipment - DOE Contact R. Eaton, (202) 586-1506; Pacific Northwest Laboratories Contact J. Currie, (509) 375-4355

- Investigate the potential impacts of HTS applications on the electric utility industry in terms of performance, cost, and market issues that will drive the acceptance of HTS technologies.

172. Prototype Testing of Dynamic Insulation Using Sol-Gel Zinc Oxide - DOE Contact R. Eaton, (202) 586-1506; University of Southern California Contact T. C. Cheng, (213) 743-6938

- Develop optimally designed ZnO insulator string for electrical insulation of overhead line transmission.

173. Interfacial Aging Phenomena in Power Cable Insulation Systems - DOE Contact R. Eaton, (202) 586-1506; University of Connecticut Contact M. S. Mashikian, (203) 486-5298

- Study the effects of semiconducting compounds on the aging of extruded power insulation.

174. Conducting Polymer Research for Electric Power Equipment Applications - DOE Contact R. Eaton, (202) 586-1506; Westinghouse Contact E. Schoch, (412) 256-1960

- Explore the technical and economical feasibility of using state-of-the-art conducting polymer materials as a replacement for traditional stress grading materials in electrical equipment.

175. Fuel Cells for Transportation - Fuel Cell Testing - DOE Contact A. Landgrebe, (202) 586-1483/FTS 896-1483; LANL Contact S. Gottesfeld, (505) 667-0853

- The objectives of this project are to measure the operating characteristics of single proton-exchange-membrane fuel cells and to determine the conditions providing optimal performance.

176. Fuel Cells for Transportation - Electrode Optimization - DOE Contact A. Landgrebe, (202) 586-1483/FTS 896-1483; LANL Contact S. Gottesfeld, (505) 667-0853

- The objective of this project is to develop fabrication techniques for fuel cell membrane/electrode assemblies that deliver high performance with low Pt loading.

177. Fuel Cells for Transportation - Non-Pt Electrocatalysts - DOE Contact A. Landgrebe, (202) 586-1483/FTS 896-1483; LANL Contact S. Gottesfeld, (505) 667-0853

- The objectives of this project are to evaluate the effectiveness of transition metal macrocyclic catalysts such as FeTMPP and CoTMPP for oxygen reduction in PEM fuel cells.

178. Fuel Cells for Transportation - State of Water and Water Transport in Proton Exchange Membranes - DOE Contact A. Landgrebe, (202) 586-1483/FTS 896-1483; LANL Contact S. Gottesfeld, (505) 667-0853

- The objectives of this project are to measure and model the state of water and the water transport properties of proton-conducting membranes available from industry and to use these data to improve fuel cell performance.

179. Fuel Cells for Transportation - CO Tolerance - DOE Contact A. Landgrebe, (202) 586-1483/FTS 896-1483; LANL Contact S. Gottesfeld, (505) 667-0853

- The objectives of this project are to quantify the effects of CO on PEM fuel cell performance and to investigate the effectiveness of oxygen injection and alloy catalysts for improving CO tolerance.

180. Fuel Cells for Transportation - Industrial Contract International Fuel Cells Inc. - DOE Contact A. Landgrebe, (202) 586-1483/FTS 896-1483; LANL Contact S. Gottesfeld, (505) 667-0853

- The objectives of this contract are to develop low cost manufacturing techniques for PEM fuel cells and to fabricate and test a 5 to 10 kW PEM fuel cell stack.

OFFICE OF SOLAR HEAT TECHNOLOGIES

	FY 1989
Office of Solar Heat Technologies - Grand Total	$4,830,000
Solar Buildings Technology Division	$1,730,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 752,000
Electrochromic Glazings (Nickel-based)	285,000
Solid State Electrochromic "Smart" Windows	120,000
Optics and Materials for Controlled Radiant Energy in Buildings	222,000
Holographic Diffractive Structures for Enhanced Daylighting	125,000
Materials Properties, Behavior, Characterization or Testing	$ 978,000
Desiccant Concepts Research	125,000
Advanced Desiccant Materials Research	100,000
Open-Cycle Absorption Solar Cooling	125,000
Solar Cooling Research Facility	425,000
Core Daylighting Systems Design	40,000
Advanced Evacuated Tubular Concentrator Research	63,000
Durability Testing Methods for Optical Switching	100,000
Solar Thermal Technology Division	$3,100,000
Materials Preparation, Synthesis, Deposition Growth or Forming	$1,000,000
Silver/Polymer Reflector Research	1,000,000
Materials Properties, Behavior, Characterization or Testing	$2,100,000
Sol-Gel Protective Films for Metal Solar Mirrors	150,000
High Flux Effects on Materials	250,000
Surface Transformations of Metals	600,000
Materials for Applications in Regenerative Thermal Electrochemical Conversion (RTEC) Technology	100,000
Catalysts for Solar-Assisted Water Detoxification	1,000,000

OFFICE OF SOLAR HEAT TECHNOLOGIES

Solar Buildings Technology Division

This program focuses on solar energy products and designs that are economically competitive and can contribute significantly to building energy requirements. The program goal is to develop a technology base that will allow industry to develop solar energy products and designs for the buildings that are reliable and economically competitive, and can contribute significantly to national building energy requirements. The objectives are:

- In the near-term, to provide industry with the information required to improve system performance and achieve acceptable equipment service life and reliability.

- In the long-term, to develop solar energy technologies that can supply up to 80 percent of residential building space heating and hot water requirements and 60 percent of its cooling requirements, and up to 60 percent of nonresidential building heating, cooling, and daylighting energy requirements, at costs competitive with conventional technologies.

R&D is conducted on new approaches for collection, conversion, storage, and delivery of solar energy using the building envelope and equipment.

Materials Preparation, Synthesis, Deposition, Growth or Forming

181. Electrochromic Glazings (Nickel-based) - DOE Contact M. M. Jenior, (202) 586-2998, FTS 896-2998; LBL Contact S. Selkowitz, (415) 486-5064, FTS 451-5064

    - Develop optical switching devices to regulate daylight and solar heat gain for all building glazing applications. These devices must switch reversibly over a large visible transmission range (e.g., 80-10 percent), should have long operating lifetimes, and must be compatible with large-area, low-cost deposition processes used by industry.

182. Solid State Tungsten-Based Electrochromic Films for Windows - DOE Contact M. M. Jenior, (202) 586-2998, FTS 896-2998; EIC Contact R. D. Rauch, (617) 769-9450

- Develop an all solid-state thin film electrochromic coating for windows that can provide active control of solar throughput in windows by the application of a small DC electric current.

- Fabricate an all-solid-state structure without cycle limitations.

183. Tungsten-Based Electrochromic Materials for Controlled Radiant Energy in Buildings - DOE Contact M. M. Jenior, (202) 586-2998, FTS 896-2998; Tufts University Contact R. B. Goldner, (617) 628-5000

- Development and modeling of all-solid optical switching devices based on films of electrochromic and other identified candidate materials in a generic electrochemical structure.

184. Holographic Diffractive Structures for Enhanced Daylighting - DOE Contact M. M. Jenior, (202) 586-2998, FTS 896-2998; Advanced Environmental Research Group Contact R. Ian-Frese, (617) 864-4982

- Develop a low-cost holographic diffractive structure (HDS) system that maximizes the utilization of sunlight for daylighting.

Materials Properties, Behavior, Characterization or Testing

185. Desiccant Concepts - DOE Contact J. Goldsmith, (202) 586-8779, FTS 896-8779; SERI Contact A. Pesaran, (303) 231-7636, FTS 327-7636

- Investigate the effect of pollutants abundant in residential areas on solid desiccant materials for dehumidifiers that may reduce their performance for solar air conditioning applications.

186. Advanced Desiccant Materials Research - DOE Contact J. Goldsmith, (202) 586-8779, FTS 896-8779; SERI Contact A. Czanderna, (303) 231-1240, FTS 327-1240

- Determine how the desired sorption performance of advanced desiccant materials can be predicted by understanding the role of their surface phenomena and materials modifications.

- Identify a next generation, low-cost material with which solar radiation or heat from another low-cost energy source can be used for regenerating the water vapor sorption activity of the desiccant.

187. Open-Cycle Absorption Solar Cooling - DOE Contact J. Goldsmith, (202) 586-8779, FTS 896-8779; Arizona State University Contact B. Wood, (602) 965-7298

- Identify a suitable mixture of absorbent-refrigerant pairs for use in a high performance open-cycle absorption system.

- Perform experiments to determine crystallization concentrations as a function of temperature.

- Develop equations for calculating the thermophysical properties of various solutions.

188. Solar Cooling Research Facility - DOE Contact M. Lopez, (415) 273-4264; Florida Solar Energy Center Contact S. Chandra, (305) 783-0300

- Identify the utility and application of desiccant materials in buildings.

- Develop innovative materials and systems.

189. Core Daylighting System Design - DOE Contact M. M. Jenior, (202) 586-2998, FTS 96-2998; LBL Contact S. Selkowitz, (415) 486-5064, FTS 451-5064

- Identify, develop, and characterize light guide materials and systems for collecting and transmitting sunlight and daylight within buildings to reduce electric lighting requirements.

190. Advanced Evacuated Tubular Concentrator Research - DOE Contact J. Goldsmith, (202) 586-8779, FTS 896-8779; University of Chicago Contact J. O'Gallagher, (312) 702-7757

- Develop a manufacturable version of an advanced evacuated compound parabolic concentrator (CPC) collector that has an annual efficiency of 50 percent at temperatures up to 350°F (175°C) and is economically competitive with flat plate collectors.

191. Durability Testing Methods for Optical Switching - DOE Contact M. M. Jenior, (202) 586-2998, FTS 896-2998; SERI Contact A. W. Czanderna, (303) 231-1240

- Identify test and measurement methods that can be used to evaluate the performance and durability of electrochromic devices in glazing applications.

Solar Thermal Technology Division

The Goal of the Solar Thermal Technology Division is to increase the use of sunlight by the design and application of solar energy concentrating systems. The concentrated energy can be used for a wide variety of applications, including electricity generation, heat for industrial processes, hazardous waste detoxification, and materials treatment. The combination of broadband energy directed in an intense (to 65,000 suns) beam can cause unique and beneficial transformations of metals, alloys, ceramics, and fibers. A major new initiative is the use of concentrated solar energy for the transformation of hazardous chemical wastes to nontoxic by-products and useful chemical feedstocks.

Materials Preparation, Synthesis, Deposition, Growth or Forming

192. Silver/Polymer Reflector Research - DOE Contact Martin Scheve, (202) 586-8110; SERI Contact Paul Schissel, (303) 231-1226

- Understand degradation mechanisms in candidate polymer/silver combinations.
- Identify silvered polymers that have a useful life of 5-10 years, at least a 90 percent reflectance, and low cost.
- Modify polymers using two approaches: bulk stabilization and surface modification.
- Improve durability of polymers in solar thermal applications.

Materials Properties, Behavior, Characterization or Testing

193. Sol-Gel Protective Films for Metal Solar Mirrors - DOE Contact Martin Scheve, (202) 586-8110; SNL Contact Tom Mancini, (505) 844-8643

- Characterize the optical and mechanical properties of a variety of sol-gel derived glass films on 400 series stainless steel substrates.

- Investigate the planarizing ability of sol-gel films on stainless steel substrates.

194. High Flux Effects on Materials - DOE Contact Frank Wilkins, (202) 586-1684; GTRI Contact Joel Shutt, (404) 894-3589

- Characterize the effects of high solar flux on carbon fibers and carbon-carbon composites.

- Compare the effects on materials caused by heat only with those produced by high solar flux.

195. Surface Transformation of Metals - DOE Contact Frank Wilkins, (202) 586-1684; SERI Contact Daniel M. Blake, (303) 231-1202

- Investigate the changes in mechanical and physical properties of alloy and transition metals when exposed to high solar flux.

- Characterize the surface transformations of ceramic powders alloyed to metal substrates with high solar flux.

196. Materials for Applications in Regenerative Thermal Electrochemical Conversion (RTEC) Technology - DOE Contact Frank Wilkins, (202) 586-1684; SERI Contact Meir Carasso, (303) 231-1353

- Test graphite based materials for use in solar electrochemical energy conversion systems.

197. Catalysts for Solar-Assisted Water Detoxification - DOE Contact Frank Wilkins, (202) 586-1684; SERI Contact Daniel M. Blake, (303) 231-1202

- Characterize and enhance transition metal oxide catalysts (such as titanium dioxide) for use in solar-assisted detoxification of toxic organic pollutants in water supplies.

OFFICE OF SOLAR ELECTRIC TECHNOLOGIES

	FY 1989
Office of Solar Electric Technologies - Grand Total	$20,900,000
Photovoltaic Energy Technology Division	$20,900,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$16,000,000
Amorphous Silicon for Solar Cells	10,500,000
Polycrystalline Thin Film Materials for Solar Cells	3,500,000
Deposition of III-V Semiconductors for High-Efficiency Solar Cells	2,000,000
Materials Properties, Behavior, Characterization or Testing	$ 2,900,000
Materials and Device Characterization	2,900,000
Device or Component Fabrication, Behavior or Testing	$ 2,000,000
High-Efficiency Crystal Silicon Solar Cells	2,000,000

OFFICE OF SOLAR ELECTRIC TECHNOLOGIES

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

198. Amorphous Silicon for Solar Cells - DOE Contact Morton B. Prince, (202) 586-1725; SERI Contact Byron Stafford, (303) 231-7126

- Plasma enhanced chemical vapor deposition (CVD), thermal CVD, and sputtering techniques with goal of developing 12 percent efficient cells of area of 1000 cm^2.

199. Polycrystalline Thin Film Materials for Solar Cells - DOE Contact Morton B. Prince, (202) 586-1725; SERI Contact Kenneth Zweibel, (303) 231-7141

- Investigation of chemical and physical vapor deposition, electrodeposition, and sputtering techniques for depositing stoichiometric films of $CuInSe_2$ and CdTe.

- Large area (1000 cm^2) control of interlayer diffusion, lattice matching and stoichiometry for long-term enhancement of 15 percent efficient large area solar cells.

200. Deposition of III-V Semiconductors for High-Efficiency Solar Cells - DOE Contact Morton B. Prince, (202) 586-1725; SERI Contact John Benner, (303) 231-1396; SNLA Contact David Hasti, (505) 844-8161

- Deposition by CVD, liquid phase epitaxy (LPE), and molecular beam epitaxy (MBE) of III-V's in order to study interfaces between layers and for precise control of thickness and uniformity.

- Long-term goal of 35 percent efficient multi-junction concentrator cells and 24 percent efficient 100 cm^2 flat plate cells.

Materials Properties, Behavior, Characterization or Testing

201. Materials and Device Characterization - DOE Contact Morton B. Prince, (202) 586-1725; SERI Contact Larry Kazmerski, (303) 231-1115

- Surface and interface analysis, electro-optical characterization and cell performance evaluation.

- Critical material/cell parameters study of such things as impurities, layer mismatch and other defects using a wide variety of instruments.

Device or Component Fabrication, Behavior or Testing

202. High-Efficiency Crystal Silicon Solar Cells - DOE Contact Morton B. Prince, (202) 586-1725; SERI Contact John Benner, (303) 231-1396; SNLA Contact David Hasti, (505) 844-8161

- Investigation of new coatings and/or dopants and other treatment that reduce electron-hole recombination at cell surfaces or in the bulk.

- Research to optimize silicon material type, material resistivity, cell thickness, surface passivation, light trapping, cell metallization, and cell processing procedures.

- Study of fundamental problems of ribbon growth.

OFFICE OF RENEWABLE ENERGY TECHNOLOGIES

	FY 1989
Office of Renewable Energy Technologies - Grand Total	$1,532,000
Geothermal Technologies Division	$ 639,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 341,000
Materials for Non-Metallic Heat Exchangers	125,000
Biochemical Concentration and Removal of Toxic Components from Geothermal Wastes	216,000
Materials Properties, Behavior, Characterization or Testing	$ 298,000
Advanced High Temperature Geothermal Well Cements	190,000
Corrosion in Binary Geothermal Systems	3,000
Advanced High Temperature Chemical Systems for Lost Circulation Control	105,000
Biofuels and Municipal Waste Technology Division	$ 893,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 325,000
Medium Temperature Solid Electrolytes: Proton Conductors	200,000
Hydrogen Production with Photoactive Semiconductor Catalysts	125,000
Materials Properties, Behavior, Characterization or Testing	$ 568,000
Cold Storage of Hydrogen on Activated Carbon	100,000
Hydrogen Production via Photoelectrolysis	118,000
Novel Methods for Solar Hydrogen Production	350,000

OFFICE OF RENEWABLE ENERGY TECHNOLOGIES

Geothermal Technology Division (GTD)

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 GTD-sponsored materials R&D.

Materials Preparation, Synthesis, Deposition, Growth or Forming

203. Materials for Non-Metallic Heat Exchangers - DOE Contact R. LaSala, (202) 896-4198; BNL Contact L. E. Kukacka, (516) 282-3065

- Development of silicon carbide-filled composites for use as corrosion resistant tubes in heat exchangers used in binary geothermal processes.

204. Biochemical Concentration and Removal of Toxic Components from Geothermal Wastes - DOE Contact G. J. Hooper, (202) 896-1146; BNL Contact E. T. Premuzic, (516) 282-2893

- Analyses of biochemical techniques for concentrating and subsequent removal of toxic metals from waste.
- Establishment of optimum conditions for microorganism-metal interactions.

Materials Properties, Behavior, Characterization or Testing

205. Advanced High Temperature Geothermal Well Cements - DOE Contact R. LaSala, (202) 896-4198; BNL Contact L. E. Kukacka, (516) 282-3065

- Characterization of promising lightweight, CO_2 resistant high temperature well cements under placement and downhole environmental conditions.
- Identification of cement binders for use in the completion of magma wells.

206. Corrosion in Binary Geothermal Systems - DOE Contact R. LaSala, (202) 896-4198; BNL Contact D. van Rooyen, (516) 282-4050

- Quantitative corrosion data from plant tests for metals presently used in binary plants and other more potentially resistive metals.

207. Advanced High Temperature Chemical Systems for Lost Circulation Control - DOE Contact R. LaSala, (202) 896-4198; BNL Contact L. E. Kukacka, (516) 282-3065

- Chemical and mechanical property characterization of advanced inorganic chemical systems added to bentonite-based drilling fluids.

Biofuels and Municipal Waste Technology (BMWT) Division

The goal of the BMWT program is to conduct research that will provide the technology necessary to increase the supply of domestically available feedstocks and convert those feedstocks plus wastes to liquid and gaseous fuels. Production research concentrates on feedstocks tailored for high production rates and suitability for conversion to liquid and gaseous fuels. The program includes the research necessary to recover the feedstocks and prepare them for conversion processes. Conversion technology research will reduce the wide range of organic materials to valuable energy commodities in the form of liquid and gaseous fuels including hydrogen. The thermal processes are particularly suited to producing liquid and gaseous fuels, which are mixtures of components that may require additional upgrading, while the biochemical processes that directly produce fuel, such as ethanol energy conversion processes, are adapted especially for the intended feedstock.

Materials Preparation, Synthesis, Deposition, Growth or Forming

208. Medium Temperature Solid Electrolytes: Proton Conductors - DOE Contact M. Gurevich, (202) 586-6104; BNL Contact J. Wegrzyn, (516) 282-7917; Stanford Contact R. Huggins, (415) 723-4110

- Investigation of candidate electrolytes capable of operating in 300-600°C temperature regime.

209. Hydrogen Production with Photoactive Semiconductor Catalysts - DOE Contact M. Gurevich, (202) 586-6104; Battelle Columbus Lab Contact R. Schwerzel, (614) 424-5637

- Obtain metallized plasma-polymerized films of suitable transparency and conductivity that exhibit stable long life and are compatible with the semiconductor band gap requirements for photo-assisted electrolysis.

- Characterization of single-crystal and powdered photocatalysts using advanced coatings prior to conducting aqueous electrolysis experiments.

Materials Properties, Behavior, Characterization or Testing

210. Cold Storage of Hydrogen on Activated Carbon - DOE Contact M. Gurevich, (202) 586-6104; Syracuse University Contact J. Schwartz, (315) 423-2807

- Verify and characterize hydrogen storage on catalyzed activated carbons.
- Identify optimum carbon/catalyst system and system design features appropriate to vehicle applications.

211. Hydrogen Production via Photoelectrolysis - DOE Contact M. Gurevich, (202) 586-6104; SERI Contact A. Nozik, (303) 231-1953

- The project focuses on the development of multiphoton photoelectrolysis devices that provide high internal photovoltages to permit the splitting of water into hydrogen and oxygen or hydrogen peroxide.

212. Novel Methods for Solar Hydrogen Production - DOE Contact M. Gurevich, (202) 586-6104; SERI Contact W. Hoagland, (303) 231-7383; Center for Electrochemical Systems and Hydrogen Research, Texas A&M University Contact John Appleby, (409) 845-8281

- Project is to develop a practical photo cell that is capable of splitting water into hydrogen and oxygen with provision for separation of the two gases.

OFFICE OF ENERGY RESEARCH

	FY 1989
Office of Energy Research - Grand Total	$207,963,249
Office of Basic Energy Sciences	$187,509,348
Division of Materials Sciences	$180,746,000
Division of Engineering and Geosciences	$ 5,881,848
Materials Properties, Behavior, Characterization or Testing	$ 5,851,848
Bounds on Dynamic Plastic Deformation	129,000
Diffusion, Fluid Flow, and Sound Propagation in Disordered Media	70,380
In-Flight Measurement of the Temperature of Small, High Velocity Particles	183,000
Experimental Measurement of the Plasma/Particle Interaction	530,000
Integrated Sensor/Model Development for Automated Welding	465,000
Nondestructive Characterization of Fracture Dynamics and Crack Growth	189,000
High-Temperature Gas-Particle Reactions	130,000
Mathematical Modeling of Transport Phenomena in Plasma Systems	98,000
Multivariable Control of the Gas-Metal Arc Welding Process	161,000
Metal Transfer in Gas-Metal Arc Welding	131,000
Modeling and Analysis of Surface Cracks	199,000
Thermal Plasma Processing of Materials	0
Transport Properties of Disordered Porous Media from the Microstructure	97,000
Inelastic Deformation and Damage at High Temperature	129,400
Energy Changes in Transforming Solids	170,000

OFFICE OF ENERGY RESEARCH (Continued)

	FY 1989
Division of Engineering and Geosciences (continued)	
Materials Properties, Behavior, Characterization or Testing (continued)	
Nondestructive Testing	0
Effective Elastic Properties of Cracked Solids	57,000
Laser Diagnostics of Plasma Assisted Chemical Vapor Deposition (PACVD) Processes	185,024
Elastic-Plastic Fracture Analysis Emphasis on Surface Flaws	454,000
Continuous Damage Theory	56,000
New Ultrasonic Imaging and Measurement Techniques for NDE	258,000
Effects of Crack Geometry and Near-Crack Materials Behavior on Scattering of Ultrasonic Waves for QNDE Applications	85,450
Diffusion and Ion Transport in Multicomponent Electrolyte Solutions	140,000
Reactive Flow Modeling	100,000
Thermophysical Property Measurements in Fluid Mixtures	538,000
Flux Flow, Pinning and Resistive Behavior in Superconducting Networks	63,594
Thermodynamics of High Temperature Brines	95,000
Thermodynamic Properties of Silicate Materials	70,000
Studies of the Interactions Between Mineral Surfaces and Ions in Solutions	80,000
Thermodynamics, Kinetics, and Transport in Aqueous Electrolyte Solutions	160,000
Thermodynamic Properties of Aqueous Solutions at High Temperatures and Pressures	125,000
Solubilities of Calcite and Dolomite in Hydrothermal Solutions	100,000
Oxygen and Hydrogen Isotope Systematics of Brines	64,000
Sulfur Diffusion in Silicate Melts	50,000
Diffusion/Dispersion Transport of Chemically Reacting Species	121,000

OFFICE OF ENERGY RESEARCH (Continued)

		FY 1989
Division of Engineering and Geosciences (continued)		
Materials Properties, Behavior, Characterization or Testing (continued)		
Experimental Database and Predictive Theories for Thermodynamic Properties of Aqueous Solutions		62,000
Physical Characterization of Magma Samples		100,000
Investigations of Ultrasonic Surface Wave Interaction with Porous Saturated Rocks		55,000
Zircons and Fluids: An Experimental Investigation with Applications for Radioactive Waste Storage		60,000
PVTX Properties of Fluid Systems: $NaCl-CaCl_2-H_2O$		91,000
Materials Structure and Composition	$	30,000
Silicate Thermochemistry		30,000
Division of Advanced Energy Projects	$	881,500
Materials Preparation, Synthesis, Deposition, Growth or Forming	$	631,500
Gas Jet Deposition of Metallic, Semiconducting and Insulating Films		154,000
Growth of High Tc Superconducting Fibers Using a Miniaturized Laser-Heated Float Zone Process		477,500
Materials Properties, Behavior, Characterization or Testing	$	250,000
Production of Fuels and Chemicals From Methane		250,000

OFFICE OF ENERGY RESEARCH (Continued)

	FY 1989
Office of Fusion Energy	$ 0*
Small Business Innovation Research Program	$20,453,901**
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 9,432,020
Phase I Projects:	
Flame Synthesis of Single Crystal Diamond Films	49,865
Low Temperature Processing of High T_c Superconductor Films for Integration of Detector Arrays with Silicon Circuitry	49,900
Fabrication of Superconducting Ceramic Filaments by a Viscous Suspension Spinning Process	49,958
N-type Boron-Carbon Based Alloys	50,000
Ultrafine Filament NbTi Superconductors	49,995
Single Crystal Fibers of Bismuth Germanate for Scintillation Detectors	49,978
Development of High Performance $MoSi_2$/SiC Laminate Composites	49,895
Membranes for a Flue Gas Treatment Process	50,000
Polymer Solid Electrolytes with Specific Anion Conduction	49,914
Polymer Solid Electrolytes with Specific Cation Conduction	49,914
Radiation Hard Plastic Scintillating Optical Fiber Spinnable Thermoplastic Polyorganosiloxanes	50,000
Techniques for the Pulsed Energy Deposition of Particle-free, Ultra-smooth High-T_c Superconducting Thin Films	49,869
Highly Conducting/Irradiation Resistant Carbon-Carbon Composites for Fusion Devices	48,204

*No submission was received from the Office of Fusion Energy for FY 1989.

**Includes 42 new Phase I and 9 new Phase II projects initiated in FY 1989, and 29 Phase II projects initiated in FY 1988. The funding shown for each Phase II project is the total allocated for the duration of the project (up to two years).

OFFICE OF ENERGY RESEARCH (Continued)

	FY 1989
Materials Preparation, Synthesis, Deposition, Growth or Forming (continued)	
Phase I Projects: (continued)	
A New Technique for High Temperature Superconducting Thin Film Production: Pulsed Electron Beam Evaporation in a Plasma Environment	50,000
Thallium Bromoiodide Detectors for Scintillation Spectroscopy	50,000
Metallurgically Engineered Nb_3Sn Superconducting Wire with High J_c	49,968
Copper Infiltrated Graphite for Improved Brazed Joints	50,000
Phase II Projects: (First Year)	
Optimized Plastic Scintillating Optical Fibers with Improved Radiation Resistance for Use at the Superconducting Super Collider	500,000
A Ceramic Membrane for Gas Separations	492,660
Radiation Modified Pyroelectric Conversion Materials	499,972
The Development of Multifilamentary Superconducting Composites	500,000
Phase II Projects: (Second Year)	
High-Flux, High-Selectivity Cyclodextrin Membranes	498,790
Novel High-Flux Antifouling Membrane Coatings	294,857
Design, Fabrication, and Interface Characterization of Ceramic Fiber-Ceramic Matrix Composites	499,995
New Low Thermal Expansion Structural Ceramics	478,473
Cost Effective Techniques for Development of Radiation-Resistant Organic Insulators for Superconducting Magnets	500,000
Composite Materials with Low Z, Self-Regenerating Coatings for In-Vessel Fusion Applications	499,915
A Tritium Permeation Resistant Polymer Coating	486,224
The Development of an Economical Process for High Quality VLV SiC Whiskers	499,993
High Performance, Distributed-Tin NbSn Superconductor Wire	356,837
Advanced Insulating Coatings for Plasma Confinement Systems	499,466

OFFICE OF ENERGY RESEARCH (Continued)

	FY 1989
Materials Preparation, Synthesis, Deposition, Growth or Forming (continued)	
Phase II Projects: (continued)	
Electrically Conductive Polymers by Ion Implantation	499,280
Process Development for Producing Nb_3Sn Multifilament Superconductors of High Current Density	491,155
The Development of a Process for Making Multifilamentary NbN	486,943
Graphite Fiber Reinforced Copper Composite for Fusion Reactor Applications	500,000
Materials Properties, Behavior, Characterization or Testing	$ 1,692,050
Phase I Projects:	
Improved Energy Resolution of Mercuric Iodide Detectors by Non-Contact Polishing Processing and Scanning Photovoltage Evaluation	49,920
The Effect of Polymer Additives & Residual Elements on the Cryogenic Performance & Radiation Resistance of Insulators for High-Field Magnets	45,000
Ceramic Composite Materials for Pyrometallurgical Reprocessing	50,000
An Investigation of High Temperature Superconductor Superlattices Containing Layers of Magnetic or Nonmagnetic Metals	47,180
Phase II Project: (First Year)	
(None)	
Phase II Projects: (Second Year)	
High Thermal Conductivity Sintered AlN	499,961
High-Speed, High-Resolution Ultrasonic NDT/E of Superconducting Magnet Mono- and Multi-filamentary Wire	500,000
Optimization of Properties of Ductile Superconducting Alloys for Operation up to 10T	499,989

OFFICE OF ENERGY RESEARCH (Continued)

	FY 1989
Device or Component Fabrication, Behavior or Testing	$ 9,329,831
Phase I Projects:	
Improved Ceramic Catalyst Supports for Coal Liquefaction	50,000
Three Dimensional Braiding Technology for Preform	
Fabrication of Structural Ceramic Composite Shapes for Fossil Energy	49,951
A Low Cost Ceramic Ultrafiltration Membrane Module	49,984
Low Cost Ceramic Support for High Temperature Gas Separation Membranes	49,984
High Rate Polymer Electrolyte-Based Rechargeable Lithium Batteries	50,000
A Low Damage SiC Grating for Synchrotron Radiation by Photoelectrochemical Etching	50,000
Highly Conductive Polymer Electrolytes	49,950
Low Cost and Improved Carbon Composites for Phosphoric Acid Fuel Cells	48,328
Materials of Improved Corrosion Resistance and Oxide Ohmic Conductivity for Molten Carbonate Fuel Cells	48,877
Corrosion Resistant Catalyst Supports for Phosphoric Acid Fuel Cells	50,000
Brazing of Graphite and Carbon Composites Using Thin Film Metallization	49,755
Development of Internal Tin Nb_3Sn Conductors by Novel Manufacturing Techniques	48,840
An Improved Brazing Technique for Graphite	49,986
Improved Thin Film Multilayer Coatings for Thermal Neutron Guides	48,786
Development of Multilayer Supermirror Coatings for Neutron Guidetubes	50,000
A Position Sensitive Neutron Detector Using Boron Phosphide Semiconductor Sensors	50,000
A High Quality Ultra-Thin Crystalline Silicon-on-Insulator for Soft X-Ray and Vacuum Ultraviolet Detectors	49,967
Development of a High J_c, Large Diameter Strand for High Field Magnets	49,991

OFFICE OF ENERGY RESEARCH (Continued)

	FY 1989
Device or Component Fabrication, Behavior or Testing (continued)	
Phase I Projects: (continued)	
High Strength, High Conductivity Plates for Application in the Compact Ignition Tokamak	49,973
Superconducting Current Leads Using High Temperature Superconductors	49,968
Corrosion Resistant Carbons for Air Cathodes in Phosphoric Acid Fuel Cells	50,000
Phase II Projects: (First Year)	
Large Area Hydrogenated Amorphous Silicon Thin Film Particle Detectors	496,222
Ultra High Resistivity Silicon Crystals for Radiation Detectors	467,558
A Laser Surface Profilometer for Steep Aspheric Surfaces	496,452
A Non-Contacting Dimensional Profiler	494,632
The Development of Method for Greatly Increasing the Count-Rate Capability and Endurance for Position-Sensitive Detector Systems	494,335
Phase II Projects: (Second Year)	
Research and Development of Multisegment Ceramic Ring Cryogenic Seals	489,634
Gate Valves for Fusion Applications	500,000
Continuous Casting of Metallic Nuclear Fuel Rods	491,018
Miniature Electromagnetic Bearings for Cryogenic Applications	499,893
Advanced Abrasive-Waterjet Techniques for Decontamination and Decommissioning of Nuclear Facilities	473,651
Non-Noble Metal Catalysts for Metal-Air or Fuel Cell Cathodes	494,430
High Energy Density Composite Flywheels for Space-Based Energy Storage Systems	454,917
Using Porous Metals for Vapor Liquid Separation in Liquid Metal Rankine Cycle Space Power Systems	497,500

OFFICE OF ENERGY RESEARCH (Continued)

	FY 1989
Device or Component Fabrication, Behavior or Testing (continued)	
Phase II Projects: (Second Year) (continued)	
The Development of Shielded X-Ray Plasma Diagnostic Detectors for High Radiation Backgrounds	499,740
Optically Enhanced Multijunction Thin-Film Silicon-Hydrogen Solar Cells	462,515
The Effect of Different Levels of Manganese on Mechanical Properties and Coupling	478,875
Advanced Heat Pipe Technology for AVLIS Processes	494,119

OFFICE OF ENERGY RESEARCH

The Director of Energy Research is responsible for three major outlay programs: Basic Energy Sciences, High Energy and Nuclear Physics, and Magnetic Fusion Energy. The Director of Energy Research also advises the Secretary on DOE physical research programs, university-based education and training activities, grants, and other forms of financial assistance. The Director also carries out additional duties assigned to the Office related to basic and advanced research, and monitors the well-being and management of the multiprogram laboratories under the jurisdiction of the Department.

Four multiprogram and seven single-purpose laboratories are administratively assigned to the Office of Energy Research. The multiprogram facilities are Argonne National Laboratory, Oak Ridge National Laboratory, Brookhaven National Laboratory, and Lawrence Berkeley Laboratory. The single-purpose or specialized laboratories are the Bates Linear Accelerator Facility at the Massachusetts Institute of Technology, the Ames Laboratory at the Iowa State University, the Fermi National Accelerator Laboratory, the Notre Dame Radiation Laboratory, the Princeton University Plasma Physics Laboratory, the Michigan State University Plant Research Laboratory, and the Stanford Linear Accelerator Center. The multiprogram laboratories conduct significant research activities for other DOE programs (Conservation, Nuclear, etc.) and other Federal agencies, while the seven specialized laboratories are funded almost totally by the Office of Energy Research.

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

- Office of Health and Environmental Research: Division of Physical and Technologies Research

- Office of Fusion Energy

- Small Business Innovation Research Program

Office of Basic Energy Sciences

Division of Materials Sciences

This basic research program has several roles. One is to increase the understanding of materials properties, behavior, and phenomena in those classes of materials that either presently or in the future might be important to the mission of the Department of Energy. Another concerns the development of new forefront analytical instruments and facilities that are used to probe the structure and behavior of matter. Thus this program carries a major responsibility for many of the nation's premier research facilities including several neutron sources, a synchrotron radiation source, processing facilities, and frontier electron microscopes. Some of the materials research has a specific relationship to an identified energy technology (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, high temperature structural metals and ceramics); and some is important to fundamental understanding of new experimental and theoretical research tools.

This research is conducted at DOE laboratories, universities, and to a lesser extent at industrial laboratories by metallurgists, ceramists, solid state physicists, and materials chemists in about 100 different institutions.

There are three subprograms:

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

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

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

The operating funds for FY 1989 for the Division of Materials Sciences were $180,746,000. This was allocated to 434 projects. Many projects cross the traditional categories and, for example, involve property-structure relationships. Nevertheless, the approximate funding distribution for FY 1989 was:

	$ (Millions)
Materials Preparation, Synthesis, Deposition, Growth or Forming	20.2
Materials Structure and Composition	26.5
Materials Properties, Behavior, Characterization or Testing	78.0
Device or Component Fabrication, Behavior or Testing	--
Facilities	56.0

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) 353-5822.

The BES Geosciences Research Program supports research that is fundamental in nature and of long-term relevance to one or more energy technologies, national security, energy conservation, or the safety objectives of the Department of Energy. It is also concerned with the extraction and utilization of such resources in an environmentally acceptable way. The purpose of this program is to develop geoscience or geosciences-related information relevant to one or more of these Department of Energy objectives or to develop the broad, basic understanding of geoscientific 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 George A. Kolstad, (301) 353-5822.

Materials Properties, Behavior, Characterization or Testing

213. Bounds on Dynamic Plastic Deformation - DOE Contact Oscar P. Manley, Contact (301) 353-5822; Argonne National Laboratory Contact C. K. Youngdahl, (312) 972-6149

   - Devise load characterization parameters using weighted integrals of time-space distributions without requiring detailed numerical analysis.

214. Diffusion, Fluid Flow, and Sound Propagation in Disordered Media - DOE Contact Oscar P. Manley, (301) 353-5822; Boston University Contact Thomas Keyes, (617) 353-4730

   - Apply modern nonequilibrium statistical mechanics methods to transport with large disorder.
   - Calculate transport coefficients, correlation functions and lattice vibrations in several disordered systems.

215. In-Flight Measurement of the Temperature of Small, High Velocity Particles - DOE Contact Oscar P. Manley, (301) 353-5822; Idaho National Engineering Laboratory Contact J. R. Fincke, (208) 526-2031

   - Measure particle temperatures and sensitivities while electrodynamically suspended.
   - Develop analog and digital signal processing techniques for in-flight property evaluation.
   - Application of developed techniques to measure particle temperatures in a high-temperature plasma.

216. Experimental Measurement of the Plasma/Particle Interaction - DOE Contact Oscar P. Manley, (301) 353-5822; Idaho National Engineering Laboratory Contacts C. B. Shaw, 208-526-8818, S. C. Snyder, (208) 526-1507 and L. D. Reynolds, (208) 526-8335

   - Describe, quantitatively, the heat, mass, and momentum transfer with metallic or oxide particles in thermal plasmas.
   - Use experimental results to validate and correct theoretical models for plasma processing and for optimal torch and fixture design.

217. Integrated Sensor/Model Development for Automated Welding - DOE Contact Oscar P. Manley, (301) 353-5822; Idaho National Engineering Laboratory Contacts H. B. Smartt, (208) 256-8333 and J. A. Johnson, 208-526-9021

- Develop model of gas metal arc welding process suitable for real-time process control

- Develop optical sensing capability to provide weld-bead geometry data.

218. Nondestructive Characterization of Fracture Dynamics and Crack Growth - DOE Contact Oscar P. Manley, (301) 353-5822; Idaho National Engineering Laboratory Contact J. A. Johnson, (208) 526-9021

- Develop instrumentation and models to measure and predict interaction between ultrasound and growing cracks in engineering materials.

- Investigate methods of sensing properties of growing cracks.

219. High-Temperature Gas-Particle Reactions - DOE Contact Oscar P. Manley, (301) 353-5822; MIT Contacts J. F. Eliott, (617) 253-3305 and P. P. Bolsaitis, (617) 253-5069

- Examine the physicochemical behavior of industrial organic particles in conditions simulating exposure to arc plasmas.

220. Mathematical Modeling of Transport Phenomena in Plasma Systems - DOE Contact Oscar P. Manley, (301) 353-5822; MIT Contact J. Szekely, (617) 253-3305

- Develop a comprehensive mathematical representation of the electromagnetic force field, velocity field, temperature field, and chemical composition of plasma flames, together with their interaction with solid particles.

221. Multivariable Control of the Gas-Metal Arc Welding Process - DOE Contact Oscar P. Manley, (301) 353-5822; MIT Contact David E. Hardt, (617) 253-2429

- Cast the GMAW process into its most general sense and examine the use of multivariable control methods.

222. Metal Transfer in Gas-Metal Arc Welding - DOE Contact Oscar P. Manley, (301) 353-5822; MIT Contact T. W. Eagar, (617) 253-3229

- Develop sensing and control methods for gas-metal arc welding processes
- Model forces controlling metal transfer.

223. Modeling and Analysis of Surface Cracks - DOE Contact Oscar P. Manley, (301) 353-5822; MIT Contacts David M. Parks, (617) 253-0033 and F. A. McClintock, (617) 253-2219

- Analyze ductile crack initiation, growth, and instability in part-through surface-cracked plates and shells.

224. Thermal Plasma Processing of Materials - DOE Contact Oscar P. Manley, (301) 353-5822; University of Minnesota Contact E. Pfender, (612) 625-6012

- Develop and diagnose a new plasma reactor to solve problems of particle injection, particle confinement, and particle dwell times.

225. Transport Properties of Disordered Porous Media from the Microstructure - DOE Contact Oscar P. Manley, (301) 353-5822; North Carolina State University Contact S. Torquato, (919) 737-2365

- Develop quantitative relationship between properties of a disordered porous medium and its microstructure.

226. Inelastic Deformation and Damage at High Temperature - DOE Contact Oscar P. Manley, (301) 353-5822; Rensselaer Polytechnic Institute Contact Erhard Krempl, (518) 266-6432

- Characterize material behavior in mathematical forms for use in inelastic stress and life prediction.
- Develop a finite element program to calculate, directly, the life-to-crack initiation of a component under a given load history.

227. Energy Changes in Transforming Solids - DOE Contact Oscar P. Manley, (301) 353-5822; Stanford University Contacts George Herrmann, David M. Barnett, (514) 723-4143

- Generalize configurational forces in deformable solids to characterize state changes accompanied by energy changes.

228. Nondestructive Testing - DOE Contact Oscar P. Manley, (301) 353-5822; Stanford University Contact G. S. Kino, (415) 497-0205

- Develop techniques for contactless nondestructive testing and range sensing in air.

229. Effective Elastic Properties of Cracked Solids - DOE Contact Oscar P. Manley, (301) 353-5822; Tufts University Contact Mark Kachanov, (617) 628-5000, ext. 2821

- Evaluate elastic properties of solids with cracks including effects of crack location and density.

230. Laser Diagnostics of Plasma Assisted Chemical Vapor Deposition (PACVD) Processes - DOE Contact Oscar P. Manley, (301) 353-5822; United Technologies Research Center Contact W. C. Roman, (203) 727-7590

- Diagnose nonequilibrium reactive plasma.

- Application of PACVD processes to hard face coatings.

231. Elastic-Plastic Fracture Analysis Emphasis on Surface Flaws - DOE Contact Oscar P. Manley, (301) 353-5822; Idaho National Engineering Laboratory Contact W. G. Reuter, (208) 526-0111

- Improve design and analytical techniques for predicting the integrity of flawed structural components.

- Experimental research with analytical evaluation guiding the direction of experimental testing. Tests are conducted on a modified ASTM A-710 material exhibiting a range of fracture toughness but essentially constant yield and ultimate tensile strength.

- Use of metallographic techniques to measure crack tip opening displacement for comparison with analytical models. Laser interferometry and infrared thermography will be used to evaluate and quantify the deformation in the crack region.

232. Continuous Damage Theory - DOE Contact Oscar P. Manley, (301) 353-5822; Arizona State University Contact D. Krajcinovic, (602) 965-8656

- Phenomenological description of the nucleation and growth of microdefects in a metallic solid and their influence on the mechanical response.

- Investigation of the interaction of fiscuous effects (reflecting boundary slip) and the brittle effects (growth of microcracks). Problems in creep rupture and fatigue will be considered using the continuum damage model developed.

233. New Ultrasonic Imaging and Measurement Techniques for NDE - DOE Contact Oscar P. Manley, (301) 353-5822; Ames Laboratory, Iowa State University Contact: D. O. Thompson, (515) 294-5320

- Demonstrate a composite multiviewing NDE transducer.

- Approach uses recent advances in ultrasonic scattering and inversion theories.

- Reconstruction protocol fits acquired data to an "equivalent" ellipsoid (3 axes and 3 angles).

234. Effects of Crack Geometry and Near-Crack Materials Behavior on Scattering of Ultrasonic Waves for QNDE Applications - DOE Contact Oscar P. Manley, (301) 353-5822; Northwestern University Contact J. D. Achenbach, (312) 491-5527

- Application of the scattered field approach to the detection of a cracklike flaw, and to the determination of its location, size, shape and orientation. Interior, as well as surface-breaking and near-surface cracks, are considered.

- Mathematical modeling of ultrasonic wave scattering by cracks adjusted to account for several typical characteristics of fatigue and stress-corrosion cracks, and the environment of such cracks.

- Investigation of local anisotropy and inhomogeneity due to near-tip voids and the effect of a zone of plastic deformation near a crack tip.

235. Thermophysical Property Measurements in Fluid Mixtures - DOE Contact Oscar P. Manley, (301) 353-5822; National Institute of Standards and Technology Contacts R. Kayser, (301) 975-2483 and J. M. H. Sengers, (301) 975-2463

- Develop accurate measurement capabilities for the thermophysical properties of complex, multiphase fluid mixtures containing hydrocarbons.

236. Flux Flow, Pinning and Resistive Behavior in Superconducting Networks - DOE Contact Oscar P. Manley, (301) 353-5822; University of Rochester Contact S. Teitel, (716) 275-4039

- Numerical simulations of finite temperature current carrying networks to provide a characterization of vortex response in non-equilibrium situations.

237. Thermodynamics of High Temperature Brines - DOE Contact George A. Kolstad, (301) 353-5822; Lawrence Berkeley Laboratory Contact K. S. Pitzer, (415) 642-3472

- Theoretical and experimental studies of the thermodynamic properties of aqueous electrolytes at high temperatures.

- Heat capacities and heats of mixing are being measured to temperatures exceeding 300°C and pressures to 1 kbar.

- Equations have been developed for the near critical and supercritical properties of $NaCl$-H_2O.

238. Thermodynamic Properties of Silicate Materials - DOE Contact George A. Kolstad, (301) 353-5822; Lawrence Berkeley Laboratory Contact D. A. Snyder, (415) 642-2577

- High temperature thermodynamic properties of silicate liquids are being measured as a function of composition.

- Measurements of the effect of temperature and oxygen fugacity on the ferri/ferrous iron ratio in natural liquids and liquids in the systems Na_2O-FeO-Fe_2O_3-SiO_2 and CaO-FeO-Fe_2O_3-SiO_2 have been combined with acoustic measurements to derive compressibilities.

239. Studies of the Interactions Between Mineral Surfaces and Ions in Solution - DOE Contact George A. Kolstad, (301) 353-5822; Lawrence Berkeley Laboratory Contact D. L. Perry, (415) 486-4819

- Use of fluorescence techniques, together with synchrotron radiation to probe surface/solution interface reactions between galena (PbS) and copper (II) and chromium (VI) aqueous solutions.

- Focus is on understanding of reduction chemisorption of a metal ion from solution as a function of parameters such as pH, ion concentrations, temperature and pressure.

240. Thermodynamics, Kinetics, and Transport in Aqueous Electrolyte Solutions - DOE Contact George A. Kolstad, (301) 353-5822; Lawrence Livermore National Laboratory Contact D. G. Miller, (415) 422-8074

- Measurement of diffusion coefficients for aqueous solutions at 25°C using optical interferometry. Systems studied include brine salts and mixtures of NaCl with $SrCl_2$ and with $MgCl_2$.

- Measurement of osmotic/activity coefficients and solubilities for a variety of aqueous electrolytes and their mixtures up to saturation or supersaturation at 25°C.

241. Thermodynamic Properties of Aqueous Solutions at High Temperatures and Pressures - DOE Contact George A. Kolstad, (301) 353-5822; Los Alamos National Laboratory Contact P. S. Z. Rogers, (505) 667-1765

- Determination of the activity coefficients of geochemically important ionic species in aqueous solutions.

- Measurement of heat capacities of concentrated electrolyte solutions to 673 K and 40 MPa with an automated flow calorimeter. Work to date on $NaCl$-Na_2SO_4-H_2O, $NaOH$-H_2O and Na_2CO_3-$NaHCO_3$-$NaCl$-H_2O to 39 MPa and 598 K.

242. Solubilities of Calcite and Dolomite in Hydrothermal Solutions - DOE Contact George A. Kolstad, (301) 353-5822; Oak Ridge National Laboratory Contact D. R. Cole, (615) 574-5473

- Determination of equilibrium constants for the principal reactions that control the solubility of dolomite and calcite in hydrothermal solutions. Co-solubility approach is used; equal molar proportions of dolomite and calcite are reacted with aqueous solutions with CO_2 concentrations varying from 0.04 to 2.3 m and ionic strengths less than 0.03.

243. Oxygen and Hydrogen Isotope Systematics of Brines - DOE Contact George A. Kolstad, (301) 353-5822; Oak Ridge National Laboratory Contact D. J. Wesolowski, (615) 574-6903

- Study of D/H ratio of water vapor in $NaCl-H_2O$ at 100°C and seven salinities ranging from 0 to 5.5 molal NaCl.

- Results suggest a small but fundamental change in the nature of bonding or the ratios of "free" versus "hydrated" water molecules in brines as temperature increases. This can lead to gross changes in the interpretation of isotopic data from natural systems.

244. Sulfur Diffusion in Silicate Melts - DOE Contact George A. Kolstad, (301) 353-5822; Oak Ridge National Laboratory Contact D. R. Cole, (615) 574-5473

- Determination of sulfur diffusivities in three compositionally different silicate melts.

- Diffusion coefficients are remarkably similar despite compositional differences.

- Reducing experimental conditions resulted in slightly higher diffusion coefficients for both high- and low-silica melts.

245. Diffusion/Dispersion Transport of Chemically Reacting Species - DOE Contact George A. Kolstad, (301) 353-5822; University of California, Berkeley Contact H. C. Helgeson, (415) 642-1251

- Project goal is quantitative understanding of chemical mass transport attending fluid flow and water-rock interaction in geochemical processes.

- Molal stepwise dissociation constants for triple ions of 14 alkali metal halides were computed for temperatures from 400 to 800°C at pressures from 500 to 4000 bars, indicating that triple ions predominate in low-pressure supercritical aqueous solutions at total concentrations $\geq$1.0 m.

246. Experimental Database and Predictive Theories for Thermodynamic Properties of Aqueous Solutions - DOE Contact George A. Kolstad, (301) 353-5822; University of Delaware Contact R. H. Wood, (302) 451-2941

- Measurements of apparent molar heat capacity of aqueous solutions of H_2S, CO_2 and CH_4 at twelve temperatures from 25 to 450°C and at pressure near 350 bar.
- Measurement of apparent molar volume of same solutions at same temperatures and two different pressures.
- Investigation of theoretical models capable of representing these data and extrapolating them to higher temperatures and pressures.

247. Physical Characterization of Magma Samples - DOE Contact George A. Kolstad, (301) 353-5822; University of Hawaii at Manoa Contact M. H. Manghnani, (808) 948-7825

- Application of ultrasonic interferometry to measure velocity and attenuation in natural and synthetic silicate melts.
- Investigation of interrelationships between physical, elastic and anelastic, and thermodynamic properties of silicate melts.
- Development of a Brillouin scattering technique for measuring the elastic and anelastic properties of melts.

248. Investigations of Ultrasonic Surface Ware Interaction with Porous Saturated Rocks - DOE Contact George A. Kolstad, (301) 353-5822; Ohio State University Contact L. Adler, (614) 292-1974

- Investigation of the interaction of ultrasonic waves with fluid-saturated porous solids.
- Numerical calculations of energy transmission and reflection coefficients for interface formed by two porous media with different porosities. Demonstration that the reflected or transmitted slow wave is strongly affected by pore interface conditions.
- Theoretical and experimental investigation of leaky Lamb wave interaction with a fluid-saturated porous plate.

249. Zircons and Fluids: An Experimental Investigation with Applications for Radioactive Waste Storage - DOE Contact George A. Kolstad, (301) 353-5822; Virginia Polytechnic Institute and State University Contact A. K. Sinha, (703) 231-5580

- Study of the relationship between hydrothermally induced mobility of uranium and lead isotopes and the chemical and mechanical properties of small populations of zircons ($ZrSiO_4$).

- Demonstrated removal of 30-40 percent of uranium from the zircon by treatment with 2M NaCl, as compared with less than 10 percent by treatment with 2 percent HNO_3.

250. PVTX Properties of Fluid Systems: $NaCl$-$CaCl_2$-H_2O - DOE Contact George A. Kolstad, (301) 353-5822; Virginia Polytechnic Institute and State University Contact R. J. Bodnar, (703) 961-7455

- Goal is to accurately and completely determine the PVTX properties of geologically important fluid systems over the complete range of conditions relevant to the Earth's crust.

- Completed studies of $NaCl$-H_2O and $NaCl$-KCl-H_2O. Near completion for $NaCl$-H_2O-CO_2. Planned studies of phase equilibria and volumetric properties of $NaCl$-$CaCl_2$-H_2O.

Materials Structure and Composition

251. Silicate Thermochemistry - DOE Contact George A. Kolstad, (301) 353-5822; Princeton University Contact A. Navrotsky, (609) 452-4674

- Examination of the effects of the charge coupled substitution $Si^{4+} = T^{3+}Na^{1+}$ (T - Al, B, Fe and Ga) on the overall stabilization of framework silicate glasses in the systems $xNaTO_2$-$(1-x)SiO_2$.

- Development of a technique for solution calorimetry of oxides of highly charged cations in molten $2PbO \cdot B_2O_3$. Measurement of thermodynamic mixing properties of glasses of the system K_2O-SiO_2-La_2O_3.

- Investigation of the structural and thermodynamic effects of aluminum substitution on tri-octahedral Fe-free micas.

Division of Advanced Energy Projects

Materials Preparation, Synthesis, Deposition, Growth or Forming

252. Gas Jet Deposition of Metallic, Semiconducting and Insulating Films - DOE Contact Walter M. Polansky, (301) 353-5995; Schmitt Technology Associates Contact Bret Halpern, (203) 432-4376

- Deposition of films by "seeding" atoms or molecules into a free jet expansion, e.g., of helium, and directing the jet at a substrate at relatively high pressure.
- Fundamentals of gas jet deposition being explored, in particular its high rate and impact energy control.

253. Growth of High T_c Superconducting Fibers Using a Miniaturized Laser-Heated Float Zone Process - DOE Contact Walter M. Polansky, (301) 353-5995; Stanford University Contact Robert S. Feigelson, (415) 723-4007

- Evaluate the laser-heated pedestal growth method for the preparation of wires using copper-oxide ceramic high temperature superconductors.
- Emphasize bismuth-containing compounds.

Materials Properties, Behavior, Characterization or Testing

254. Production of Fuels and Chemicals From Methane - DOE Contact Walter M. Polansky, (301) 353-5995; Argonne National Laboratory Contact Victor A. Maroni, (312) 972-4547

- Novel bifunctional catalyst materials are being developed that can convert methane into fuels and industrial chemicals under moderate conditions of temperature and pressure.
- The types of catalysts under investigation are molecular sieve materials that are incorporated with transition metals having unique oxidation state chemistries and coordination geometry.

Office of Health and Environmental Research

The Office of Health and Environmental Research supports a broad multidisciplinary program in basic and applied life sciences research for the purpose of achieving a comprehensive understanding of the health and environmental effects associated with energy technologies. Research is conducted to characterize and measure energy-related hazards, study transport and transformations in the environment, determine the biological and ecological response and define the potential impact on human health. In addition, new applications of nuclear science and energy technologies are developed for use in the diagnosis and treatment of human disease. Material interests are primarily in development of sensors for radiation and chemical detection.

This Office sponsored no materials research in FY 1989.

Office of Fusion Energy*

The main goal of the magnetic fusion program is to establish the scientific and technological base required for an assessment of the feasibility of fusion energy. The strategy for providing this scientific and technological base is two-fold: (1) maintenance of a domestic R&D program that covers the necessary range of fusion science and technology adequately, and (2) use of international collaboration to advance the program in a timely way, especially through joint projects.

The work that must be accomplished to reach the program goal can be summarized by defining four key technical issues. The issues are associated with determining the properties of burning plasmas, improving magnetic confinement systems, formulating fusion materials and developing fusion nuclear technology. These issues have been agreed to by the Economic Summit Member's Fusion Working Group as the focus for planning future international research facilities. The U.S. program research on these issues constitutes the basis for participation in the world fusion program including participation in the four part ITER Design with the European community, Japan and the Soviet Union.

The third key issue is of specific relevance to this report. It addresses the identification and testing of materials for fusion systems. Not only is materials research vital to a successful experimental fusion program today but it is also the key to realizing the benefits of fusion. Materials play a central role in determining the environmental characteristics of a fusion reactor. Achievement of the program goal requires the development of new materials to enhance the economic and environmental potential of fusion. As part of the program's international strategy, this issue is being pursued through cooperative agreements which provide significant foreign contributions toward the operation of U.S. research facilities.

*No submission was received from the Office of Fusion Energy for FY 1989.

Small Business Innovation Research Program

The Small Business Innovation Research (SBIR) program was established in compliance with the Small Business Innovation Development Act of 1982, Public Law 97-219. 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 are limited to $50,000. Phase II is the principal research or research and development effort, and awards can be as high as $500,000 for work to be performed in periods of up to two years. Under Phase III, commercial applications of the research or research and development are to be pursued by small businesses with non-Federal capital or, alternatively, Phase III may involve follow-on non-SBIR Federal contracts for products or processes desired by the Government.

The materials-related projects, like all other projects in the DOE SBIR program, were selected using the specific evaluation criteria listed in the program solicitation. Conclusions were reached on the basis of detailed reports returned by reviewers drawn from DOE laboratories, universities, private industry, and government. In the case of Phase II, if several proposals were judged to be of approximately equal technical merit, preference was given to those proposals that had demonstrated third phase, non-Federal capital commitments.

The work supported in this program represents high-risk research, but the potential benefits are also high if the objectives are met. Brief descriptions of all DOE SBIR projects (not just those of interest in materials research) are given in the following publications: Abstracts of Phase I Awards, 1989 (DOE/ER-0417), Abstracts of Phase II Awards, 1989 (DOE/ER-0418), and Abstracts of Phase II Awards, 1988 (DOE/ER-0379). Copies of these publications may be obtained by calling Mrs. Gerry Washington on (301) 353-5867.

Materials Preparation, Synthesis, Deposition, Growth or Forming

Phase I Projects:

Flame Synthesis of Single Crystal Diamond Films - DOE Contact Jerry Smith, (301) 353-3426; Advanced Fuel Research, Inc. Contact Dr. Philip W. Morrison, Jr., (203) 528-9806

Low Temperature Processing of High T_c Superconductor Films for Integration of Detector Arrays with Silicon Circuitry - DOE Contact Walter Polansky, (301) 353-5935; Advanced Fuel Research, Inc., Contact Dr. David G. Hamblen, (203) 528-9806

Fabrication of Superconducting Ceramic Filaments by a Viscous Suspension Spinning Process - DOE Contact Walter Polansky, (301) 353-5935; HiTc Superconco, Inc., Contact Dr. Robert D. De Luca, (215) 862-9722

N-type Boron-Carbon Based Alloys - DOE Contact William J. Barnett, (301) 353-3097; Hi-Z Technology, Inc., Contact Mr. Norbert B. Elsner, (619) 535-9343

Ultrafine Filament NbTi Superconductors - DOE Contact Robert Diebold, (301) 353-5490; IGC Advanced Superconductors, Inc. Contact Dr. Hem Kanithi, (203) 753-5215

Single Crystal Fibers of Bismuth Germanate for Scintillation Detectors - DOE Contact Stanley Whetstone, (301) 353-3613; LaserGenics Corporation Contact Dr. Richard G. Schlecht, (408) 433-0161

Development of High Performance $MoSi_2$/SiC Laminate Composites - DOE Contact Jerry Smith, (301) 353-3426; Materials Technologies Corporation Contact Dr. Yogesh Mehrotra, (203) 261-5200

Membranes for a Flue Gas Treatment Process - DOE Contact Soung S. Kim, PETC, (412) 675-6007; Membrane Technology and Research, Inc. Contact Dr. Johannes G. Wians, (415) 328-2222

Polymer Solid Electrolytes with Specific Anion Conduction - DOE Contact Albert Landgrebe, (301) 353-1483; Moltech Corporation Contact Dr. Terje A. Skotheim, (516) 282-4490

Polymer Solid Electrolytes with Specific Cation Conduction - DOE Contact Albert Landgrebe, (301) 353-1483; Moltech Corporation Contact Dr. Terje A. Skotheim, (516) 282-4490

Radiation Hard Plastic Scintillating Optical Fiber Spinnable Thermoplastic Polyorganosiloxanes - DOE Contact Robert Diebold, (301) 353-5490; Nanoptics, Inc., Contact Dr. Julie P. Harmon, (904) 392-9244

Techniques for the Pulsed Energy Deposition of Particle-free, Ultra-smooth High-T_c Superconducting Thin Films - DOE Contact Walter Polansky, (301) 353-5935; Neocera Associates Contact Dr. Roger Edwards, (201) 647-2694

Highly-Conducting/Irradiation Resistant-Carbon-Carbon Composites for Fusion Devices - DOE Contact Marvin M. Cohen, (301) 353-4253; Nuclear and Aerospace Materials Corporation Contact Mr. Glen B. Engle, (619) 487-0325

A New Technique for High Temperature Superconducting Thin Film Production: Pulsed Electron Beam Evaporation in a Plasma Environment - DOE Contact Walter Polansky, (301) 353-5935; Plasma and Materials Technologies, Inc., Contact Dr. Gregor A. Campbell, (818) 841-1094

Thallium Bromoiodide Detectors for Scintillation Spectroscopy - DOE Contact Stanley Whetstone, (301) 353-3613; Radiation Monitoring Devices, Inc., Contact Dr. Michael R. Squillante, (617) 926-1167

Metallurgically Engineered Nb_3Sn Superconducting Wire with High J_c - DOE Contact Donald Beard, (301) 353-4958; Supercon, Inc., Contact Dr. Donald W. Capone II, (508) 842-0174

Copper Infiltrated Graphite for Improved Brazed Joints - DOE Contact Marvin M. Cohen, (301) 353-4253; Technical Research Associates, Inc. Contact Mr. Joseph K. Weeks, (801) 582-8080

Phase II Projects: (First Year)

Optimized Plastic Scintillating Optical Fibers with Improved Radiation Resistance for Use at the Superconducting Super Collider - DOE Contact Robert Diebold, (301) 353-5490; Bicron Corporation Contact Charles R. Hurlbut, (216) 564-2251

A Ceramic Membrane for Gas Separations - DOE Contact Dan Cicero, (304) 291-4826; CeraMem Corporation Contact Robert L. Goldsmith, (617) 489-0467

Radiation-Modified Pyroelectric Conversion Materials - DOE Contact Richard Kelley, (301) 353-3426; Chronos Research Laboratories, Inc., Contact Randall B. Olsen, (691) 455-8200

The Development of Multifilamentary Superconducting Composites - DOE Contact Walter Polansky, (301) 353-5995; EIC Laboratories, Inc., Contact Stuart F. Cogan, (617) 769-9450

Phase II Projects: (Second Year)

High-Flux, High-Selectivity Cyclodextrin Membranes - DOE Contact Robert Marianelli, (301) 353-5804; Bend Research, Inc., Contact Paul van Eikeren, (503) 382-4100

Novel High-Flux Antifouling Membrane Coatings - DOE Contact Robert Marianelli, (301) 353-5804; Bend Research, Inc. Contact Scott B. McCray, (503) 382-4100

Design, Fabrication, and Interface Characterization of Ceramic Fiber-Ceramic Matrix Composites - DOE Contact Eugene Hoffman, (615) 574-0735; Ceramatec, Inc., Contact David W. Richerson, (801) 972-2455

New Low Thermal Expansion Structural Ceramics - DOE Contact Richard Kelley, (301) 353-3426; Ceramatec, Inc., Contact Santosh Y. Limaye, (801) 972-2455

Cost Effective Techniques for Development of Radiation-Resistant Organic Insulators for Superconducting Magnets - DOE Contact Donald Beard, (301) 353-4958; Composite Technology Development Contact Maurice B. Kasen, (303) 494-8999

Composite Materials with Low Z, Self-Regenerating Coatings for In-Vessel Fusion Applications - DOE Contact Marvin Cohen, (301) 353-4253; Corium Industries, Inc., Contact Han Pak, (404) 872-5620

A Tritium Permeation Resistant Polymer Coating - DOE Contact Gene Nardella, (301) 353-4956; KMS Fusion, Inc. Contact Richard L. Crawley, (313) 769-8500

The Development of an Economical Process for High Quality VLS SiC Whiskers - DOE Contact Robert Schulz, (202) 596-8032; Materials and Electrochemical Research Corporation Contact Cheng-Tsin Lee, (602) 746-9442

High Performance, Distributed-Tin NbSn Superconductor Wire - DOE Contact Donald Beard, (301) 353-4958; Pyromet, Inc. Contact Jaydee W. Miller, (215) 497-1743

Advanced Insulating Coatings for Plasma Confinement Systems - DOE Contact Donald Beard, (301) 353-4958; Spire Corporation Contact Ward Halverson, (617) 275-6000

Electrically Conductive Polymers by Ion Implantation - DOE Contact Earle Fowler, (301) 353-4958; Spire Corporation Contact Ih-Huang Loh, (617) 275-6000

Process Development for Producing Nb_3Sn Multifilament Superconductors of High Current Density - DOE Contact Donald Beard, (301) 353-4958; Supercon, Inc., Contact James Wong, (508) 842-0174

The Development of a Process for Making Multifilamentary NbN - DOE Contact Donald Beard, (301) 353-4958; Supercon, Inc., Contact Donald Capone, (508) 842-0174

Graphite Fiber Reinforced Copper Composite for Fusion Reactor Applications - DOE Contact Marvin Cohen, (301) 353-4253; Technical Research Associates, Inc., Contact Joseph K. Weeks, (801) 582-8080

Materials Properties, Behavior, Characterization or Testing

Phase I Projects:

Improved Energy Resolution of Mercuric Iodide Detectors by Non-Contact Polishing Processing and Scanning Photovoltage Evaluation - DOE Contact Stanley Whetstone, (301) 353-3613; Advanced Research and Applications Corporation Contact Dr. L. J. Palkuti, (408) 733-7780

The Effect of Polymer Additives & Residual Elements on the Cryogenic Performance and Radiation Resistance of Insulators for High-Field Magnets - DOE Contact Donald Beard, (301) 353-4958; Composite Technology Development, Inc., Contact Dr. Naseem A. Munshi, (303) 447-2226

Ceramic Composite Materials for Pyrometallurgical Reprocessing - DOE Contact Clinton Bastin, (301) 353-5259; Materials and Electrochemical Research Corporation Contact J. C. Withers, (602) 574-1980

An Investigation of High Temperature Superconductor Superlattices Containing Layers of Magnetic or Nonmagnetic Metals - DOE Contact Jerry Smith, (301) 353-3426; Talandic Research Corporation Contact Dr. Christine Carmichael, (818) 334-3000

Phase II Project: (First Year)

(None)

Phase II Projects: (Second Year)

High Thermal Conductivity Sintered AlN - DOE Contact Richard Kelley, (301) 353-3426; Ceramatec, Inc. Contact Raymond A. Cutler (801) 972-2455

High-Speed, High-Resolution Ultrasonic NDT/E of Superconducting Magnet Mono-and Multi-filamentary Wire - DOE Contact Earle Fowler, (301) 353-4801; Sonoscan, Inc., Contact Michael G. Oravecz, (312) 766-7088

Optimization of Properties of Ductile Superconducting Alloys for Operation up to 10T - DOE Contact Earle Fowler, (301) 353-4801; Supercon, Inc. Contact T. Scott Krelick, (508) 842-0174

Device or Component Fabrication, Behavior or Testing

Phase I Projects:

Improved Ceramic Catalyst Supports for Coal Liquefaction - DOE Contact James Carr, (301) 353-6519; Aker Industries, Inc. Contact Dr. Glendon M. Benson, (415) 658-7248

Three Dimensional Braiding Technology for Preform Fabrication of Structural Ceramic Composite Shapes for Fossil Energy - DOE Contact James Carr, (301) 353-6519; Braidtech, Inc., Contact Dr. Robert A. Florentine, (215) 296-3830

A Low Cost Ceramic Ultrafiltration Membrane Module - DOE Contact Robert Marianelli, (301) 353-5804; CeraMem Corporation Contact Dr. Robert L. Goldsmith, (617) 489-0467

Low Cost Ceramic Support for High Temperature Gas Separation Membranes - DOE Contact Lisa A. Jarr, METC, (304) 291-6252; CeraMem Corporation Contact Dr. Robert L. Goldsmith, (617) 899-0467

High Rate Polymer Electrolyte-Based Rechargeable Lithium Batteries - DOE Contact Albert Landgrebe, (202) 586-1483; Covalent Associates, Inc. Contact Dr. Victor R. Koch, (617) 938-1140

A Low Damage SiC Grating for Synchrotron Radiation by Photoelectrochemical Etching - DOE Contact Jerry Smith, (301) 353-3426; EIC Laboratories, Inc., Contact Dr. Michael M. Carrabba, (617) 769-9450

Highly Conductive Polymer Electrolytes - DOE Contact Albert Landgrebe, (202) 586-1483; EIC Laboratories, Inc. Contact Dr. K. M. Abraham, (617) 769-9450

Low Cost and Improved Carbon Composites for Phosphoric Acid Fuel Cells - DOE Contact James Carr, (301) 353-6519; Energy Research Corporation Contact Dr. Larry G. Christner, (203) 792-1460

Materials of Improved Corrosion Resistance and Oxide Ohmic Conductivity for Molten Carbonate Fuel Cells - DOE Contact James Carr, (301) 353-6519; Energy Research Corporation Contact Dr. Chao-Yi Yuh, (203) 792-1460

Corrosion Resistant Catalyst Supports for Phosphoric Acid Fuel Cells - DOE Contact James Carr, (301) 353-6519; Giner,Inc. Contact Dr. John A. Kosek, (617) 899-7270

Brazing of Graphite and Carbon Composites Using Thin Film Metallization - DOE Contact Marvin M. Cohen, (301) 353-4253; Hittman Materials and Medical Components, Inc., Contact Mr. Harold N. Barr, (301) 730-7800

Development of Internal Tin Nb_3Sn Conductors by Novel Manufacturing Techniques - DOE Contact Earle Fowler, (301) 353-4801; IGC Advanced Superconductors, Inc., Contact Mr. Gennady Ozeryansky, (203) 753-5215

An Improved Brazing Technique for Graphite - DOE Contact Marvin M. Cohen, (301) 353-4253; Lintel Technology, Inc. Contact Dr. Chou H. Li, (516) 484-1719

Improved Thin Film Multilayer Coatings for Thermal Neutron Guides - DOE Contact Jerry Smith, (301) 353-3426; Opto-Line Associates, Inc. Contact Mr. John H. Bradshaw, (508) 470-3275

Development of Multilayer Supermirror Coatings for Neutron Guidetubes - DOE Contact Jerry Smith, (301) 353-3426; Ovonic Synthetic Materials Company Contact Mr. James L. Wood, (313) 326-1290

A Position Sensitive Neutron Detector Using Boron Phosphide Semiconductor Sensors - DOE Contact Jerry Smith, (301) 353-3426; Radiation Monitoring Devices, Inc., Contact Dr. Gerald Entine, (617) 926-1167

A High Quality Ultra-Thin Crystalline Silicon-on-Insulator for Soft X-Ray and Vacuum Ultraviolet Detectors - DOE Contact Charles Finfgeld, (301) 353-3423; Spire Corporation Contact Dr. Fereydoon Namavar, (617) 275-6000

Development of a High J_c, Large Diameter Strand for High Field Magnets - DOE Contact Earle Fowler, (301) 353-4801; Supercon, Inc., Contact Mr. T. Scott Kreilick, (508) 842-0174

High Strength, High Conductivity Plates for Application in the Compact Ignition Tokamak - DOE Contact Donald G. Beard, (301) 353-4958; Supercon, Inc., Contact Mr. Charles Renaud, (508) 842-0174

Superconducting Current Leads Using High Temperature Superconductors - DOE Contact Walter Polansky, (301) 353- 5935; Superconductive Components, Inc., Contact Dr. Edward R. Funk, (614) 486-0261

Corrosion Resistant Carbons for Air Cathodes in Phosphoric Acid Fuel Cells - DOE Contact James Carr, (301) 353-6519; The Electrosynthesis Company, Inc., Contact Dr. Norman L. Weinberg, (716) 684-0513

Phase II Project: (First Year)

Large Area Hydrogenated Amorphous Silicon Thin Film Particle Detectors - DOE Contact Robert Diebold, (301) 353-5490; Glasstech Solar, Inc., Contact Arun Madan, (303) 425-6600

Ultra High Resistivity Silicon Crystals for Radiation Detectors - DOE Contact Robert Diebold, (301) 353-5490; Intraspec, Inc., Contact John Walter, (615) 483-1859

A Laser Surface Profilometer for Steep Aspheric Surfaces - DOE Contact Richard Kelley, (301) 353-3426; Optra, Inc., Contact Michael Hercher, (617) 535-7670

A Non-Contacting Dimensional Profiler - DOE Contact Stanley Sobczynski, (202) 586-1878; Optra, Inc., Contact Michael Hercher, (617) 535-7670

The Development of Method for Greatly Increasing the Count-Rate Capability and Endurance for Position-Sensitive Detector Systems - DOE Contact Richard Kelley, (301) 353-3426; ORDELA, Inc., Contact Manfred K. Kopp, (615) 483-8675

Phase II Projects: (Second Year)

Research and Development of Multisegment Ceramic Ring Cryogenic Seals - DOE Contact Earle Fowler, (301) 353-4801; Aspen Systems, Inc. Contact Kang P. Lee, (617) 481-5058

Gate Valves for Fusion Applications - Radial-Directed, Fluid- Pressure-Loaded, All-Metal-Sealed Double Gates - DOE Contact T. V. George, (301) 353-4957; Batzer and Associates Contact Thomas H. Batzer, (415) 447-8804

Continuous Casting of Metallic Nuclear Fuel Rods - DOE Contact Clint Bastin, (301) 252-5259; Creare, Inc., Contact Thomas Jasinski, (603) 643-3800

Miniature Electromagnetic Bearings for Cryogenic Applications - DOE Contact Earle Fowler, (301) 4801; Creare, Inc., Contact Herbert Sixsmith, (603) 643-3800

Advanced Abrasive-Waterjet Techniques for Decontamination and Decommissioning of Nuclear Facilities - DOE Contact Henry Walter, (301) 353-5510; Flow Research Company Contact Dougles C. Echert, (206) 872-8500

Non-Noble Metal Catalysts for Metal-Air or Fuel Cell Cathodes - DOE Contact Ira Helms, (301) 353-5845; GINER, Inc., Contact S. Sarangapani, (617) 899-7270

High Energy Density Composite Flywheels for Space-Based Energy Storage Systems - DOE Contact Ira Helms, (301) 353-5845; Materials Sciences Corporation Contact Crystal H. Newton, (215) 542-8400

Using Porous Metals for Vapor Liquid Separation in Liquid Metal Rankine Cycle Space Power Systems - The Membrane Liquid Trap - DOE Contact Ira Helms (301) 353-5845; PAI Corporation Contact Robert E. MacPherson, Jr., (615) 483-0666

The Development of Shielded X-Ray Plasma Diagnostic Detectors for High Radiation Backgrounds - DOE Contact Charles Finfgeld, (301) 353-3421; Radiation Science, Inc. Contact Allen S. Krieger, (617) 494-0335

Optically Enhanced Multijunction Thin-Film Silicon-Hydrogen Solar Cells - DOE Contact Richard King, (202) 586-1693; Spectracom Contact Stephen Chad Miller, (818) 341-4087

The Effect of Different Levels of Manganese on Mechanical Properties and Coupling - DOE Contact Earle Fowler, (301) 353-4801; Supercon, Inc., Contact T. Scott Krelick, (508) 842-0174

Advanced Heat Pipe Technology for AVLIS Processes - DOE Contact Arnold Litman, (301) 353-5777; Thermacore, Inc., Contact Jerome E. Toth, (717) 569-6551

OFFICE OF NUCLEAR ENERGY

	FY 1989
Office of Nuclear Energy - Grand Total	$142,746,000
Office of Remedial Action and Waste Technology	$ 3,391,000
Division of Waste Treatment Projects	$ 3,391,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 1,641,000
Technical Support to West Valley Demonstration Project	1,641,000
Materials Properties, Behavior, Characterization or Testing	$ 1,750,000
Materials Characterization Center Testing of West Valley Formulation Glass	600,000
Development of Test Methods and Testing of West Valley Reference Formulation Glass	900,000
Process and Product Quality Optimization for the West Valley Waste Form	250,000
Office of Uranium Enrichment	$ 21,660,000
Gaseous Diffusion	
Device or Component Fabrication, Behavior or Testing	$ 6,060,000
Gaseous Diffusion: Barrier Quality	2,587,000
Gaseous Diffusion: Materials and Chemistry Support	3,473,000
Uranium-Atomic Vapor Laser Isotope Separation (U-AVLIS)	$ 15,600,000
U-AVLIS: Separator Materials	8,700,000
U-AVLIS: Uranium Processing	6,900,000

OFFICE OF NUCLEAR ENERGY (Continued)

	FY 1989
Office of Civilian Reactor Development	$ 38,865,000
Office of Advanced Reactor Programs	$ 5,315,000
Division of High Temperature Gas-Cooled Reactors	$ 5,315,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 775,000
Fuel Process Development	775,000
Materials Properties, Behavior, Characterization orTesting	$ 4,540,000
Fuel Materials Development	515,000
Fuel Development and Testing	2,500,000
Graphite Development	65,000
Graphite Development and Testing	460,000
Metals Technology Development	30,000
Structural Materials Development	800,000
Advanced Gas Reactor Materials Development	170,000
Office of Technology Support Programs (LMRs)	$ 33,550,000
Fuels and Core Materials	$ 28,300,000
Materials Properties, Behavior, Characterization or Testing	$ 28,300,000
Fuel Performance Demonstration	7,600,000
Pyroprocess Development	5,000,000
Fuel Safety Experiments and Analysis	4,000,000
Core Design Studies	4,300,000
Fuel Cycle Studies	5,300,000
LMR Technology R&D	2,100,000

OFFICE OF NUCLEAR ENERGY (Continued)

	FY 1989
Structural Materials and Design Methodology	$ 5,250,000
Materials Properties, Behavior, Characterization or Testing	$ 5,250,000
Structural Design/Life Assurance Technology (funded by JAPC)	0
Modified 9 Cr-1 Mo Steel Design Properties (funded by JAPC)	0
Nondestructive Testing Technology for Heat Exchangers	0
Nuclear Systems Materials Handbook	0
MOTA Fabrication and Operation	1,100,000
Absorber Development	700,000
FFTF Metal Fuel Testing	1,100,000
Core Demonstration Experiment (CDE)	1,600,000
International Collaboration	750,000
Office of Space and Defense Power Systems	$ 1,830,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 1,280,000
Development of Improved Thermoelectric Materials for Space Nuclear Power Systems	30,000
Development of an Improved Process for the Manufacture of DOP-26 Iridium Alloy Blanks	600,000
Carbon Bonded Carbon Fiber Insulation Manufacturing Process Development and Product Characterization	650,000
Device or Component Fabrication, Behavior or Testing	$ 150,000
Nondestructive Testing Methods Development and Application to Thermoelectric Materials and Devices	150,000

OFFICE OF NUCLEAR ENERGY (Continued)

	FY 1989
Materials Properties, Behavior, Characterization or Testing	$ 400,000
Characterization of State-of-the-Art Improved Silicon-Germanium Thermoelectric Device/Materials and Silicon-Germanium Materials Development	400,000
Office of Naval Reactors	$ 77,000,000*

*Approximate

OFFICE OF NUCLEAR ENERGY

The Office of Nuclear Energy conducts research projects in the Office of Remedial Action and Waste Technology, the Office of Uranium Enrichment, 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 Remedial Action and Waste Technology

Division of Waste Treatment Projects

The mission of the Division of Waste Treatment Projects is to facilitate development of a reliable national system for managing low-level waste and to carry out a demonstration of immobilization of high-level radioactive waste in borosilicate glass at the West Valley Demonstration Project.

Materials Preparation, Synthesis, Deposition, Growth or Forming

255. Technical Support to West Valley Demonstration Project - DOE Contact T. W. McIntosh, (301) 353-3589; PNL Contact W. A. Ross, (509) 376-3644

- Provide technical assistance for the preparation of Waste Qualification Reports for West Valley, as required for the Department's high-level waste acceptance process.
- Determine the effects of borosilicate glass composition on chemical durability and develop an empirical model to relate composition and durability.
- Chemically characterize the high-level waste sludge from tank 8D-2 at West Valley.
- Develop ion exchange media tailored for plutonium removal from liquid high-level waste and waste rinse waters.

Materials Properties, Behavior, Characterization or Testing

256. Materials Characterization Center Testing of West Valley Formulation Glass - DOE Contact H. F. Walter, (301) 353-5510; PNL Contact G. B. Mellinger, (509) 376-9318

- Fabricate and test a glass having the expected reference composition of West Valley borosilicate glass incorporating actual West Valley high-level waste.

257. Development of Test Methods and Testing of West Valley Reference Formulation Glass - DOE Contact E. A. Maestas, (716) 942-4314; CUA Contact P. B. Macedo, (202) 635-5327

- Develop methods to test borosilicate glass waste form for durability.
- Test nonradioactive and uranium/thorium containing reference waste formulation glass for the West Valley Demonstration Project.
- Study means to maximize the region of acceptable quality around the point of optimal durability for the borosilicate glass waste form.
- Prepare Waste Qualification Reports.

258. Process and Product Quality Optimization for the West Valley Waste Form - DOE Contact E. A. Maestas, (716) 942-4314; AU Contact L. D. Pye, (607) 871-2432

- Study properties and crystallization behavior of the West Valley glass composition.
- Develop methods for control of product quality during routine manufacture of the West Valley Demonstration Project waste form.
- Prepare Waste Qualification Reports.

Office of Uranium Enrichment

The Department of Energy is authorized by the Atomic Energy Act of 1954, as amended, to provide toll uranium enrichment services. Customers deliver natural uranium to one of DOE's plants and, for a fee, DOE returns material enriched to the desired level in the isotope uranium 235. The goal of the Uranium Enrichment program is to maintain this activity as a strong viable enterprise retaining a market share that preserves a long term competitive position. It is intended that these services be done for commercial and defense customers to help ensure our national and energy security in an economical, reliable, safe, secure, and environmentally acceptable manner that will also assure a reasonable recovery of the Government's investment.

Uranium as found in nature contains about 7/10ths of 1 percent uranium 235 which is fissionable. The remainder is essentially uranium 238 which is non-fissionable. The fissionable characteristics of uranium 235 make it desirable for use as nuclear fuel. To date, most nuclear reactors designed for producing electrical power require uranium 235 concentrations between 2 and 5 percent. Presently, uranium is enriched to the desired uranium 235 assay levels in gaseous diffusion plants. These plants operate on the principle that lighter weight gaseous isotopes have slightly higher average velocities and thus can be made to diffuse through a porous barrier more rapidly than heavier species. Two streams can be created, one enriched in the lighter isotope and one depleted. Because enrichment for a single cycle, or stage, is very small, a cascade of stages is required. For example, a plant constructed for producing 4 percent assay U-235 would contain about 1200 stages. Although many other methods for enrichment are still being investigated and another production technique is being used in parts of Europe, diffusion plants today provide the vast majority of the world's enrichment services. The United States' gaseous diffusion 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.

Until 1974, the United States held a virtual monopoly in the world enrichment market. Since that time, competition from foreign suppliers has reduced DOE's share of the world market to below 50 percent. The ability of foreign suppliers to penetrate DOE's previously exclusive market was due principally to significant price differences and more favorable contract terms.

The Administration and Congress have reaffirmed that the United States must be a reliable and economic source of uranium enrichment services for domestic and military purposes. As a result, in 1984 DOE announced that it was embarking on a major initiative to restore the competitive position of the United States in enrichment. The elements of the Department's initiative were designed to: stabilize DOE's market share through the issuance of a new more flexible enrichment contract; reduce prices to competitive levels; enhance DOE customer services and marketing activities; and reduce program costs in all major areas, including diffusion operations and advanced technology research and development activities. The underlying philosophy of the DOE approach was to operate the program as much like a competitive business as possible keeping in mind that an oversupply of world uranium enrichment capacity will exist well into the 1990s. Today, DOE is still the world's leader in enrichment services with competitive prices and flexible terms, but a substantial portion of operating requirements are being met or will be met in the future by spot market transactions which reflect utility interests in shorter term contracting. To this end, legislation has been introduced which could restructure the program into a government-owned corporation. The bill has been approved by the Senate and is under review by the House.

One major element in the initiative to recapture the enrichment market was the selection of the Uranium-Atomic Vapor Laser Isotope Separation (U-AVLIS) process in June 1985 as having the best potential for providing the lowest cost uranium enrichment in the future. Because the enrichment market will be dynamic for at least the next decade, the timing and extent of integration of U-AVLIS into the enrichment enterprise is being carefully evaluated.

The U-AVLIS process is based on utilizing the differences in the electronic spectra of atoms and uranium isotopes to induce the selective absorption required for isotopic separation. The process utilizes the controlled vaporization of uranium atoms from metal feed followed by selective excitation and ionization of uranium 235 using tunable lasers in the visible regions of the spectrum. The resulting plasma of uranium enriched in uranium 235 ions can then be removed from the vapor in a separator using electromagnetic methods. Collection of the metal product is as a liquid that is allowed to solidify upon withdrawal.

The Deputy Assistant Secretary for Uranium Enrichment, reporting to the Assistant Secretary for Nuclear Energy, is responsible for managing the uranium enrichment enterprises four offices: Business Operations; Marketing, Technology Deployment and Strategic Planning; Operations and Facility Reliability; and Advanced Technology Projects and Technology Transfer. The Office of Business Operations is responsible for supply policy formulation, financial management, pricing, enterprise budgets, and enrichment demand/economic analyses. The Marketing, Technology Deployment and Strategic Planning Office is responsible for enrichment service sales and contracting, marketing, and for integrating production, business, marketing and technology development into a single strategic plan for the uranium enrichment enterprise. Operations and Facility Reliability is responsible for overseeing all operations and maintenance activities of the gaseous diffusion plants including the electrical power contracts which are a major cost element. Operations and Facility Reliability assures compliance with the growing body of Federal and State environmental, health, safety and security requirements for the gaseous diffusion plants. The Office of Advanced Technology Projects and Technology Transfer is responsible for all research/development/demonstration and generation of production plant designs for U-AVLIS. This office monitors foreign enrichment technology and is the focal point for U-AVLIS security, safeguards, non-proliferation and export controls.

Revenues received by DOE for the enrichment of uranium are 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 the Revised Statutes (31 USC 484). The sum appropriated is reduced as uranium enrichment revenues are received during a fiscal year so as to result in no net fiscal year appropriations. Total obligations for all uranium enrichment activities in FY 1989 were about $1.3 billion.

Materials R&D activities within the Office of Uranium Enrichment are varied and, for the most part, classified Restricted Data. In FY 1989, approximately $21.6 million was used in these endeavors and $20.3 million is planned for FY 1990. Paragraph summaries of these activities are presented in the second part of this report. The DOE contact is A. P. Litman, (301) 353-5777.

Gaseous Diffusion

Device or Component Fabrication, Behavior or Testing

259. Gaseous Diffusion: Barrier Quality

- Studies of the short- and long-term changes in the separative capability of the diffusion barrier.

- Methods to recover and maintain barrier quality and demonstration in the production facilities.

260. Gaseous Diffusion: Materials and Chemistry Support

- Characterization of contaminant-process gas cascade reactions, physical/chemical properties of UF_6 substances, corrosion of materials, failure analyses, trapping technology, alternative materials replacement.

Uranium-Atomic Vapor Laser Isotope Separation (U-AVLIS)

261. U-AVLIS: Separator Materials

- Selection and testing of alternative candidate structural and component materials and coatings for the U-AVLIS separator system.

- Fabrication of full size components and subsystems for U-AVLIS verification tests.

262. U-AVLIS: Uranium Processing

- Bench-scale experiments and design studies on three alternatives for preparation of U-AVLIS feed from precursor oxide.

- Design of a demonstration system for U-AVLIS metal product conversion to precursor oxide for light water power reactor fuel.

- Environmental, safety and health compliance activities.

- Interaction with fuel fabricators to assure integration into the nuclear fuel cycle.

Office of Civilian Reactor Development

Office of Advanced Reactor Programs

Division of High Temperature Gas-Cooled Reactors

The objective of this division is to develop the base technology, systems concepts, and reactor designs which will permit the Government, in cooperation with utilities and private industry, to commercialize the High Temperature Gas-Cooled Reactor (HTGR). The materials interests of this division include those required for the development of coated particle fuels, graphite moderator and reflector blocks, graphite core support blocks and posts, and heat exchanger tubing and tube sheets. The DOE contact for these projects is J. E. Fox, (301) 353-3985.

Materials Preparation, Synthesis, Deposition, Growth or Forming

263. Fuel Process Development - DOE Contact J. E. Fox, (301) 353-3985; GA Technologies Contact R. F. Turner, (619) 455-2306

- Production of depleted and enriched uranium oxycarbide microspheres.
- Coating of microspheres with multiple ceramic layers of pyrolytic carbon and silicon carbide.
- Consolidation of coated fissile and fertile fuel particles into fuel rods.

Materials Properties, Behavior, Characterization or Testing

264. Fuel Materials Development - DOE Contact J. E. Fox, (301) 353-3985; GA Technologies Contact R. F. Turner, (619) 455-2306

- Development of technology base required to design, qualify, and license fuel systems for near-term steam cycle HTGRs.
- Preparation and characterization of irradiation specimens.
- Development and verification of fuel performance models.

265. Fuel Development and Testing - DOE Contact J. E. Fox, (301) 353-3985; ORNL Contact M. J. Kania, (615) 576-4856

- Fabrication, testing, and evaluation of irradiation experiments; development of post-irradiation examination equipment and methods.

- Evaluation of fuel performance and development of fission product release mechanism and models.

266. Graphite Development - DOE Contact J. E. Fox, (301) 353-3985; GA Technologies Contact R. Vollman, (619) 455-3310

- Selection, characterization, and qualification of graphite materials for application in HTGRs.

- Development of failure and design criteria.

267. Graphite Development and Testing - DOE Contact J. E. Fox, (301) 353-3985; ORNL Contact T. D. Burchell, (615) 576-8595

- Selection, characterization, and qualification of graphite materials; evaluation of high temperature corrosion resistance and mechanical properties (tensile, creep, fatigue, fracture mechanics, etc.)

- Fabrication, testing, and evaluation of irradiation experiments; development of high strength, oxidation resistant graphites with high resistance to irradiation damage.

268. Metals Technology Development - DOE Contact J. E. Fox, (301) 353-3985; GA Technologies Contact R. F. Turner, (619) 455-2306

- Characterize and qualify the metallic materials selected for application in the near-term steam cycle/cogeneration HTGR system.

- Develop base technology required for design validation and code qualifications.

269. Structural Materials Development - DOE Contact J. E. Fox, (301) 353-3985; ORNL Contact P. L. Rittenhouse, (615) 574-5103

- Selection, characterization, and qualification of high temperature alloys; evaluation of effects of exposures in simulated environments on mechanical properties (creep, fatigue, fracture mechanics).

- Development of the database and correlations required for qualification.

270. Advanced Gas Reactor Materials Development - DOE Contact J. E. Fox, (301) 353-3985; ORNL Contact O. F. Kimball, (615) 574-8258

- Testing and evaluation of high temperature alloys for effects of exposure in simulated reactor environments on mechanical properties.

- Generation of database for development of design criteria and code qualification rules for temperatures above 760°C (1400°F).

Office of Technology Support Programs (LMRs)

The applied research and development technology activities, conducted at several national laboratories, industrial organizations, universities, and through bilateral and trilateral technology programs and exchanges with foreign nations, relate to current and advanced reactor systems. The scope of these activities include the following areas: fuel cycles; design and performance of high quality core components for fuels, blanket, and control systems; development of the structural materials used in these components and systems; development and demonstration of equipment, processes, and procedures for fabricating, processing, handling, and producing mixed oxide bearing fuels, binary and ternary metal fuels, materials, and components; sodium technology; standards and quality assurance; assuring a reliable high quality economical fuel supply for LMRs; destructive and nondestructive testing, examination, and evaluation of core components and the facilities and capabilities for conducting such examinations; responsibility for engineering and supporting facilities; associated safety, safeguards, and nonproliferation; maintaining competent capabilities in the several contractor organizations that conduct the pertinent R&D activities and programs. These activities are responsive to the administration's policies and goals and, to the DOE programs that support them.

In-reactor and out-of-reactor property evaluations are being conducted on core materials, clad/ducts, fuels and absorber materials. Through irradiation testing in FFTF and EBR-II, the Technology Support Programs are developing, qualifying, and verifying the use of reference, improved and advanced mixed oxide and metal fuels and boron carbide absorbers, including full-size driver and blanket fuels, and absorber element pins and assemblies—same for carbide fuels. Fabrication development, evaluation, qualification, and verification (raw material processing, melting, hot working, cold working, and finishing) are conducted on reference, improved, and advanced alloys including in-reactor qualification of pins, ducts, and assemblies. Improved and advanced materials are being tested for use in future cores. The testing for these programs is primarily conducted at government laboratories: Argonne National Laboratory at Chicago, Illinois and Idaho Falls, Idaho; Oak Ridge National Laboratory at Oak Ridge, Tennessee; and Westinghouse Hanford Company at Richland, Washington.

Fuels and Core Materials

Materials Properties, Behavior, Characterization or Testing

271. Fuel Performance Demonstration - DOE Contact Andrew Van Echo, (301) 353-3930/FTS 233-3930; ANL Contact Leon C. Walters, (208) 526-7384/ FTS 583-7384

- Develop and demonstrate U-Pu-Zr ternary fuel clad with ferritic steel alloy HT-9 or austenitic stainless steel alloy D-9 to at least 150,000 MWD/T burnup.

272. Pyroprocess Development - DOE Contact Eli I. Goodman, (301) 353-2966/ FTS 233-2966; ANL Contact James E. Battles, (312) 972-4538/FTS 972-4538

- Develop and demonstrate a pyroprocess that includes electrorefining of binary (U-Zr) and ternary (U-Pu-Zr) metal fuel for recycle in the Integrated Fast Reactor (IFR) and process waste treatment.

273. Fuel Safety Experiments and Analysis - DOE Contact Philip B. Hemmig, (301) 353-3579/FTS 233-3579; ANL Contact John Marchaterre, (312) 972-4561/ FTS 972-4561

- Conduct TREAT tests on irradiated ternary metal fuels on U-Pu-Zr to demonstrate safety performance of metallic fuel in fast reactor systems.

274. Core Design Studies - DOE Contact Philip B. Hemmig, (301) 353-3579/ FTS 233-3579; ANL Contact D. C. Wade, (312) 972-4858/FTS 972-4858

- Conduct metallic fuel core designs for advanced innovative liquid metal reactors. Evaluate core reactivity coefficients and neutronics performance and actinide self-consumption in closed fuel cycle. Support conversion of oxide fuel core to metal fuel in EBR-II and develop optimized metal fuel core designs for advanced LMR systems.

275. Fuel Cycle Studies - DOE Contact Eli I. Goodman, (301) 353-2966/FTS 233-2966; ANL Contact M. J. Lineberry, (312) 972-7434/FTS 972-7434

- Program will develop equipment for remotized in-cell application, including reusable mold concept for injection-casting furnace, semi-automated pin processor and engineering-scale pyroprocessing equipment for the ultimate commercial fuel cycle facility design and costs.

276. LMR Technology R&D - DOE Contacts Philip B. Hemmig, (301) 353-3579/FTS 233-3579 and C. Chester Bigelow (Seismic), (301) 353-4299/FTS 233-4299; ANL Contact D. C. Wade, (312) 972-4858/FTS 972-4858

- Continue seismic analyses and test support for design. Provide test and analyses support for the ALMR mechanical components. Continue inherent safety controllability testing and analyses to demonstrate the passive safety aspects of the IFR concept and how they could be applied in the ALMR design.

Structural Materials and Design Methodology

Materials, Properties, Behavior, Characterization and Testing

277. Structural Design/Life Assurance Technology - DOE Contact Andrew Van Echo, (301) 353-3930/FTS 233-3930; ORNL Contact Jim Corum, (615) 574-0718/FTS 624-0718

- Develop the structural design methods and criteria for use of modified 9 Cr-1 Mo steel in liquid metal reactor environment. It has been closed out in FY 1989. The program is now supported under a DOE/Japanese exchange agreement, funded jointly by DOE and Japanese Atomic Power Company (JAPC).

278. Modified 9 Cr-1 Mo Steel Design Properties - DOE Contact Andrew Van Echo, (301) 353-3930/FTS 233-3930; ORNL Contact Phil Rittenhouse, (615) 574-5103/FTS 624-5103

- Conduct long-term creep-rupture tests on base metal, weldments, castings and effects of long-term (up to 10 years) thermal aging on tensile and toughness behavior of modified 9 Cr-1 Mo steel. The program is now supported under a DOE/Japanese exchange agreement, funded jointly by DOE and Japanese Atomic Power Company (JAPC).

279. Nondestructive Testing Technology for Heat Exchangers - DOE Contact Andrew Van Echo, (301) 353-3930/FTS 233-3930; ORNL Contact Donald J. McGuire, (615) 574-4835/FTS 624-4835

- Program had been conducting eddy-current and ultrasonic probes, equipment and operating procedures for use at 400 degrees Fahrenheit in liquid sodium for LMR systems for use on intermediate heat exchangers and steam generators. However, program has been phased out in FY 1989.

280. Nuclear Systems Materials Handbook - DOE Contact C. Chester Bigelow, (301) 353-4299/FTS 233-4299; ORNL Contact Martin F. Marchbanks, (615) 574-1091/FTS 624-1091

- Program was developing correlations on mechanical properties, such as creep, cyclic fatigue and effects of thermal aging on modified 9 Cr-1 Mo steel to incorporate into the NSMH. Program was phased out in FY 1988.

281. MOTA Fabrication and Operation - DOE Contact Andrew Van Echo, (301) 353-3930/FTS 233-3930; WHC Contact Ray J. Puigh, (509) 376-3766/ FTS 444-3766

- Fabricate MOTA test train and vehicle to irradiate and test materials, HT-9, Dispersion Strengthened Ferritic Steel (DSF) and others, in a controlled environment in FFTF.

282. Absorber Development - DOE Contact C. Chester Bigelow, (301) 353-4299/ FTS 233-4299, Andrew Van Echo, (301) 353-3930/FTS 233-3930; WHC Contact Alan E. Waltar, (509) 376-5514/FTS 444-5514

- Conduct, test, and evaluate irradiated absorber experiments to extend the FFTF absorber lifetimes, support Series III control rod design and update design codes CONRD and CRPBOW.

283. FFTF Metal Fuel Testing - DOE Contact Andrew Van Echo, (301) 353-3930/ FTS 233-3930; WHC Contact Alan E. Waltar, (509) 376-5514/FTS 444-5514

- Conduct metal fuel (MFF-2) irradiation testing in FFTF, transient testing in TREAT with HT-9 clad to support conversion of the ALMR from an oxide-fuel core to a binary U-Zr fuel core.

284. Core Demonstration Experiment (CDE) - DOE Contact Jacob Glatter, (301) 353-3921/FTS 233-3921; WHC Contact Alan E. Waltar, (509) 376-5514/ FTS 444-5514

- Continue CDE irradiation in FFTF to extend the fuel lifetime to 1,200 EFPD, conduct post-irradiation examination (PIE), conduct TREAT tests, and TREAT tests on pins from ACO-1 and FO-2 lead tests. Evaluate data to justify continued irradiation beyond 1,200 EFPDs.

285. International Collaboration - DOE Contact Jacob Glatter, (301) 353-3921/ FTS 233-3921; WHC Contact J. David Watrous, (509) 376-1002/FTS 444-1002

- Complete fabrication of the DSF-1 fuel test with cladding types agreed to with DOE and PNC. Monitor irradiation performance in FFTF of PNC fuel (MFA-1 and -2) and blanket (MBA-1) assemblies. Characterize production lots of MA-957 cladding. Reconstitute MOTA NAM-1 test specimens. Ship C-1 pins to PNC.

Office of Space and Defense Power Systems

The Office of Space and Defense Power Systems is responsible for the development, system safety and production of radioisotope 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

286. Development of Improved Thermoelectric Materials for Space Nuclear Power Systems - DOE Contact W. Barnett, (303) 353-3097; General Electric Co., Space Systems Division Contact P. D. Gorsuch, (215) 354-5047

- Study of Si-Ge type thermoelectric alloys. Key variables include alloy and dopant additions, processing parameters, and structure control. Goal is an average Figure of Merit, Z, of 1×10^{-3} per °C from 300-1000°C.

287. Development of an Improved Process for the Manufacture of DOP-26 Iridium Alloy Blanks - DOE Contact W. Barnett, (303) 353-3097; ORNL Contact E. K. Ohriner, (615) 574-8519

- Development of a consumable arc melt/extrusion route process for the production of DOP-26 iridium alloy sheet and foil. Improve product quality and yield and scaleup size of units processed.

288. Carbon Bonded Carbon Fiber Insulation Manufacturing Process Development and Product Characterization - DOE Contact W. Barnett, (303) 353-3097; ORNL Contact R. L. Beatty, (615) 574-4536

- Improve process control systems, optimization of process parameters, and accommodate a new type carbon fiber for the manufacture of CBCF, carbon bonded carbon-fiber thermal insulation.

Device or Component Fabrication, Behavior or Testing

289. Nondestructive Testing Methods Development and Application to Thermoelectric Materials and Devices - DOE Contact W. Barnett, (303) 353-3097; ORNL Contact B. E. Foster, (615) 574-4837

- Develop and apply state-of-the-art nondestructive examination (NDE) techniques for Si-Ge thermoelectric materials, multicouple devices and multicouple subassemblies.

Materials Properties, Behavior, Characterization or Testing

290. Characterization of State-of-the-Art Improved Silicon-Germanium Thermoelectric Device/Materials and Silicon-Germanium Materials Development - DOE Contact W. Barnett, (303) 353-3097; Iowa State University Contact B. Beaudry, (515) 294-1366

- Evaluation and characterization of state-of-the-art Si-Ge/GaP and other "improved" silicon-germanium type thermoelectric materials.

Office of Naval Reactors

The Materials Research and Development Program is in the Reactor Materials Division under the Deputy Assistant Secretary for Naval Reactors. The 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 in the high power density and long life 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 $77 million in FY 1989 including approximately $42 million as the cost for irradiation testing in the Advanced Test Reactor. The Naval Reactors contact is Robert H. Steele, (703) 557-5565.

OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT

	FY 1989
Office of Civilian Radioactive Waste Management - Grand Total	$13,513,000
Office of Systems Integration and Regulations	0*
Office of Civilian Radioactive Waste Management/ Yucca Mountain Project (OCRWM/YMP)	$13,138,000
Materials Properties, Behavior, Characterization or Testing	$ 9,806,000
Waste Package Environment	1,699,000
Waste Form Testing	2,342,000
Metal Barrier Testing	2,264,000
Other Engineered Barrier Waste Package Components	4,000
Integrated Testing	1,435,000
Waste Package: Performance Assessment	686,000
Research on Geochemical Modeling of Radionuclide Interaction with a Fractured Rock Matrix	1,376,000
Device or Component Fabrication, Behavior or Testing	$ 3,332,000
Waste Package: Design, Fabrication and Prototype Testing	1,748,000
Waste Package Environmental Field Tests	1,584,000
Sandia National Laboratories: Brittle Fracture Technology Program	$ 375,000
Materials Structure and Composition	$ 25,000
Microstructure Investigations of Nodular Cast Iron	15,000
Composition Investigation of Nodular Cast Iron	10,000

*No submission was received from this office for FY 1989.

OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT (Continued)

	FY 1989
Sandia National Laboratories: Brittle Fracture Technology Program (Continued)	
Materials Properties, Characterization, Behavior or Testing	$ 330,000
Generate Material Property Database for Nodular Cast Iron	50,000
Mosaik Brittle Fracture Test Program	75,000
Investigate Thickness Effects on Impact and Toughness Properties of Ferritic Steel	80,000
Investigate the Feasibility of Using Depleted Uranium as a Structural Component in Cask Construction	25,000
Use State-of-the-Art Data Acquisition Ductile Cast Iron Drop Test	100,000
Instrumentation and Facilities	$ 20,000
Evaluate Current NDE Methods for Applicability to Thick Section Nodular Cast Iron	20,000

OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT

Office of Systems Integration and Regulations*

Office of Civilian Radioactive Waste Managemnent/Yucca Mountain Project (OCRWM/YMP)

The primary goal of the OCRWM/YMP materials program is the development of tuff specific waste packages that meet the NRC's performance requirements. This work includes the definition of physical and chemical conditions of the site, evaluation of the package materials, waste package design and performance assessment, prototype waste package fabrication, and performance testing. (As a result of the Nuclear Waste Policy Act Amendments, the Salt Repository Project and the Basalt Waste Isolation Project were terminated effective March 1988.)

Materials Properties, Characterization or Testing

291. Waste Package Environment - DOE Contact C. P. Gertz, (702) 794-7920; LLNL Contact David Short, (415) 422-1287

- Characterize the time-dependent behavior of the hydrogeologic environment in which the waste packages will reside in order to establish the envelope of conditions that define package design parameters, materials testing conditions, and boundary conditions for performance analysis.

292. Waste Form Testing - DOE Contact C. P. Gertz, (702) 794-7920; LLNL Contact David Short, (415) 422-1287

- Perform the testing and evaluation necessary to identify the waste package components required by specific host rock and to select the materials for those components.

- Characterize the behavior of and determine the radionuclide release rates for the various waste forms in the geological tuff environment and as modified by corrosion products in the Metal Barrier Testing.

*No submission was received from this office for FY 1989.

293. Metal Barrier Testing - DOE Contact C. P. Gertz, (702) 794-7920; LLNL Contact David Short, (415) 422-1287

- Characterize the behavior of the metal barrier and determine corrosion rates and corrosion mechanisms, including the interaction between the metal barrier and its surrounding environment.

- Six austenitic phase alloys and copper/copper based alloys are being evaluated as candidate materials.

294. Other Engineered Barrier Waste Package Components - DOE Contact C. P. Gertz, (702) 794-7920; LLNL Contact David Short, (415) 422-1287

- Characterize the properties and behavior of other engineered barrier waste package components that may be present in a repository.

295. Integrated Testing - DOE Contact C. P. Gertz, (702) 794-7920; LLNL Contact David Short, (415) 422-1287

- Characterize the integrated behavior of the waste form, barrier materials, and surrounding environment.

296. Waste Package: Performance Assessment - DOE Contact C. P. Gertz, (702) 794-7920; LLNL Contact David Short, (415) 422-1287

- Provide a quantitative prediction of long-term waste package performance.

297. Research on Geochemical Modeling of Radionuclide Interaction with a Fractured Rock Matrix - DOE Contact C. P. Gertz, (702) 794-7920; LLNL Contact David Short, (415) 422-1287

- Further develop the geochemical modeling code EQ3/6 for use in long-term predictions for site suitability and radionuclide release from a nuclear waste repository.

Device or Component Fabrication, Behavior or Testing

298. Waste Package: Design, Fabrication and Prototype Testing - DOE Contact C. P. Gertz, (702) 794-7920; LLNL Contact David Short, (415) 422-1287

- Develop, analyze, fabricate, and test waste package designs that incorporate qualified materials and that are fully compatible with the repository design.
- Supports license application by demonstrating conformance with requirements for safe handling, emplacement, possible retrieval, and credible accident conditions per NRC 10 CFR 60 and EPA 40 CFR 191 in a cost-effective manner.

299. Waste Package Environmental Field Tests - DOE Contact C. P. Gertz, (702) 794-7920; LLNL Contact David Short, (415) 422-1287

- Develop and conduct field experiments designed to determine and evaluate the thermal, mechanical, thermomechanical, hydrothermal and chemical phenomena for welded tuff.
- Determine the responses of tuff to excavation of an underground facility in order to evaluate effects of the heat released by the waste on the hydrologic behavior and effects on components of the engineered barrier system.

Sandia National Laboratories: Brittle Fracture Technology Program

The objective of this program is to qualify alternate materials (other than stainless steel) for use in nuclear spent fuel cask construction. Candidate materials include nodular cast iron and ferritic steel. The main technical issue which must be addressed is the application of fracture mechanics to cask analysis and design. Materials such as nodular cast iron exhibit a ductile/brittle failure mode transition. Hence, a cask constructed out of this material may be susceptible to brittle fracture under certain environmental and loading conditions. The application of fracture mechanics can provide the cask analyst/designer the ability to guarantee ductile cask material response to design loadings.

Materials Structure and Composition

300. Microstructure Investigations of Nodular Cast Iron - DOE Contact F. Falci, (301) 353-3595; SNL Contact K. B. Sorenson, (505) 845-8431

- Investigation of the effect of microstructure on material properties.
- Study of the effect of graphite nodule size and spacing on fracture toughness.

301. Composition Investigation of Nodular Cast Iron - DOE Contact F. Falci, (301) 353-3595; SNL Contact K. B. Sorenson, (505) 845-8431

- Investigation of the effect of material composition on material properties.
- Study of the effect of material composition on fracture toughness and tensile properties.

Materials Properties, Behavior, Characterization or Testing

302. Generate Material Property Database for Nodular Cast Iron - DOE Contact F. Falci, (301) 353-3595; SNL Contact K. B. Sorenson, (505) 845-8431

- Generate a database for nodular cast iron which includes material properties pertinent to fracture mechanics.

303. Mosaik Brittle Fracture Test Program - DOE Contact F. Falci, (301) 353-3595; SNL Contact K. B. Sorenson, (505) 845-8431

- Perform a series of drop tests using a ductile cast iron cask to demonstrate a proof of principle for the fracture mechanics design approach.

304. Investigate Thickness Effects on Impact and Toughness Properties of Ferritic Steel - DOE Contact F. Falci, (301) 353-3595; SNL Contact K. B. Sorenson, (505) 845-8431

- Generate a database of nilductility (NDT) transition temperature, Charpy and fracture toughness measurements as a function of thickness.

305. Investigate the Feasibility of Using Depleted Uranium as a Structural Component in Cask Construction - DOE Contact F. Falci, (301) 353-3595; SNL Contact K. B. Sorenson, (505) 845-8431

- Investigate the feasibility of using depleted uranium (DU) as a structural component in cask body construction.

306. Use State-of-the-Art Data Acquisition for Ductile Cast Iron Drop Test - DOE Contact F. Falci, (301) 353-3595; SNL Contact K. B. Sorenson, (505) 845-8431

- The Mosaik Instrumentation Data Acquisition System (MIDAS) will be used to support data acquisition needs for drop tests being conducted in Albuquerque, New Mexico, and West Germany under DOE sponsorship.

OFFICE OF DEFENSE PROGRAMS

	FY 1989
Office of Defense Programs - Grand Total	$49,499,246
Office of Waste and Transportation Management	$ 12,746
Waste Research and Development Division*	$ 12,746
Materials Properties, Behavior, Characterization or Testing	$ 12,746
Waste Form Qualification	6,000
Immobilization/Volume Reduction/In-place Stabilization	6,746
Office of Weapons Research, Development, and Testing	$49,486,500
Weapons Research Division	$49,486,500
Sandia National Laboratories - Albuquerque	$21,064,500
Solid State Sciences Directorate, 1100	$ 8,770,000
Ion Interactions and Surface Sciences Research Department, 1110	$ 1,370,000
Materials Properties, Behavior, Characterization or Testing	$ 1,370,000
Ion Implantation Studies for Friction, Wear and Microhardness	300,000
Silicon-Based Radiation Hardened Microelectronics	670,000
Surface Science	400,000

*In November 1989, this program was transferred from Defense Programs to the new Office of Environmental Restoration and Waste Management and placed under the Office of Waste Operations.

OFFICE OF DEFENSE PROGRAMS (Continued)

	FY 1989
Sandia National Laboratories - Albuquerque (continued)	
Laser and Chemical Physics Research Department, 1120	$ 1,650,000
Materials Properties, Behavior, Characterization or Testing	$ 1,650,000
Plasma Etching	500,000
Plasma-Enhanced Chemical Vapor Deposition	100,000
Laser-Controlled Etching and Deposition of Materials	250,000
Surface Chemistry of Organometallics for Compound Semiconductor Epitaxy	300,000
Metallorganic Chemical Vapor Deposition	500,000
Compound Semiconductor and Device Research Department, 1140	$ 2,000,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 2,000,000
Materials Growth by Molecular Beam Epitaxy (MBE)	500,000
Materials Growth by MOCVD	400,000
Strained Layer Superlattices for IR Detectors	300,000
Novel Processing Technology for Semiconductor Technologies	500,000
Thin Film Superconductors	300,000

OFFICE OF DEFENSE PROGRAMS (Continued)

	FY 1989
Sandia National Laboratories - Albuquerque (continued)	
Condensed Matter Research Department, 1150	$ 3,000,000
Materials Properties, Behavior, Characterization or Testing	$ 3,000,000
Superconductivity	650,000
Shock Physics and Chemistry	500,000
Semiconductors	600,000
Surface Science	650,000
Disordered Materials	600,000
Optoelectronics and Microsensor Research Department, 1160	$ 750,000
Materials Properties, Behavior, Characterization or Testing	$ 750,000
New Concepts in Microsensors	750,000
Organic and Electronic Materials Department, 1810	$ 1,789,500
Chemistry of Organic Materials Division, 1811	$ 475,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 250,000
Sulfonated Aromatic Polysulfones	100,000
Carbon Foams	150,000
Materials Properties, Behavior, Characterization or Testing	$ 225,000
Radiation Hardened Dielectrics	100,000
Organic Nonlinear Optical Materials	125,000

OFFICE OF DEFENSE PROGRAMS (Continued)

	FY 1989
Sandia National Laboratories - Albuquerque (continued)	
Physical Chemistry and Mechanical Properties of Polymers Division, 1812	$ 555,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 130,000
Chemistry of Plasma Etching and Deposition Processes	130,000
Materials Structure and Composition	$ 425,000
Materials Structure, Dynamics, and Property Studies by Multinuclear Pulsed NMR Spectroscopy	75,000
Mechanistic and Kinetic Studies of Polymer Aging	250,000
Theory of Polymer Dynamics	100,000
Physical Properties of Polymers Division, 1813	$ 459,500
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 315,000
Microporous Foam Development	157,500
Development of Removable Encapsulants	157,500
Materials Properties, Behavior, Characterization or Testing	$ 144,500
Mechanical Properties of Encapsulants	21,000
Deformation of Kevlar Fabrics	73,500
Moisture Permeation in Encapsulants, Adhesives, and Seals	50,000

OFFICE OF DEFENSE PROGRAMS (Continued)

	FY 1989
Sandia National Laboratories - Albuquerque (continued)	
Electronic Property Materials Division, 1815	$ 300,000
Materials Properties, Behavior, Characterization or Testing	$ 300,000
Nonlinear Optical Materials	100,000
Hydrogen Effects in Silicon	100,000
Rapid Thermal Processing of Gate Oxides	100,000
Materials Characterization Department, 1820	$ 990,000
Analytical Chemistry Division, 1821	$ 250,000
Instrumentation and Facilities	$ 250,000
Development of Automated Methods for Chemical Analysis	250,000
Electron Optics and X-ray Analysis Division, 1822	$ 240,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 40,000
Thermomechanical Treatment of U Alloys	40,000
Instrumentation and Facilities	$ 200,000
Advanced Methods for Electron Optical, X-ray, and Image Analysis	200,000
Surface Chemistry and Analysis Division, 1823	$ 500,000
Instrumentation and Facilities	$ 500,000
Advanced Methods for Surface and Optical Analysis	500,000

OFFICE OF DEFENSE PROGRAMS (Continued)

	FY 1989
Sandia National Laboratories - Albuquerque (continued)	
Metallurgy Department, 1830	$ 3,115,000
Physical Metallurgy Division, 1831	$ 525,000
Materials Properties, Behavior, Characterization or Testing	$ 525,000
Analytical Electron Microscopy of Engineering Alloys	50,000
Segregation Behavior During Solidification of Alloys	100,000
Solid State Reactions Between Metal Substrates and Solders	150,000
Fluxless Soldering	75,000
Stress Voiding of Aluminum Interconnect Lines	100,000
Grain Boundary Segregation in Al-Cu Metallization Interconnect Lines	50,000
Mechanical Metallurgy Division, 1832	$ 630,000
Materials Properties, Behavior, Characterization or Testing	$ 630,000
Micromechanical Testing	100,000
Toughness of Ductile Alloys	330,000
Low Melting Point Alloy Studies	200,000
Process Metallurgy Division, 1833	$ 1,400,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 300,000
Vacuum Arc Remelting	300,000

OFFICE OF DEFENSE PROGRAMS (Continued)

	FY 1989
Sandia National Laboratories - Albuquerque (continued)	
Process Metallurgy Division, 1833 (continued)	
Device or Component Fabrication, Behavior or Testing	$ 1,100,000
Electronbeam Melting	200,000
Electroslag Remelting	300,000
Welding of Nickel-Based Alloys	250,000
Plasma Arc Welding	100,000
Laser Welding	50,000
Development of Materials for Magnetic Fusion Reactors	200,000
Surface and Interface Technology Division, 1834	$ 560,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 80,000
Development of Hard, Wear-Resistant Coatings for Mechanical Applications	80,000
Materials Properties, Behavior, Characterization or Testing	$ 190,000
Modification of Mechanical Properties by Ion Implantation	40,000
Corrosion Predictions	100,000
Solvent Substitutive Programs	50,000
Device or Component Fabrication, Behavior or Testing	$ 150,000
Process Control Ultrasonic Cleaning of Delicate Parts	70,000
Plasma Oxidation and Reduction Studies	80,000

OFFICE OF DEFENSE PROGRAMS (Continued)

	FY 1989
Sandia National Laboratories - Albuquerque (continued)	
Surface and Interface Technology Division, 1834 (continued)	
Instrumentation and Facilities	$ 140,000
Ion Beam Reactive Deposition System	50,000
Deposition and Evaluation of Titanium Nitride Films	50,000
In Situ Friction, Wear, and Electrical Contact Resistance Systems	40,000
Chemistry and Ceramics Department, 1840	$ 6,400,000
Inorganic Materials Chemistry Division, 1846	$ 6,400,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 3,800,000
Electrolytic and Electrophoretic Methods for Materials Processing	400,000
Aerosol Production of Fine Ceramic Powders	200,000
Chemically Prepared Ceramic Films for Opto-electronic Applications	1,200,000
Development of New Glasses and Glass-Ceramics	500,000
Preparation of Ceramic Powders by Chemical Techniques	1,500,000
Materials Structure and Composition	$ 400,000
Structure of Novel Glasses	250,000
Structure of Sol-Gel Films	150,000

OFFICE OF DEFENSE PROGRAMS (Continued)

	FY 1989
Sandia National Laboratories - Albuquerque (continued)	
Inorganic Materials Chemistry Division, 1846 (continued)	
Materials Properties, Behavior, Characterization and Testing	$ 1,800,000
Molecular Beam Studies of Hydrogen in Metals	400,000
Electronic Ceramics	600,000
Ceramic Fracture	300,000
Superplastic Ceramics	100,000
Reactivity and Bonding of Glasses and Ceramics to Metals	400,000
Device or Component Fabrication, Behavior or Testing	$ 400,000
Sensor Development	200,000
SAW Development	200,000
Sandia National Laboratories - Livermore	$ 4,080,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 1,100,000
Powder Metallurgy	200,000
Advanced Electrodeposition Studies	100,000
Metal Forming	200,000
Advanced Organic Materials	200,000
Particulate Technology	50,000
Tritium Getter Technology	50,000
Molded Desiccant Foam	100,000
Plasma Processing	200,000

OFFICE OF DEFENSE PROGRAMS (Continued)

	FY 1989
Sandia National Laboratories - Livermore (continued)	
Materials Properties, Behavior, Characterization or Testing	$ 2,180,000
Tritium and Decay Helium Effects on Crack Growth in Metals and Alloys	700,000
Joining Science and Technology	400,000
Composites: Characterization and Joining	150,000
Compatibility, Corrosion, and Cleaning of Materials	20,000
Tritium-Metal Interaction	350,000
Measurement of Multilayer Thin Film Structures	60,000
Helium in Metal Tritides	200,000
Analysis of Defects and Interfaces in Metals	300,000
Instrumentation and Facilities	$ 800,000
New Spectroscopy	50,000
Tritium Facility Upgrade for Materials Characterization and Testing	500,000
New Analytical Techniques	50,000
New High Resolution Electron Microscopy Facility	200,000
Lawrence Livermore National Laboratory	$ 9,131,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 2,480,000
Inorganic Aerogels	600,000
Photoactivated Catalysis on Aerogels	80,000

OFFICE OF DEFENSE PROGRAMS (Continued)

	FY 1989
Lawrence Livermore National Laboratory (continued)	
Materials Preparation, Synthesis, Deposition, Growth or Forming (continued)	
Synthesis Project (Explosives)	250,000
Synthesis and Reactivity of Transition Metal Fluorocarbon Complexes	150,000
Sputtering (Plutonium Alloys)	100,000
Organic Aerogels	200,000
Polymer Coating and Foam Development	1,000,000
Atomic Engineering	100,000
Materials Structure and Composition	$ 1,647,000
Theory of the Structure and Dynamics of Molecular Fluids	300,000
Site-Specific Chemistry Using Synchrotron Radiation	197,000
Capillary Structures (in Foams)	100,000
Plutonium Pyrochemical Research	160,000
Electronic Structure in Superconducting Oxides	290,000
Theory of Superconducting Oxides	450,000
A New Method for the Calculation of the Electronic Structure of Surfaces and Interfaces	150,000
Materials Properties, Behavior, Characterization or Testing	$ 3,874,000
Nuclear Spin Polarization	1,100,000
Measurement of Tritium Permeation Through Resistant Materials at Low Temperatures	90,000
Pretransformation Behavior in Alloys	175,000
Interfacial Bonding in Multilayer X-ray Mirrors	25,000
$\Delta N=O$ Spectroscopy Using Multilayer Gratings	152,000
Multilayer X-ray Optics Development	250,000
Thin Film X-ray Studies	80,000
In Situ Reversed Deformation Experiments	20,000

OFFICE OF DEFENSE PROGRAMS (Continued)

	FY 1989
Lawrence Livermore National Laboratory (continued)	
Materials Properties, Behavior, Characterization or Testing (continued)	
Dislocation Microstructure of Aluminum and Silver Deformed to Large Steady-State Creep	90,000
Delayed Failure of Silver-Aided Diffusion Bonds	190,000
Constitutive and Failure Behavior of Metals at High Rates of Tensile Strain	290,000
Theoretical and Experimental Studies of Solid Combustion Reactions	190,000
Fracture Behavior of Refractory Metals and Alloys in Liquid Actinides	100,000
Modeling and Experimental Measurement of Residual Stress	160,000
Failure Characterization of Composite Materials	117,000
Surface Modification to Reduce Abrasion and Friction	100,000
Numerical Modeling of Crack Growth	145,000
Interfaces, Adhesion and Bonding	600,000
Device or Component Fabrication, Behavior or Testing	$ 945,000
IC Protective Coatings	720,000
Characterization of Solid-State Microstructures in High Explosives by Synchrotron X-ray Tomography	50,000
Optical Diagnostics of High Explosives Reaction Chemistry	175,000

OFFICE OF DEFENSE PROGRAMS (Continued)

	FY 1989
Lawrence Livermore National Laboratory (continued)	
Instrumentation and Facilities	$ 185,000
Scanning Tunneling Microscope	165,000
Scanning Tunneling Microscopy (STM) and Atomic Force Microscope (AFM) as a Detector	20,000
Tritium Facility Upgrade	(11,900,000)*
Decontamination and Waste Treatment Facility (DWTF)	(7,700,000)[1]
Los Alamos National Laboratory	$15,211,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 7,638,000
Actinide Alloy Development	1,350,000
Plutonium Oxide Reduction	150,000
Ion-Beam Implantation	200,000
Electroplating Low Atomic Number Materials	100,000
Liquid Crystal Polymer Development	200,000
Surface Property Modified Plastic Components	50,000
Low-Density, Microcellular Plastic Foams	300,000
Target Coatings	400,000
Physical Vapor Deposition and Surface Analysis	700,000
Chemical Vapor Deposition (CVD) Coatings	200,000
Synthesis of Metallic Glasses	75,000
Polymers and Adhesives	803,000
Tritiated Materials	511,000
Salt Fabrication	379,000
Slip Casting of Ceramics	150,000
Whisker Growth Technology	120,000
New Hot Pressing Technology	300,000
Glass and Ceramic Coatings	40,000
Cold Pressing, Cold Isostatic Pressing and Sintering	10,000

*Line-item construction projects: not included in subtotal or total.

OFFICE OF DEFENSE PROGRAMS (Continued)

	FY 1989
Los Alamos National Laboratory (continued)	
Materials Preparation, Synthesis, Deposition, Growth or Forming (continued)	
Plasma-Flame Spraying Technology	185,000
Rapid Solidification Technology	100,000
Superplastic Forming	150,000
Microwave Sintering/Processing	120,000
Predictions of Super Strong Polymers	565,000
High Energy Storage Material	200,000
Synthesis of Ceramic Coatings	30,000
Laser Surface Treatment of Materials	250,000
Materials Structure or Composition	$ 1,112,000
Actinide Surface Properties	700,000
Neutron Diffraction of Pu and Pu Alloys	237,000
Surface, Material and Analytical Studies	175,000
Materials Properties, Behavior, Characterization or Testing	$ 3,881,000
Mechanical Properties of Plutonium and Its Alloys	450,000
Phase Transformation in Pu and Pu Alloys	450,000
Isobaric Expansion of Actinides	200,000
Plutonium Shock Deformation	350,000
Non-Destructive Evaluation	500,000
Powder Characterization	50,000
Shock Deformation in Actinide Materials	200,000
Dynamic Mechanical Properties of Weapons Materials	225,000

OFFICE OF DEFENSE PROGRAMS (Continued)

	FY 1989
Los Alamos National Laboratory (continued)	
Materials Properties, Behavior, Characterization or Testing (continued)	
Dynamic Testing of Materials for Hyper-Velocity Projectiles	280,000
Mechanical Properties	300,000
Radiation Damage in High-Temperature Superconductors	281,000
Structural and Superconducting Ceramics	595,000
Device or Component Fabrication, Behavior or Testing	$ 2,580,000
Radiochemistry Detector Coatings	200,000
Target Fabrication	1,500,000
Filament Winder	150,000
Polymeric Laser Rods	150,000
High Energy Density Joining Process Development	410,000
Arc Welding Process Development	150,000
Solid State Bonding	20,000

OFFICE OF DEFENSE PROGRAMS

Assistant Secretary for Defense Programs

The Assistant Secretary for Defense Programs directs the Nation's nuclear weapons research, development, testing, production, and surveillance programs. In addition, the Assistant Secretary coordinates a safeguards and security program to provide accountability and physical protection of special nuclear materials, including research and development for improvements, testing, evaluation, and implementation of safeguards systems. Additional responsibilities include management of the inertial fusion development and nuclear materials production programs, classification and declassification of sensitive weapons information, analysis and coordination of international activities related to nuclear technology and materials, and the management of waste from defense program activities.

Materials activities in Defense Programs are concentrated in the Office of Weapons Research, Development, and Testing and in the Office of Nuclear Materials Production. Within the Office of Weapons Research, Development, and Testing, materials activities are supported by the Inertial Fusion Division and by the Weapons Research Division. The bulk of these activities are performed at the three weapons program national laboratories: Sandia, Lawrence Livermore, and Los Alamos.

Office of Defense Waste and Transportation Management

Waste Research and Development Division*

The objective of the Defense High-Level Waste (HLW) Technology Program is to develop the technology for ending interim storage and achieving permanent disposal of all U.S. defense HLW. Defense HLW generated by atomic energy defense activities is stored on an interim basis at three U.S. Department of Energy (DOE) operating locations: the Savannah River Site in South Carolina, the Hanford Site in Washington, and the Idaho National Engineering Laboratory in Idaho. HLW will be immobilized for disposal in a geologic repository. Other waste will be stabilized in-place, if, after completion of the National Environmental Policy Act (NEPA) process, it is determined, on a site-specific basis, that this option is safe, cost effective and environmentally sound.

The orderly transition from interim storage to permanent disposal at the three DOE sites will proceed sequentially in order to permit technical developments at the first site to

*In November 1989, this program was transferred from Defense Programs to the new Office of Environmental Restoration and Waste Management and placed under the Office of Waste Operations.

be utilized at the other sites and thereby achieve a more efficient use of resources. The immediate program focus is on implementing the waste disposal strategy selected in compliance with the NEPA process at Savannah River and Hanford, while continuing progress toward development of final waste disposal strategy at Idaho.

At Savannah River HLW will be retrieved from underground storage tanks, immobilized as borosilicate glass, stored on-site for an interim period, and eventually shipped to a geologic repository. A Defense Waste Processing Facility (DWPF) to immobilize Savannah River waste is under construction.

At Hanford a final Environmental Impact Statement (EIS) was prepared to support selection of a disposal strategy for Hanford high-level, transuranic and tank wastes. The Preferred Alternative recommended proceeding with disposal of double-shell tank waste, retrievably-stored transuranic waste and encapsulated cesium and strontium. Further development and evaluation is required for the remaining three types of wastes: single-shell tank waste, TRU-contaminated soil site, and pre-1970 buried suspect TRU-contaminated solid waste. A Record of Decision was signed in April 1988, selecting the Preferred Alternative.

At Idaho several alternative waste management strategies have been identified and their relative rankings evaluated. One of these strategies will eventually be selected in compliance with the NEPA process for disposal of Idaho HLW.

Materials Properties, Behavior, Characterization or Testing

307. Waste Form Qualification - DOE Contact Ken Chacey, (301) 427-1621 and Marv Furman (509) 376-7062; Westinghouse Hanford Company Contact Steve Schaus, (509) 376-8365

- Fundamental data for immobilizing defense waste (e.g., borosilicate glass, crystalline ceramics).

308. Immobilization/Volume Reduction/In-place Stabilization - DOE Contacts Ken Chacey, (301) 427-1621 and Marv Furman, (509) 376-7062; Westinghouse Hanford Company Contact Steve Schaus, (509) 376-8365

- Process flowsheets for treatment of HLW streams at Richland and Idaho.

Office of Weapons Research, Development, and Testing

Weapons Research Division

Sandia National Laboratories - Albuquerque

Solid State Sciences Directorate, 1100

Ion Solid Interactions and Surface Sciences Research Department, 1110

The mission of Department 1110 is to provide Sandia National Laboratories with a comprehensive research program and technology base in ion implantation, ion-solid microanalysis/channeling thin film kinetics and epitaxy, and defects and hydrogen in solids. The research is designed to enhance fundamental understanding of the physical and chemical processes necessary to control the near-surface and interfacial regions of solids as well as to develop new techniques for the controlled synthesis, modification and analysis of these near-surface and interfacial regions. A major aspect of the work is thus to develop an underlying understanding and control of thin film kinetics, epitaxy, defects, hydrogen-materials interactions, alloying processes, and the formation of metastable and amorphous phases. In addition, the mission of the department is to relate this knowledge to laboratory problems and needs in the development of advanced weapons and energy systems.

Materials Properties, Behavior, Characterization or Testing

309. Ion Implantation Studies for Friction, Wear and Microhardness - DOE Contact A. E. Evans, (301) 353-3098; Sandia Contacts D. M. Follstaedt, (505) 844-2102, S. M. Myers, (505) 844-6076 and L. E. Pope, (505) 844-5041

- Ion implantation is used to modify the surface and near-surface regions of metals and these implantation-modified materials are evaluated for their improved friction and wear characteristics.

310. Silicon-Based Radiation Hardened Microelectronics - DOE Contact A. E. Evans, (301) 353-3098; SNL Contacts H. J. Stein, (505) 844-6279, K. L. Brower, (505) 844-6131 and J. A. Knapp, (505) 844-2305

- Optical, electrical and compositional measurements, in conjunction with electron paramagnetic resonance and related techniques are used to determine the fundamental defect structures and materials properties required for radiation-hardened Si-based microelectronics.

311. Surface Science - DOE Contact A. E. Evans, (301) 353-3098; Sandia Contact T. A. Michalski, (505) 844-5829

- Scanning tunneling microscopy, field ion microscopy, Auger electron spectroscopy, UV photoemission spectroscopy, and thermal desorption are being used to understand at an atomic level the early stages of epitaxy of oxidation and corrosion of metals and semiconductors, the nature of the adhesion of polymers to metals and how to improve it.

- Novel chemical vapor deposition techniques are being developed to produce more uniform and reliable multicomponent pyrotechnics.

Laser and Chemical Physics Research Department, 1120

Materials processing science studies emphasizing chemical vapor deposition and plasma- and photo-enhanced vapor deposition and etching are carried out. Emphasis is on microelectronic and optoelectronic materials and processing methods. Examples of ongoing studies are provided below.

Materials Properties, Behavior, Characterization or Testing

312. Plasma Etching - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; SNL Contacts K. E. Greenberg, (505) 844-1243 and P. J. Hargis, (505) 844-2821

- Fundamental studies of plasmas of the type widely used in the manufacture of large-scale and very-large-scale integrated electronic circuits to etch small features in semiconductors, dielectrics and conductors.

- Improved understanding of the underlying physics and chemistry of technologically-important processes occurring both in the volume and on the surface.

- New process methods and methodologies that give improved pattern-transfer fidelity and less damage to the underlying material.

- Process monitors that may lead to improved process reliability.

313. Plasma-Enhanced Chemical Vapor Deposition - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; SNL Contacts K. E. Greenberg, (505) 844-1243 and P. J. Hargis, (505) 844-2821

- Fundamental studies to gain new understanding of plasma-enhanced chemical vapor deposition, PECVD, of thin film materials of the type that are used in the manufacture of microelectronic devices.

- Processes that give higher quality materials having good adhesion to the underlying structure.

- *In situ* monitors for process control.

314. Laser-Controlled Etching and Deposition of Materials - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; SNL Contact A. Wayne Johnson, (505) 844-8782

- Underlying science and the technological limits of laser-controlled deposition and etching of conductors and insulators on microelectronic circuits.

- Expected to find important applications for the correction of design errors in prototype circuits and for customization of large-scale integrated circuits.

315. Surface Chemistry of Organometallics for Compound Semiconductor Epitaxy - DOE Contact A. E. Evans, (301) 353-3098; Sandia Contact J. R. Creighton, (505) 844-3955

- The motivation for this study stems from the extensive use of organometallic compounds ($Ga(CH_3)_3$, $Al(CH_3)_3$, etc.) as sources of elemental constituents for the growth of compound semiconductors by such techniques as metallorganic chemical-vapor deposition (MOCVD), chemical-beam epitaxy (CBE), and atomic layer epitaxy (ALE).

- Probe the primary chemical surface reactions to gain a scientific understanding of these technologically important systems.

316. Metallorganic Chemical Vapor Deposition - DOE Contact A. E. Evans, (301) 353-3098; SNL Contacts K. P. Killeen, (505) 844-5164 and M. E. Coltrin, (505) 844-7843

- The deposition of thin films of III-V compound semiconductor materials to produce scientifically tailored semiconductor structures is often done by thermal chemical vapor deposition using Group III organometallic compounds ($Ga(CH_3)_3$, $Al(CH_3)_3$, etc.), and Group V hydrides (AsH_3, PH_3, etc.) or alkyls ($As(CH_3)_3$, $P(C_2H_5)_3$, etc.).

- We are applying comprehensive theoretical modelling of the fluid dynamics and both the volume and the surface chemistry, as well as an extensive array of *in situ* measurement tools to gain new insight into the underlying physics and chemistry of the process.

- Goal of this work is the development of processes and process control procedures that yield higher quality materials and more abrupt heterointerfaces.

- Identify chemical precursors that are less toxic and otherwise more safe to handle.

Compound Semiconductor and Device Research Department, 1140

Study and application of semiconductor strained-layer superlattices and heterojunction materials to explore solutions to new and existing semiconductor materials problems, by coordination of semiconductor physics (theory and experiment) and materials science. This program investigates fundamental material properties including band structure, electronic transport, crystal stability, and linear and nonlinear optical properties. It also includes investigation of thin film high temperature superconductors for hybrid compound semiconductor/superconductor applications. The materials under study have a wide range of applications for high speed and microwave technology, optical detectors, lasers, and optical modulation and switching.

Materials Preparation, Synthesis, Deposition, Growth or Forming

317. Materials Growth by Molecular Beam Epitaxy (MBE) - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; Sandia Contacts L. R. Dawson, (505) 846-3451, T. M. Brennan, (505) 844-3233 and J. F. Klem, (505) 844-9102

- Growth of AlGaAs/GaAs, InAsSb/InAl, InGaAs/GaAs, and AlInAs/GaInAs strained layer superlattice (SLS) and strained quantum well (SQW) structures for electronic and optoelectronic applications.

318. Materials Growth by MOCVD - DOE Contact A. E. Evans, (301) 353-3098/ FTS 233-3098; Sandia Contact R. M. Biefield, (505) 844-1556

- Growth of GaP/GaAsP and InAsSb/InSb SLS's for high temperature radiation-hard electronic devices and for long wavelength IR detectors, respectively. A primary goal of this effort is to identify suitable dopants for n and p type InAsSb/InSb SLSs. A further goal is to fabricate p-n junction photodiodes from these materials for IR detectors in the 8-12 μm wavelength region.

319. Strained Layer Superlattices for IR Detectors - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; Sandia Contact P. S. Peercy, (505) 844-4309

- Strained layer superlattices based on the InAsSb/InSb and InAsSb/InSb/AlSb systems are being investigated for use as attractive alternatives to the unstable HgCdTe alloys for IR detector applications in the 8-12 μm range. These IR materials are being grown by both MBE and MOCVD techniques. Photovoltaic detector with $D^* > 1 \times 10^{10}$ cm $\sqrt{HZ}/W$ at 10 μm and 77K and photoconductive detection to 15 μm have been demonstrated.

320. Novel Processing Technology for Semiconductor Technologies - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; Sandia Contact D. S. Ginley, (505) 844-8863

- This program involves studies of new technologies for formation of diffusion barriers for improved epitaxial growth, novel metallurgies for Shottky barrier and Ohmic contact formation, passivation layer development, and development of new metallurgical techniques for deposition of reactive alloys, and deposition and patterning of high temperature superconductors for interconnects on semiconductor devices.

321. Thin Film Superconductors - DOE Contact A. E. Evans, (301) 353-3098/ FTS 233-3098; Sandia Contact D. S. Ginley, (505) 844-8863/FTS 844-8863

- Thin films of the high temperature superconductors in the Y-Ba-Cu-O and Tl-Ca-Ba-Cu-O systems are being prepared by MBE, E-beam evaporation and sputtering. Strongly-linked polycrystalline films with critical currents approaching 1,000,000 A/cm^2 or 77K have been demonstrated. Patterning and contacting technology for the films for device applications is also being developed.

Condensed Matter Research Department, 1150

The mission of Department 1150 is to provide fundamental understanding and strong technology bases in novel materials and structures, surface physics and shock wave physics and chemistry. Both experimental and theoretical research are performed. Current areas of emphasis include high T_c superconductors, shock-induced solid state chemistry, disordered materials, high temperature semiconducting borides, defects in semiconductors, surface desorption and ferroelectrics.

Materials Properties, Behavior, Characterization or Testing

322. Superconductivity - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; Sandia Contact B. Morosin, (505) 844-8169

- Transport, magnetic and structural measurements to access the fundamental factors which limit the performance of ceramic superconductors.
- Development of theoretical models of high temperature superconductivity.
- Development of new processing technologies for ceramic superconductors, in particular high pressure, high temperature oxygen treatments.

323. Shock Physics and Chemistry - DOE Contact A. E. Evans, (301) 353-3098/ FTS 233-3098; Sandia Contact R. A. Graham, (505) 844-1931

- Both organic and inorganic solids are being investigated to determine the influence of molecular structure on shock-induced bond scission, and the influence of line and point defects on the observed, enhanced, shock-induced solid state reactivity.
- The influence of shock modification on the properties and synthesis of high T_c superconductors is being explored. Shock-activated thermal batteries are being studied to determine the mechanisms and materials parameters which influence electrical output.
- A revolutionary time-resolved dynamic stress gauge using the piezoelectric polymer PVF_2 is being developed.

324. Semiconductors - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; Sandia Contacts D. Emin, (505) 844-3431 and H. P. Hjalmarson, (505) 846-0355

- Theoretical and experimental studies of electronic properties of boron carbide at high temperatures.
- Radiation-induced defects and their deep electronic levels in silicon and compound semiconductors and the role of these defects in device degradation.
- Physics of light-hole devices based on strained layer superlattices.

325. Surface Science - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; Sandia Contact D. R. Jennison, (505) 844-5909

- Detection and analysis of neutral atoms and molecules desorbed from surfaces.
- Theory of electronically stimulated desorption.
- Theory of surface electronic structure.
- Hydrogen in metals.

326. Disordered Materials - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; Sandia Contact G. A. Samara, (505) 844-6653

- Application of polymeric synthesis routes to ceramic materials.
- Gas phase materials processing.
- Gelation in foam precursors and sol-gel glasses.
- Fundamentals of film formation.
- The physics and formation of microemulsions.

Optoelectronics and Microsensor Research Department, 1160

The mission of Department 1160 is to provide Sandia National Laboratories with a comprehensive science and technology base in photonics and microsensor research. A fundamental understanding of the interaction of materials with both electromagnetic and mechanical forms of energy as well as their chemical environment are used to facilitate the design of new photonic and sensor devices. Activities include research into advanced materials and devices for optical sources; modulators and detectors; information processing; and chemical sensing.

Materials Properties, Behavior, Characterization or Testing

327. New Concepts in Microsensors - DOE Contact A. E. Evans, (301) 353-3098; Sandia Contacts R. C. Hughes, (505) 844-8172, A. J. Ricco, (505) 844-4947; M. A. Butler, (505) 844-6897

- Radiation-sensing field-effect transistor (RADFET) which operates by the trapping of radiation-produced holes in the silicon dioxide gate dielectric of the FET.

- Chemical sensors which operate by inducing charged layers at the metal-silicon dioxide interface in response to the chemical species.

- Acoustic wave devices for detection of solid-liquid interface phenomena like viscosity, freezing, and low level chemical detection.

- Optically-based corrosion and energy impulse detectors for high speed impulse detection and remote corrosive species detection.

- A miniature optical fiber micromirror chemical detector that can distinguish between water and common organic solvents.

Organic and Electronic Materials Department, 1810

Department 1810 provides support to Sandia projects through selection, development, and characterization of organic and electronic materials and associated manufacturing processes. Responsibilities span exploratory development through design, production, and stockpile life. The Department provides the Laboratories with knowledge and engineering data on properties and reliability of organic and electronic materials pertinent to our unique applications and conducts in-depth studies in order to understand and improve these properties. Department 1810 investigates unique and innovative approaches to applying organic materials to problems of interest at Sandia.

Chemistry of Organic Materials Division, 1811

Division 1811 supports the Laboratories in the area of chemistry of organic materials. It is responsible for selecting, formulating, and characterizing polymer films and coatings, adhesives, and resins for casting and molding as well as developing or synthesizing new organic materials for unique and innovative applications. This division coordinates aging and compatibility studies throughout the Laboratories. To accomplish these goals, the

Division carries out in-depth chemical investigations to characterize the reaction chemistry of these materials which influence their formulation, processing, or aging.

Materials Preparation, Synthesis, Deposition, Growth or Forming

328. Sulfonated Aromatic Polysulfones - DOE Contact A. E. Evans, (301) 353-3098; Sandia Contacts R. L. Clough, (505) 844-3492, C. Arnold, Jr., (505) 844-8728, and R. A. Assink, (505) 844-6372

- Sulfonated aromatic polysulfones have been developed as stable ionic battery membranes and are now in testing in prototype batteries.

329. Carbon Foams - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; Sandia Contract R. L. Clough, (505) 844-3492

- Development of a new type of microporous carbon foam.

- High-temperature carbonization of polymer foams.

Materials Properties, Behavior, Characterization or Testing

330. Radiation Hardened Dielectrics - DOE Contact A. E. Evans, (301) 353-3098; Sandia Contacts R. L. Clough, (505) 844-3492 and C. Arnold, Jr., (505) 844-8728

- Polymer dielectrics have been developed that display a minimum radiation-induced conductivity (RIC).

- These materials will be used in capacitors and cables exposed to high dose-rate radiation so that little charge is lost due to RIC in this environment.

- Processing parameters have been optimized.

331. Organic Nonlinear Optical Materials - DOE Contact A. E. Evans, (301) 353-3098/ FTS 233-3098; Sandia Contacts R. L. Clough, (505) 844-3492; P. A. Cahill, (505) 844-5754, G. E. Pike, (505) 844-7562, and M. B. Sinclair, (505) 844-5506

- Research on fabrication of organic nonlinear optical devices on semiconductor substrates has been initiated.

Physical Chemistry and Mechanical Properties of Polymers Division, 1812

Division 1812 develops new organic materials, structurally and chemically characterizes organic materials, and studies their mechanical properties. It is responsible for characterizing the molecular, electronic, and microphase structure of organic materials and their chemical reactivity toward the use environment as well as formulation of organic composites and adhesives.

Materials Preparation, Synthesis, Deposition, Growth or Forming

332. Chemistry of Plasma Etching and Deposition Processes - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; Sandia Contacts C. L. Renschler, (505) 844-0324 and R. J. Buss, (505) 844-7494

- Study of chemistry of glow discharge plasmas using molecular beam and laser techniques.
- Application to selectivity in etching for microelectronic fabrication.
- Also applied to production of solar cell materials and their carbon/hydrogen films.

Materials Structure and Composition

333. Materials Structure, Dynamics, and Property Studies by Multinuclear Pulsed NMR Spectroscopy - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; Sandia Contacts C. L. Renschler, (505) 844-0324 and R. H. Assink, (505) 844-6372

- Use of ^{13}C and ^{1}H spectroscopy of precursor liquids for encapsulants and foams.
- Studies of coal liquefaction catalysts and processes.
- Study of degradation pathways and products in organic materials.
- Imaging techniques for liquid and solid foams.

334. Mechanistic and Kinetic Studies of Polymer Aging - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; Sandia Contacts C. L. Renschler, (505) 844-0324, K. T. Gillen, (505) 844-7494, and R. L. Clough, (505) 844-3492

- Mechanistic studies of thermo-oxidative degradation routes in polymers.
- Development of novel tools and techniques to quantify polymer aging.
- Development of kinetic theory and validation with experimental data.

335. Theory of Polymer Dynamics - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; Sandia Contact J. M. Zeigler, (505) 844-0324

- Extension of Mode-Mode-Coupling Theory to polymeric liquids.
- Calculation of structure-property relationships from first principles, with no adjustable parameters.
- Develop understanding of important length scales, as observed in scattering experiments.

Physical Properties of Polymers Division, 1813

Division 1813 provides support to Sandia projects through selection, development, and processing of foams, elastomers, encapsulants, and molding compounds. It is responsible for characterizing the physical properties and aging behavior of these materials. This Division also carries out in-depth physical property studies when necessary in order to understand or improve these properties.

Materials Preparation, Synthesis, Deposition, Growth or Forming

336. Microporous Foam Development - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; Sandia Contacts J. G. Curro, (505) 844-3963, J. H. Aubert, (505) 844-3305, and P. B. Rand, (505) 844-7953

- Development of new polymer and carbon foams which have both low density and small cell sizes (0.1 to 10 microns).
- Process utilizes thermally induced phase separation followed by solvent removal steps such as extraction or freeze-drying.

337. Development of Removable Encapsulants - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; Sandia Contacts J. G. Curro, (505) 844-3963, D. B. Adolf, (505) 844-4773, and P. B. Rand, (505) 844-7953

- Development of removable encapsulant to allow rework of electronic components.

- Use of thermoplastic-coated glass microballoons poured into assembly and heated to fuse polymer. Encapsulant removed with solvent.

Materials Properties, Behavior, Characterization or Testing

338. Mechanical Properties of Encapsulants - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; Sandia Contacts J. G. Curro, (505) 844-3963 and D. B. Adolf, (505) 844-4773

- Measurement of linear elastic properties (coefficient of thermal expansion, bulk modulus, and shear modulus) as functions of temperature that lead to stresses upon thermal cycling for common polymeric encapsulants.

- Future studies will focus on the ultimate properties of these materials for use in determining failure criteria using computer codes.

339. Deformation of Kevlar Fabrics - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; Sandia Contacts J. G. Curro, (505) 844-3963 and W. E. Warren, (505) 844-4445

- The effect of specific fabric microstructure and Kevlar yarn properties on the effective elastic properties of the fabric are being investigated theoretically and experimentally to allow optimization of the mechanical properties of parachute fabrics.

340. Moisture Permeation in Encapsulants, Adhesives and Seals - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; Sandia Contacts J. G. Curro, (505) 844-3963 and P. F. Green, (505) 846-2466

- Polymeric materials are used as encapsulants, seals and adhesives in weapon components.

- Program is initiated to study moisture permeation in commonly used encapsulants, adhesives and seals.

Electronic Property Materials Division, 1815

Division 1815 provides support to Sandia programs through selection, development, and characterization of electronic materials. Responsibilities span exploratory development through design, production, and stockpiling. The Division also performs in-depth studies in order to understand material properties and associated electronic phenomena. Areas of activity include electronic materials, dielectrics, and optical materials.

Materials Properties, Behavior, Characterization or Testing

341. Nonlinear Optical Materials - DOE Contact A. E. Evans, (301) 353-3098/ FTS 233-3098; SNL Contacts G. E. Pike, (505) 844-7562 and M. L. Sinclair, (505) 844-5506

- Specially synthesized organic molecules are being characterized for nonlinear hyperpolarizabilities.

342. Hydrogen Effects in Silicon - DOE Contact A. E. Evans, (301) 353-3098/ FTS 233-3098; Sandia Contacts G. E. Pike, (505) 844-7562 and R. A. Anderson, (505) 844-7676

- Measurements mode of hydrogen diffusion through metal contacts into boron-doped silicon.
- Hydrogen bonds to boron and phosphorous and passivates them as dopants.
- Affects formation of Schottky barriers.

343. Rapid Thermal Processing of Gate Oxides - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; Sandia Contact G. E. Pike, (505) 844-7562 and W. K. Schubert, (505) 846-6548

- Characterization of 20 nm layers of SiO_2.
- Capacitance-voltage techniques to study X-ray radiation defects.
- Fowler-Nordheim current measurements for dielectric breakdown measurements.

Materials Characterization Department, 1820

Department 1820 performs chemical, physical, and thermophysical analyses of materials in support of weapons and energy programs throughout the Laboratories. The department also has the responsibility for the development of advanced analytical techniques to meet existing or anticipated needs. Consulting and process reviews are other important functions of the department.

Analytical Chemistry Division, 1821

The Analytical Chemistry Division, 1821, is responsible for performing chemical analyses in support of weapon and energy programs at Sandia. The division is equipped to analyze a variety of samples such as gases, polymers, liquids, solutions, solids, organics, inorganics, glasses, alloys, ceramics, and geological materials. Analyses are performed by a variety of techniques using absorption and emission spectroscopy, gas chromatography, gas chromatography/mass spectrometry, ion chromatography, neutron activation analysis, electrochemistry, combustion, and classical methods of chemical analysis.

Instrumentation and Facilities

344. Development of Automated Methods for Chemical Analysis - DOE Contact A. E. Evans, (301) 353-3098; Sandia Contact S. H. Weissman, (505) 846-0820

- New automated methods for the chemical analysis of materials are being developed to meet new or anticipated needs and to improve accuracy, precision and efficiency of analyses.

Electron Optics and X-ray Analysis Division, 1822

The Electron Optics and X-ray Analysis Division, 1822, characterizes the microstructures of engineering materials and develops a basis for understanding processing microstructure property relationships in a wide range of materials including metals, ceramics, and semiconductor materials.

Materials Preparation, Synthesis, Deposition, Growth or Forming

345. Thermomechanical Treatment of U Alloys - DOE Contact A. E. Evans, (301) 353-3098; Sandia Contact K. H. Eckelmeyer, (505) 844-7775

- Strengthening mechanisms were investigated in U-Ti and U-Nb alloys with the goals of simplifying processing procedures and increasing strength-ductility combinations.

Instrumentation and Facilities

346. Advanced Methods for Electron Optical, X-ray, and Image Analysis - DOE Contact A. E. Evans, (301) 353-3098; Sandia Contact W. F. Chambers, (505) 844-6163

- Advanced methods of automated electron and X-ray instrumental analysis are being developed to improve resolution, accuracy, and efficiency and to allow us to undertake and solve more difficult problems.

Surface Chemistry and Analyses Division, 1823

The Surface Chemistry and Analyses Division 1823 provides analytical surface and optical analyses of materials in support of Sandia programs throughout the Laboratories. In addition, staff members in the division engage in advanced materials research and in research funded by specific weapons or energy programs which can be uniquely investigated using their expertise. Specific techniques employed within the division include Auger spectroscopy, X-ray photoelectron spectroscopy, low energy ion scattering and secondary ion mass spectroscopies, energetic ion analysis methods, fluorescence and Raman spectroscopies, dispersive and Fourier transform infrared spectroscopies.

Instrumentation and Facilities

347. Advanced Methods for Surface and Optical Analysis - DOE Contact A. E. Evans, (301) 353-3098; Sandia Contact J. A. Borders, (505) 844-8855

- An ion microscope is being added, primarily to support semiconductor materials development and processing.

- Chemometric statistical data correlation methods have been developed for infrared spectroscopy and are now being extended to Auger electron spectroscopy.

Metallurgy Department, 1830

Department 1830 selects, develops, and characterizes the non-electronic behavior of all metals and processes that may be needed to meet systems and components requirements. Responsibilities span exploratory development through design, production, and stockpile life. If either current or anticipated demands cannot be met by commercially-available metals and processes, Department 1830 is responsible for the necessary development. Understanding mechanisms of alloy bulk and surface behavior provides the basis for alloy and process development and increases the confidence of predictions of behavior. Surface treatment and coating processes receive special emphasis because of the close coupling of the surface and "bulk" behavior.

Physical Metallurgy Division, 1831

The Physical Metallurgy Division selects, develops and characterizes the physical behavior of all metals that may be needed to meet systems and components requirements. This includes the selection and development of alloys to insure a sufficiently long service life while maintaining fabricability. Responsibilities span exploratory development through design, production and stockpile life. If commercial technology does not meet engineering requirements, Division 1831, working with the other divisions in Department 1830, will develop the required technology. Understanding the relationship between alloy processing, alloy microstructure and alloy behavior is the basis for alloy selection and development and provides the input required to predict, via thermodynamic and kinetic modeling, the physical behavior of the alloy through its service life. The objective of Division 1831 is, therefore, to use this understanding to extend the capabilities of the design engineers and to increase confidence in alloy performance.

Materials Properaties, Behavior, Characterization or Testing

348. Analytical Electron Microscopy of Engineering Alloys - DOE Contact A. E. Evans, (301) 353-3098/FTS 223-3098; Sandia Contacts A. D. Romig, (505) 844-8358, M. J. Carr, (505) 846-1405, and T. J. Headley, (505) 844-4787

- Experimental techniques and the appropriate mathematical manipulation (with Monte Carlo simulations of electron trajectories in solids) of the experimental data are being applied to establish chemical concentrations at high spatial resolutions in Fe-Ni based and Ni-based superalloys, intermetallic compound alloys, IC metallizations and Si used for microelectronic applications.

349. Segregation Behavior During Solidification of Alloys - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; Sandia Contacts C. V. Robino, (505) 844-6557, A. D. Romig, (505) 844-8358, and M. J. Cieslak, (505) 846-7500

- The distribution of elements following solidification is being studied more rigorously than has been done in the past. Diffusion in the solid, solidification in multicomponent systems and for non-planar front solidification are being treated.

350. Solid State Reactions Between Metal Substrates and Solders - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; Sandia Contacts A. D. Romig, (505) 844-8358, J. J. Stephens, (505) 846-9962, M. M. Karnowsky, (505) 844-4134, and G. C. Nelson, (505) 844-5200

- An integrated experimental and diffusion modeling program aimed at determining the stability of the intermediate phases in a solder joint as a function of temperature and at determining the rates at which they form.

- Systems currently under study include Au/Pb-In, Au-Pd/Pb-In, Cu/Pb-Sn, Cu/Pb-In, and Pd/Pb-In.

351. Fluxless Soldering - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; Sandia Contacts F. M. Hosking, (505) 844-4925, C. V. Robino, (505) 844-6557, and D. R. Frear, (505) 846-4713

- The feasibility of using nonmolecular hydrogen and other atmospheres to reduce surface oxides and enhance wetting is being examined.

- The goal of this work is to find a reactive gas and specific processing conditions which produce solder joints which are comparable to those produced using rosin based fluxes, but are not environmentally hazardous either alone or with subsequent cleaning operations.

352. Stress Voiding of Aluminum Interconnect Lines - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; Sandia Contacts A. D. Romig, (505) 844-8358, F. G. Yost, (505) 846-5446, and J. A. Van Den Avyle, (505) 844-1016

- A diffusion model has been developed which predicts the rate of void formation in Al interconnects as a function of stress.

- Current efforts are addressing the measurement of the stress as a guide to assessing product reliability and the development of a suitable accelerated aging test.

353. Grain Boundary Segregation in Al-Cu Metallization Interconnect Lines - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; Sandia Contacts A. D. Romig, (505) 844-8358, D. R. Frear, (505) 846-4713, and C. R. Hills, (505) 844-4787

- Integrated theoretical and experimental program directed at understanding the microstructural role of Cu in Al interconnects.
- Initial results have shown that the grain boundaries are free of Cu, except for the formation of $CuAl_2$ precipitates.
- Work in progress on time-temperature dependent evolution of these microstructures, especially with respect to the distribution of Cu.

Mechanical Metallurgy Division, 1832

The mission of the Mechanical Metallurgy Division 1832 is to provide the characterization and understanding of the mechanical and corrosion properties of metals and alloys. This includes the selection of alloys and the conduct of research in alloy design and thermomechanical effects on material behavior. Sophisticated mechanical testing and corrosion capabilities are part of this division, and extensive use is made of the analytical capabilities at Sandia.

Materials Properties, Behavior, Characterization or Testing

354. Micromechanical Testing - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; Sandia Contacts W. B. Jones, (505) 845-8301 and R. J. Bourcier, (505) 844-6638

- Development of techniques for conducting tensile and creep tests on structures with dimensions of a few micrometers.
- Development of constitutive models that describe time independent inelastic and time dependent creep and relaxation response of these structures.

355. Toughness of Ductile Alloys - DOE Contact A. E. Evans, (301) 353-3098/ FTS 233-3098; Sandia Contacts R. J. Salzbrenner, (505) 844-5041 and J. A. VanDenAvyle, (505) 844-1016

- Elastic-plastic fracture toughness (J_{Ic}) is being studied to determine if it can be used as the basis for structural design. This includes a study of both the experimental techniques used to measure toughness at high loading rates and the application of the parameter in computer code calculations. The correlation between microstructure and toughness is also examined. Current emphasis is on the study of ductile cast iron for nuclear material shipping casks.

356. Low Melting Point Alloy Studies - DOE Contact A. E. Evans, (301) 353-3098/ FTS 233-3098; Sandia Contacts W. B. Jones, (505) 845-8301 and D. R. Frear, (505) 846-4713

- Examination of solder alloys under conditions of isothermal mechanical fatigue and thermomechanical fatigue.

- Demonstration that microstructural instability plays a large role in strain localizations; development of mechanistic models useful for solder joint design.

Process Metallurgy Division, 1833

This Division supports the Laboratories by selecting, characterizing, and developing metallurgical processes needed in the manufacture of components and systems. The objective is to provide process definition and control by understanding the mechanisms which operate. Attention is devoted toward structure-property modifications that occur during manufacturing processes. Principal processes currently under study include laser welding, arc welding (GTA and plasma), vacuum induction melting, vacuum arc remelting, electroslag remelting, and investment casting.

Materials Preparation, Synthesis, Deposition, Growth or Forming

357. Vacuum Arc Remelting - DOE Contact A. E. Evans, (301) 353-3098; Sandia Contact F. J. Zanner, (505) 844-7073

- Vacuum arc remelting is being studied with the objective of reducing inhomogeneities and defects in structural alloys and uranium alloys. The melt characteristics have been related to the types and pressures of gases in the arc atmosphere.

Device or Component Fabrication, Behavior or Testing

358. Electronbeam Melting - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; SNL Contact F. J. Zanner, (505) 844-7073

- Study of the control of melting and solidification during electronbeam melting, directed toward the recycling of uranium scrap.

359. Electroslag Remelting - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; SNL Contact M. C. Maquire, (505) 844-4925

- Study directed at the control of the electroslag remelting system, which refines ingot microstructure and eliminates impurities via electrochemical reactions. Goal is a control methodology to produce uniform optimum properties throughout the length of the ingot.

360. Welding of Nickel-Based Alloys - DOE Contact A. E. Evans, (301) 353-3098; Sandia Contacts M. J. Cieslak, (505) 846-7500 and M. C. Maguire, (505) 844-1109

- Mechanisms of hot-cracking during the fusion welding of both solid solution strengthened and precipitation-strengthened nickel-based alloys are under study. Hot-cracking in Hastelloys C-22 and C-276 and Inconel 718 appears to be related to solidification segregation resulting in formation of topologically-close-packed phases. New precipitation strengthened alloys are being developed.

361. Plasma Arc Welding - DOE Contact A. E. Evans, (301) 353-3098; Sandia Contacts P. W. Fuerschbach, (505) 846-2464 and J. L. Jellison, (505) 844-6397

- Variable polarity plasma arc welding of aluminum is under development. Calorimetry studies show that a high period of negative polarity can be used than has been commonly believed.

362. Laser Welding - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; Sandia Contact J. L. Jellison, (505) 844-6397

- Both pulsed and CW laser welding is being developed for application to component closures. Mechanisms of beam-plume interactions are being evaluated for various material-process combinations. These results, along with a new understanding of the roles of reflectivity and convention, are being incorporated into models of the processes. The roles of surface-driven convection and refraction of the beam by the plume are being studied.

- The plume modifies conversions flow in the weld pool. New CW Nd:YAG laser capability is being developed.

363. Development of Materials for Magnetic Fusion Reactors - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; Sandia Contact M. F. Smith, (505) 846-4270

- Materials used in magnetic confined fusion energy devices experience severe environments. A low-pressure plasma spray process has been successfully developed to deposit ceramic/metal coatings. The coatings are being considered for first wall surfaces or for graded thermal expansion layers.

Surface Engineering and Thin Film Technology Division, 1834

The Surface Engineering and Thin Film Technology Division 1834 is concerned with the influence of surface and near-surface regions on the engineering application of materials. Basic and applied research is conducted to understand and control deposition processes for reproducible surface modification and to correlate surface composition and microstructure with surface properties, friction, wear, and corrosion resistance. Controlled deposition of materials by physical vapor deposition of thin films and surface modification by ion implantation are techniques used to tailor surface properties. This division also supports design and component groups in areas where surface properties are critical.

Materials Preparation, Synthesis, Deposition, Growth or Forming

364. Development of Hard, Wear-Resistant Coatings for Mechanical Applications - DOE Contact A. E. Evans, (301) 353-3098; Sandia Contact J. K. G. Panitz, (505) 844-8604

- A study of the friction and wear properties of carbon coatings has begun. The objective will be to deposit hard diamond-like or diamond coatings with low coefficients of friction without the high levels of residual stress and poor adhesion that are typically characteristic of the diamond coatings currently produced by chemical vapor deposition.

Materials Properties, Behavior, Characterization or Testing

365. Modification of Mechanical Properties by Ion Implantation - DOE Contact A. E. Evans, (301) 353-3098; Sandia Contact M. Dugger, (505) 844-8778

- The dual implantation of titanium and carbon into stainless steels produces an amorphous layer; the amorphous layer reduces both friction and wear. The effects of implantation species on friction and wear are being explored. A project to evaluate ion-implanted uranium has begun.

366. Corrosion Predictions - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; Sandia Contact N. F. Sorenson, (505) 846-6024

- Acoustic plate mode sensors are being developed to allow for the measurement of small amounts of metallic corrosion. These data will be used to generate determined rate coefficients for corrosion reaction in non-accelerated experiments, allowing for realistic corrosion lifetime predictions.

367. Solvent Substitutive Programs - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; Sandia Contact M. C. Oborny, (505) 844-1038

- A program to evaluate alternative solvents to halogenerated solvents for use in cleaning and coating processes has begun. Long term materials compatibility issues are being addressed.

Device or Component Fabrication, Behavior or Testing

368. Process Control Ultrasonic Cleaning of Delicate Parts - DOE Contact A. E. Evans, (301) 353-3098; Sandia Contact M. C. Oborny, (505) 844-1038

- Ultrasonic cavitation, which has long been used to improve the effectiveness of solvent cleaning, can cause surface damage and fatigue failures in some materials and parts. A new generation of ultrasonic cleaner claims to avoid these problems by operating in a swept frequency mode and also controlling the energy injection rate into the cleaning solution by the control of five physical parameters associated with the ultrasonic bath.

369. Plasma Oxidation and Reduction Studies - DOE Contact A. E. Evans, (301) 353-30908/FTS 233-3098; Sandia Contact E. P. Lopez, (505) 846-8979

- Plasma treatments employing both oxidizing and reducing atmospheres are being studied using a Branson Barrel Etcher. Preliminary results indicate that a reducing atmosphere will restore an oxidized surface.

Instrumentation and Facilities

370. Ion Beam Reactive Deposition System - DOE Contact A. E. Evans, (301) 353-3098; Sandia Contact D. E. Peebles, (505) 844-1647

- A system is in use to study the properties of deposited films by controlled use of atom/molecule/ion beams. These films are being evaluated for tribological performance.

371. Deposition and Evaluation of Titanium Nitride Films - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; Sandia Contacts D. E. Peebles, (505) 844-1647 and L. E. Pope, (505) 844-5041

- Effects of parameters such as substrate material, deposition temperature, deposition pressure, ionization, contamination, stoichiometry and film thickness on titanium nitride film microstructure, adhesion and wear behavior.

372. In Situ Friction, Wear, and Electrical Contact Resistance Systems - DOE Contact A. E. Evans, (301) 353-3098; Sandia Contact M. Dugger, (505) 844-8778

- An *in situ* friction, wear, and electrical contact resistance device has been assembled to do complete oscillatory or unidirectional sliding friction experiments in a scanning Auger system, without exposure to ambient environments that can mask compositional measurements.

Chemistry and Ceramics Department, 1840

Department 1840 supports Sandia weapons and energy programs by selecting, developing, and characterizing ceramics, glasses and glass-ceramics. A variety of approaches are used, including gas-phase synthesis and reactions, solution preparation, as well as more traditional ceramic processing. The department promotes advanced weapons and energy concepts by providing new materials and developing new prototype components.

Interfacial Chemistry and Coating Research Division, 1841

Division 1841 is responsible for developing an understanding of the materials and processes involved in the formation of coatings and thin film structures. This work may be applicable to processes in use at Sandia, such as CVD tungsten films, as well as to new types of coatings, such as electrophoretic formation of dielectric films. The division develops CVD and aerosol techniques for preparing ceramic powders. There is a major effort in understanding the interaction of hydrogen with metals.

Electronic Ceramics Division, 1842

Division 1842 develops and determines the properties of new ceramics for electronic and optical applications in Sandia systems. Examples are PZT for nonvolatile, radiation hard semiconductor memories, high-field ZnO varistors, $KNbO_3$ for optical switches, and cuprate high temperature superconductors.

Ceramics Development Division, 1845

Division 1845 is responsible for supporting laboratory programs involving glass- or ceramic-to-metal seals and other uses of glass or ceramics in moderate temperature environments. Expertise in the division includes the following areas: fracture surface analysis of brittle materials; seal design and fabrication processes; and glass and ceramic properties, i.e., strength, electrical conductivity. The division also maintains an active materials development program to formulate new glass or glass ceramics to meet particular requirements, e.g., corrosion resistance or high thermal expansion.

Inorganic Materials Chemistry Division, 1846

Division 1846 develops new processes for making ceramic powders and films using solution chemistry techniques. Understanding the structure and chemistry of sol-gel bulk and film materials is a significant part of this activity. The division also develops understanding of small particle-metal interactions that has led to new catalyst materials.

Materials Preparation, Synthesis, Deposition, Growth or Forming

373. Electrolytic and Electrophoretic Methods for Materials Processing - DOE Contact A. E. Evans, (301) 353-3098; Sandia Contact Sylvia Tsao, (505) 846-6753

- These techniques are being used to apply organic and ceramic coatings to large irregularly-shaped objects. Applications are for composite coatings, insulators and IEMP hardeners.

374. Aerosol Production of Fine Ceramic Powders - DOE Contact A. E. Evans, (301) 353-3098; Sandia Contact Sylvia Tsao, (505) 846-6753

- Aerosol techniques are being used to prepare fine particle, unagglomerated ceramic powders that are then further processed for electronic and structural applications.

375. Chemically Prepared Ceramic Films for Opto-electronic Applications - DOE Contact A. E. Evans, (301) 353-3098; Sandia Contact B. C. Bunker, (505) 844-8940

- Chem-prep techniques are applied to preparation of thin films of $KNbO_3$, PZT, PNZT, and other ceramics. The properties of those films are being studied and modified to enhance their performance in opto-electronic devices.

376. Development of New Glasses and Glass-Ceramics - DOE Contact A. E. Evans, (301) 353-3098; Sandia Contact J. W. Rogers, Jr., (505) 844-1141

- New formulations of glasses and glass-ceramics are being developed, primarily for sealing applications. Examples are high thermal expansion glass ceramics for sealing to stainless steel, high thermal conductivity germanate glass-ceramics, and Li-corrosion resistant glasses for battery headers.

377. Preparation of Ceramic Powders by Chemical Techniques - DOE Contact A. E. Evans, (301) 353-3098; Sandia Contact D. H Doughty, (505) 844-1933

- Chemical precipitation techniques are being developed for preparation of a wide variety of ceramic powders such as varistors, ferroelectrics, and high Tc superconductors.

Materials Structure and Composition

378. Structure of Novel Glasses - DOE Contact A. E. Evans, (301) 353-3098; Sandia Contact J. W. Rogers, Jr., (505) 844-1141

- The structures of novel glasses in the phosphate tellurate and germanate systems are being studied and related to properties such as durability and thermal conductivity.

379. Structure of Sol-Gel Films - DOE Contact A. E. Evans, (301) 353-3098; Sandia Contact D. H. Doughty, (505) 844-1933

- Structures of sol-gel films suitable for optical or environmentally protective coatings are being studied by ellipsometric techniques.

Materials Properties, Behavior, Characterization or Testing

380. Molecular Beam Studies of Hydrogen in Metals - DOE Contact A. E. Evans, (301) 353-3098; Sandia Contact Sylvia Tsao, (505) 846-6753

- Dynamics of chemical reactions on metal surfaces are studied by quantum-resolved molecular beam techniques.

381. Electronic Ceramics - DOE Contact A. E. Evans, (301) 353-3098; Sandia Contact B. C. Bunker, (505) 844-8940

- Electric properties of ceramics such as varistors, ferroelectrics and ceramic superconductors are being studied and related to composition and structure.

382. Ceramic Fracture - DOE Contact A. E. Evans, (301) 353-3098; Sandia Contact J. W. Rogers, Jr., (505) 844-1141

- Research is being conducted on ceramic fracture to understand the phenomenon better and to develop tougher ceramics.

383. Superplastic Ceramics - DOE Contact A. E. Evans, (301) 353-3098; Sandia Contact J. W. Rogers, Jr., (505) 844-1141

- The relation between ceramic microstructure composition and plastic deformation is being studied to develop superplasticity in ceramics such as Y_2O_3 and ZrO_2.

384. Reactivity and Bonding of Glasses and Ceramics to Metals - DOE Contact A. E. Evans, (301) 353-3098; Sandia Contact J. W. Rogers, Jr., (505) 844-1141

- Reactivity of metals and ceramics are being studied to improve their bonding for hermetic seal applications.

Device or Component Fabrication, Behavior or Testing

385. Sensor Development - DOE Contact A. E. Evans, (301) 353-3098; Sandia Contact Sylvia Tsao, (505) 846-6753

- Environmental sensors for gases such as H_2O are being developed using porous ceramic films grown by electrolytic techniques.

386. SAW Development - DOE Contact A. E. Evans, (301) 353-3098; Sandia Contact D. H. Doughty, (505) 844-1933

- Surface acoustic wave devices are being developed as sensitive and selective detectors are adsorbed species in gas and liquid environments.

Sandia National Laboratories - Livermore

Materials Preparation, Synthesis, Deposition, Growth or Forming

387. Powder Metallurgy - DOE Contact A. E. Evans, (301) 353-3098; Sandia Contacts M. I. Baskes, (415) 294-3226) and J. E. Smugeresky, (294) 422-2910

- Inert gas atomization, and melt spinning processes are being used to advance development of the powder metallurgy and rapid solidification processing of a variety of alloy systems. Advanced techniques are being developed and applied to powder characterization.

388. Advanced Electrodeposition Studies - DOE Contact A. E. Evans, (301) 353-3098; Sandia Contacts R. E. Stoltz, (415) 294-2162, H. R. Johnson, (415) 294-2822 and W. D. Bonivert, (415) 294-2987

- Engineering applications, electroanalytical development, and fundamental investigations are being pursued in the area of electrodeposition and electroforming.

389. Metal Forming - DOE Contact A. E. Evans, (301) 353-3098; Sandia Contacts J. Lipkin, (415) 422-2417, T. C. Lowe, (415) 294-3187 and D. A. Hughes, (415) 294-2686

- Inelastic deformation and failure are examined through crystal plasticity modeling and experimentation. Results are used to help interpret finite element metal forming simulations and guide the development of phenomenological constitutive relations for large strain deformation.

390. Advanced Organic Materials - DOE Contact A. E. Evans, (301) 353-3098; Sandia Contacts D. L. Lindner, (415) 294-3306, J. G. Curro, (505) 844-3963, W. R. Even, (415) 294-3217 and C. B. Frost, (415) 294-2048

- An understanding of methods for producing microstructural modifications in organic foams has enabled the production of polymeric foams with unique physical properties.

391. Particulate Technology - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; Sandia Contacts D. L. Lindner, (415) 294-3306 and W. R. Even, (415) 294-3217

- We have developed methods to produce extremely fine actinide oxide particles of controlled morphology: spheres, plates and needles.

392. Tritium Getter Technology - DOE Contact A. E. Evans, (301) 353-3098/ FTS 233-3098; Sandia Contacts D. L. Lindner, (415) 294-3306 and T. Shepodd, (415) 294-2791

- We have demonstrated a system that is capable of gettering large amounts of tritium gas even in the presence of contained amounts of oxygen and water without releasing radioactive species as it ages.

393. Molded Desiccant Foam - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; Sandia Contacts D. L. Lindner, (415) 294-3306 and C. B. Frost, (415) 294-2048

- We have developed a desiccant-loaded polymer foam material that can be effectively used in applications in which both structural and desiccating properties are needed.

394. Plasma Processing - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; Sandia Contact W. L. Hsu, (415) 294-2379

- The synthesis of diamond and amorphous carbon by plasma processing is being studied.

Materials Properties, Behavior, Characterization or Testing

395. Tritium and Decay Helium Effects on Crack Growth in Metals and Alloys - DOE Contact A. E. Evans, (301) 353-3098; Sandia Contacts S. L. Robinson, (415) 294-2209, S. H. Goods, (415) 294-3274 and N. R. Moody, (415) 294-2622

- Experimental and theoretical studies are underway to determine the effects of tritium and decay helium on mechanical properties and crack growth susceptibility in fcc alloys.

396. Joining Science and Technology - DOE Contact A. E. Evans, (301) 353-3098; Sandia Contacts J. A. Brooks, (415) 294-2051 and K. W. Mahin, (415) 294-3582

- This program is developing a science-based methodology for improving the fundamental understanding of the behavior of welded structures and modeling of the complex fusion weld process. Advanced joining techniques using solid state welding, and adhesives are being developed for advanced structural materials.

397. Composites: Characterization and Joining - DOE Contact A. E. Evans, (301) 353-3098; Sandia Contacts D. L. Lindner, (415) 294-3306 and J. R. Spingarn, (415) 294-2719

- The stability, compatibility, and joining of polymer matrix composite materials are under investigation. Focus is upon graphite fiber reinforced materials. Identification of moisture adsorption sites in thermosetting resins is underway. Coatings to increase stability for special designs are being studied. Joining studies include adhesives, mechanical fasteners and the welding of thermoplastics.

398. Compatibility, Corrosion, and Cleaning of Materials - DOE Contact, A. E. Evans, (301) 353-3098; Sandia Contacts H. R. Johnson, (415) 294-2822, R. E. Stoltz, (415) 294-2162, J. M. Hrubu, (415) 294-2596 and D. K. Ottesen, (415) 294-2787

- We have developed special techniques using FTIR that allow interior surface of small diameter tubes or external surfaces of wire are examined for corrosion and cleaning techniques.

399. Tritium-Metal Interaction - DOE Contact A. E. Evans, (301) 353-3098/ FTS 233-3098; Sandia Contact A. E. Pontau, (415) 294-3159 and M. E. Malinowski, (415) 294-2069

- The interactions of tritium gas with metals is characterized by a number of experimental techniques including tritium-imaging and nuclear reaction ion micro-beam analysis.

400. Measurement of Multilayer Thin Film Structures - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; Sandia Contacts B. E. Mills, (415) 294-3230

- We have developed a dual-energy beta backscatter measurement technique that we have used to measure layer thicknesses in multilayer thin film structures.

401. Helium in Metal Tritides - DOE Contact A. E. Evans, (301) 353-3098; Sandia Contacts W. A. Swansiger, FTS 234-2496, S. E. Guthrie, FTS 234-2360 and D. F. Cowgill, (505) 844-7480

- Helium evolution in metal tritides is being studied by NMR, gas sampling and dilatometry techniques.

402. Analysis of Defects and Interfaces in Metals - DOE A. E. Evans, (301) 353-3098; Sandia Contacts T. C. Lowe, (415) 294-3187 and S. H. Goods, (415) 294-3247

- Inelastic deformation and failure near interfaces is being examined through crystal plasticity modeling and experimentation. Results are used to understand the mechanisms of failure in metals and alloys subject to gas embrittlement.

Instrumentation and Facilities

403. New Spectroscopy - DOE Contact A. E. Evans, (301) 353-3098; Sandia Contacts D. L. Lindner, (415) 294-3305, M. C. Nichols, (415) 294-2906 and B. E. Mills, (415) 294-3230

- New spectroscopic techniques are being developed for special applications. For example, micro-fluorescence spectroscopy, high resolution energy loss spectroscopy (HREELS), and X-ray photoelectron spectroscopy (XPS) are being implemented.

404. Tritium Facility Upgrade for Materials Characterization and Testing - DOE Contact A. E. Evans, (301) 353-3098; Sandia Contacts S. H. Goods, (415) 294-3274 and S. L. Robinson, (415) 294-2209

- New experimental capabilities in surface analysis, fractography, and thermomechanical history are improving both the characterization of tritium-induced degradation of material properties, and the development of predictive abilities.

405. New Analytical Techniques - DOE Contact A. E. Evans, (301) 353-3098/ FTS 233-3098; Sandia Contacts D. L. Lindner, (415) 294-3306, M. C. Nichols, (415) 294-2906 and B. E. Mills, (415) 294-3230

- We have developed a system for X-ray microtomography that can be used for spatial elemental analysis for materials and structures.

406. New High Resolution Electron Microscopy Facility - DOE Contact A. E. Evans, (301) 353-3098; Sandia Contacts G. J. Thomas, (415) 294-3224 and M. J. Mills, (415) 294-3018

- A new high resolution transmission electron microscope laboratory is now operational. It includes an intermediate voltage high resolution microscope, sample preparation and photoprocessing facilities, and computational facilities for image simulations and image processing. It will be utilized to determine the atomistic structures of a number of material systems, including (a) metal-metal interfaces such as grain boundaries, (b) defect structures in undeformed and deformed metals and alloys, (c) helium-induced defect evolution in metal tritides, and (d) semiconductor-oxide interfaces. These studies are important to gas transfer technologies and to semiconductor device fabrication.

Lawrence Livermore National Laboratory

Materials Preparation, Synthesis, Deposition, Growth or Forming

407. Inorganic Aerogels - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; LLNL Contact L. W. Hrubesh, (415) 423-1691/FTS 543-1691

- The objective of this project is to develop the chemistry and procedures for processing monolithic pieces of micro-porous, inorganic aerogel materials and to extend the range of bulk densities over which such materials can be directly made.

408. Photoactivated Catalysis on Aerogels - DOE Contact A. E. Evans, (301) 353-3098; LLNL Contact C. A. Colmenares, (415) 422-6352/FTS 532-6352

- We have demonstrated that SiO_2 aerogels doped with uranyl ions are catalytically active for the production hydrocarbons from simple gas mixtures (i.e., Co + H_2, $H_2 + C_2H_4$, and H_2 + C_2H_6) using sunlight as the energy source. We are currently investigating other dopants (i.e., Ce^{IV}, Eu^{IV}, Fe^{+3}, and others) and the basic energy transfer mechanism using surface-sensitive and optical spectroscopies.

409. Synthesis Project (Explosives) - DOE Contact A. E. Evans, (301) 353-3098/ FTS 233-3098; LLNL Contact C. L. Coon, (415) 422-6311

- Synthesize new, energetic materials which have the potential of surpassing HMX in terms of performance and safety.

- Developing new synthetic approaches to the synthesis of nitro and nitroamine compounds.

410. Synthesis and Reactivity of Transition Metal Fluorocarbon Complexes - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; LLNL Contact Robert D. Sanner, (415) 423-3875/FTS 543-3875

- The objectives are to synthesize new transition metal fluorocarbon complexes and to investigate the reactivity of the compounds.

411. Sputtering (Plutonium Alloys) - DOE Contact A. E. Evans, (301) 353-3098/ FTS 233-3098; LLNL Contact H F. Rizzo, (415) 422-6369

- Synthesize Pu-rich alloys using the triode sputtering system under various conditions to determine the influence of different solute elements on the stability of Pu-rich alloys.

412. Organic Aerogels - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; LLNL Contact R. W. Pekala, (415) 422-0152

- This project examines the synthesis of aerogels from organic precursors using sol-gel chemistry.

413. Polymer Coating and Foam Development - DOE Contact A. E. Evans, (301) 353-3098; LLNL Contact S. A. Letts, (415) 423-2681/FTS 543-2681

- Low density, porous, polymer foams are being developed to hold liquid DT fuel for direct-drive laser fusion targets. Ultra smooth, uniform plasma polymer coatings are being developed as ablator layers for direct-drive laser targets.

414. Atomic Engineering - DOE Contact A. E. Evans, (301) 353-3098; LLNL Contact Troy W. Barbee, Jr., (415) 423-7796/FTS 543-7796

- Physical vapor deposition techniques are being used to synthesize ordered compounds by a sequential atomic layer technique. Particular emphasis is being placed on superconducting oxides and dimensionality sensitive compounds.

Materials Structure and Composition

415. Theory of the Structure and Dynamics of Molecular Fluids - DOE Contact A. E. Evans, (301) 353-3098; LLNL Contact D. F. Calef, (415) 422-7797/ FTS 532-7797

- Develop improved theoretical models for the thermodynamic and kinetic behavior of molecular fluids, especially under the conditions of extreme pressure and temperature found in detonations.

416. Site-Specific Chemistry Using Synchrotron Radiation - DOE Contact A. E. Evans, (301) 353-3098; LLNL Contact Joe Wong, (415) 423-6385

- Utilize a couple of advanced X-ray spectroscopic tools, EXAFS and XANES, to investigate the local atomic structure and chemical bonding of selected constituent elements in a variety of materials that are of relevance to current and/or future programmatic needs.

417. Capillary Structures (in Foams) - DOE Contact A. E. Evans, (301) 353-3098/ FTS 233-3098; LLNL Contact R. W. Hopper, (415) 423-2420

- The objectives of this study are understanding of the characteristics and evolution of the structures in real and reciprocal space, and of the mechanical properties of foams.

418. Plutonium Pyrochemical Research - DOE Contact A. E. Evans, (301) 353-3098/ FTS 233-3098; LLNL Contact O. H. Krikorian, (415) 422-8076

- The objective of this research is to determine the thermodynamics, kinetics, and mechanisms of reactions of Pu with Si and Aℓ in molten metal systems that have relevance to pyrochemical recovery processes for Pu from residual waste materials.

419. Electronic Structure in Superconducting Oxides - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; LLNL Contact M. J. Fluss, (415) 423-6665/ FTS 543-6665

- We have put into place a multidisciplinary program involving the chemistry, physics, and technology of high-temperature superconductors with the goal of deducing the mechanism underlying their properties.

420. Theory of Superconducting Oxides - DOE Contact A. E. Evans, (301) 353-3098/ FTS 233-3098; LLNL Contact A. McMahan, (415) 422-7198/FTS 532-7198

- A diverse theoretical effort looking at both new superconducting mechanisms and the details of the electronic properties of superconducting oxides and related compounds.

421. A New Method for the Calculation of the Electronic Structure of Surfaces and Interfaces - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; LLNL Contact A. Gonis, (415) 423-5836/FTS 543-5836

- The objective of this research is to develop first-principles, charge self-consistent methods for the determination of the electronic structure of surfaces and grain boundaries.

Materials Properties, Behavior, Characterization or Testing

422. Nuclear Spin Polarization - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; LLNL Contact P. C. Souers, (415) 422-1302

- In order to eventually make high-cross section nuclear fusion fuel, it is necessary to discover the magnetic resonance parameters needed to ensure the best chance of creating sizeable nuclear polarization of solid deuterium-tritium and to undertake the actual polarization with the best equipment available.

423. Measurement of Tritium Permeation Through Resistant Materials at Low Temperatures - DOE Contact A. E. Evans, (301) 353-3098; FTS 233-3098; LLNL Contact Jon L. Maienschein, (415) 423-1816/FTS 543-1816

- Measuring tritium permeation through resistant materials at 10-170°C, using a very sensitive method developed in this laboratory, to enhance our understanding of the permeation process at low temperatures.

424. Pretransformation Behavior in Alloys - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; LLNL Contact L. E. Tanner, (415) 423-2653

- This investigation characterizes the structural behavior of metallic solid solutions as they approach phase transformations. The emphasis is on premartensitic modulated microstructures.

425. Interfacial Bonding in Multilayer X-ray Mirrors - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; LLNL Contact A. F. Jankowski, (415) 523-2519/FTS 543-2519

- The motivation for this study was to determine the cause for differences measures in the X-ray reflectivities between W/C and newly developed W/B_4C multilayer X-ray mirrors.

426. ΔN=O Spectroscopy Using Multilayer Gratings - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; LLNL Contacts T. W. Barbee, Jr., (415) 423-7796 and D. D. Dietrich, (415) 422-7868

- Normal incidence multilayer focusing gratings operating in the spectral range 15 to 300 eV are being developed for experimental studies of the ΔN=O transitions in helium-like heavy ions.

427. Multilayer X-ray Optics Development - DOE Contact A. E. Evans, (301) 353-3098/ FTS 233-3098; LLNL Contact Troy W. Barbee, Jr., (415) 423-7796

- Development of X-ray multilayer optic elements and instrumentation has been the objective of this program. Specific optics studied include concave figured optics, flat multilayers and diffraction gratings for Cassegrain telescopes, monochromators and spectrometers.

428. Thin Film X-ray Studies - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; LLNL Contact Troy W. Barbee, Jr., (415) 423-7796

- Development of techniques for characterization of ultra thin films (0.1 monolayer to 5 monolayer thick) using X-ray scattering and fluorescence EXAFS has been the objective of this study. This will allow development of an understanding of interface formation.

429. In Situ Reversed Deformation Experiments - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; LLNL Contact M. E. Kassner, (415) 423-2329/ FTS 543-2329

- Continue the world's first *in situ* cyclic or reversed plastic deformation tests in the high-voltage transmission electron microscope (HVEM).

430. Dislocation Microstructure of Aluminum and Silver Deformed to Large Steady-State Creep - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; LLNL Contact M. E. Kassner, (415) 423-2329/FTS 543-2329

- The objectives of this work are to experimentally identify (a) the phenomenology and theory of extended ductility of pure aluminum and other high-stacking fault metals and alloys, (b) the source for large-strain softening of aluminum at elevated temperature, (c) the phenomenology and theory of steady-state deformation of silver at ambient temperature, which provides insight into the mechanism for intermediate creep in pure metals, (d) the dynamic restoration mechanism of Al-Mg alloys deformed to large strains at elevated temperature.

431. Delayed Failure of Silver-Aided Diffusion Bonds - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; LLNL Contact M. E. Kassner, (415) 423-2329/ FTS 543-2329

- To determine the mechanisms of delayed failure in silver-aided diffusion bonds.

432. Constitutive and Failure Behavior of Metals at High Rates of Tensile Strain - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; LLNL Contact W. H. Gourdin, (415) 422-8093/FTS 532-8093

- Stress-strain data from expanding ring experiments has been combined with results from tests at lower rates to derive a new set of parameters for the mechanical threshold stress constitutive model for oxygen free electronic (OFE) grade copper of various grain sizes.

433. Theoretical and Experimental Studies of Solid Combustion Reactions - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; LLNL Contact J. B. Holt, (415) 422-8003/FTS 532-8003

- The objectives of this work were to develop a mathematical model for condensed phase combustion involving a sequential reaction mechanism and to determine kinetic constants for a model reaction such as Ti and C.

434. Fracture Behavior of Refractory Metals and Alloys in Liquid Actinides - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; LLNL Contact J. S. Huang, (415) 422-5645

- This investigation characterizes the mechanical behaviors of refractory metals and alloys in liquid actinides. The emphasis is on the study of micromechanisms of fracture and of the relations between phase diagrams and micromechanisms of fracture.

435. Modeling and Experimental Measurement of Residual Stress - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; LLNL Contact E. Flower, (415) 423-1572/FTS 543-1572

- The objective of this work is to further understand the evolution of residual stress in metal components and to determine strengths and limitations of measurement techniques.

436. Failure Characterization of Composite Materials - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; LLNL Contact Scott E. Groves, (415) 422-1331/ FTS 532-1331

- The primary objective of this research is to characterize the three-dimensional failure response of continuous fiber graphite epoxy composite materials.

437. Surface Modification to Reduce Abrasion and Friction - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; LLNL Contact Herman R. Leider, (415) 423-1884/ FTS 543-1884

- The objective of this program is to determine enhanced resistance to particle abrasion of surfaces covered by ceramic-like hair (i.e., filters).

438. Numerical Modeling of Crack Growth - DOE Contact A. E. Evans, (301) 353-3098/ FTS 233-3098; LLNL Contact R. A. Riddle, (415) 423-7541/FTS 543-7541

- We are developing new analytical tools to predict the effect of cracks and other defects on the strength of structural components. We have updated a J integral post-processor for the finite code NIK2D to calculate the energy release rate at crack tips due to thermal and residual stresses, and body forces.

439. Interfaces, Adhesion and Bonding - DOE Contact A. E. Evans, (301) 353-3098/ FTS 233-3098; LLNL Contact Wayne E. King, (415) 423-6547/FTS 543-6547

- The interface, adhesion, and bonding thrust area is investigating the influence of impurities, flaws, and inclusions on adhesion and bonding at internal interfaces. The initial phase of a work requires characterization of the structure and properties of pure interfaces as a baseline for future research.

Device or Component Fabrication, Behavior or Testing

440. IC Protective Coatings - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; LLNL Contact M. O. Riley, (415) 422-6865/FTS 532-3045

- The goal of this work is the development of protective coatings to safeguard microelectronic chips.

441. Characterization of Solid-State Microstructures in High Explosives by Synchrotron X-ray Tomography - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; LLNL Contact W. C. Tao, (415) 423-0499/FTS 543-0499

- The objectives of this research are to characterize non-destructively the type and distribution of microstructural defects in high explosive single crystals and composite formulation, and to examine their respective influences on Hot-Spot generation and propagation.

442. Optical Diagnostics of High Explosives Reaction Chemistry - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; LLNL Contact S. F. Rice, (415) 423-3258/FTS 543-3258

- The objectives of this research are to develop time resolved techniques to study the molecular and microscopic behavior of the reaction zone of detonating and deflagrating energetic materials. Special emphasis is placed on pulsed laser probes designed to study the chemical kinetics of reactions under these conditions.

Instrumentation and Facilities

443. Scanning Tunneling Microscope - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; LLNL Contact W. Siekhaus, (415) 422-6884/FTS 532-6884

- The technical objectives of this program are to develop STM's capable of performing structural analysis and spectroscopic analysis in fluids (air, water, oil) and in ultrahigh vacuum (UHV).

444. Scanning Tunneling Microscopy (STM) and Atomic Force Microscope (AFM) as a Detector - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; LLNL Contact W. Siekhaus, (415) 422-6884/FTS 532-6884

- Scanning tunneling microscopy, in conjunction with the atomic force microscope, can now be used to detect and characterize submicron defects on optical components which may be conductors or insulators.

445. Tritium Facility Upgrade - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; LLNL Contact G. M. Morris, (415) 423-1770/FTS 543-1770

- Consists of three line items: (1) a new 5,700 square foot office addition along with the modification of 2,000 square feet of the existing facility, (2) a Vacuum Effluent and Recovery System (VERS) designed to recover over 90 percent of the existing routine stack emissions, (3) a Secondarily Contained Tritium System (SCOTS) which replaces the existing low and high pressure systems with a modern totally secondarily contained system.

446. Decontamination and Waste Treatment Facility (DWTF) - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; LLNL Contact R. Quong, (415) 422-7093/FTS 532-7093

- The proposed Decontamination and Waste Treatment Facility (DWTF) will provide complete radioactive, mixed, and hazardous waste treatment capability of laboratory generated wastes.

Los Alamos National Laboratory

Materials Preparation, Synthesis, Deposition, Growth or Forming

447. Actinide Alloy Development - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-098; LANL Contact D. C. Christensen, (505) 667-2556/FTS 843-2556

- Development of new alloys of plutonium, including casting, thermomechanical working, sputtering, and stability studies.

- Measurements of resistivity, thermal expansion and bend ductility to evaluate fabrication processes and alloy stability.

448. Plutonium Oxide Reduction - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; LANL Contact D. Peterson, (505) 667-5181/FTS 843-5181

- Determination of thermodynamics of interactions used in direct-oxide reduction of plutonium.

449. Ion-Beam Implantation - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; LANL Contact D. V. Duchane, (505) 667-6887/FTS 843-6887

- Exploration of ion implantation for surface modification.

- Goals of improved surface hardness and corrosion resistance.

450. Electroplating Low Atomic Number Materials - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; LANL Contact D. V. Duchane, (505) 667-3238/ FTS 843-3238

- Investigation of electroplating low atomic number metals (aluminum and beryllium) by using non-aqueous plating baths.

451. Liquid Crystal Polymer Development - DOE Contact A. E. Evans, (301) 353-3098/ FTS 233-3098; LANL Contact Dave Duchane, (505) 667-6887/FTS 843-6887

- Synthesis of a liquid crystal polymer with strength in three dimensions.

452. Surface Property Modified Plastic Components - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; LANL Contact D. V. Duchane, (505) 667-6887/ FTS 843-6887

- Modification of surface properties of plastic components by a solvent infusion process.
- Use of process to improve the biocompatibility properties of such plastics as acrylics and silicones.

453. Low-Density, Microcellular Plastic Foams - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; LANL Contact D. V. Duchane, (505) 667-6887/ FTS 843-6887

- Manufacture of microstructural polyolefin foams with densities between 0.01 g/cc and 0.2 g/cc by a nonconventional foaming process.

454. Target Coatings - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3912; LANL Contact D. V. Duchane, (505) 667-6887/FTS 843-6887

- Development of single and multilayer metallic and nonmetallic thin film coatings, smooth and uniform in thickness.

455. Physical Vapor Deposition and Surface Analysis - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; LANL Contact D. V. Duchane, (505) 667-6887/ FTS 843-6887

- Physical vapor deposition and sputtering to produce materials for structural applications, corrosion resistance, optical properties, and thin film transducers.

456. Chemical Vapor Deposition (CVD) Coatings - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; LANL Contacts J. R. Laia and D. W. Carroll, (505) 667-3239/FTS 843-3239

- Development of CVD thin film and bulk coatings by a variety of techniques including conventional flow-by, fluid-bed, plasma-assisted, MOCVD, and chemical vapor infiltration (CVI) in support of DoE, DoD, and other Federal agency programs.
- Synthesis/application of new CVD organometallic precursors for low temperature (<300°C) deposition.
- *In-situ* diagnostics of CV reactors/processes using various spectroscopies to feed back data for process control (intelligent processing).
- Modeling activities in support of CVD coating systems—reactor systems, chemical systems, and fluid dynamics.
- Laser-assisted CVD and laser material interactions.

457. Synthesis of Metallic Glasses - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; LANL Contact A. Mayer, (505) 667-1146/FTS 843-1146

- Investigation of feasibility of synthesis of a broad range of metallic glasses by electrodeposition.
- Investigate the feasibility of synthesizing amorphous metallic powders by chemical reduction techniques from aqueous solutions.
- Applications: hard coating, corrosion-resistant coatings, biomedical applications, weapons physics, inertial confinement fusion.

458. Polymers and Adhesives - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; LANL Contact D. A. Hemphill, (505) 667-8335/FTS 843-8335

- Development of fabrication processes and evaluation and testing of commercial and special plastic and composite materials for weapons programs.

- Development of highly filled polymers, high strength composites, cushioning materials, high-explosive compatible adhesives, potting materials, and castable loaded thermoplastics.

- Apply commercial and developmental plastics and composites fabrication techniques to specific weapons materials and components for the purpose of improving weapon efficiency and economy.

459. Tritiated Materials - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; LANL Contact D. H. W. Carstens, (505) 667-5849/FTS 843-5849

- Advanced R&D on low-Z, tritiated materials with the emphasis on Li(D,T) (salt) and other metal tritides.

- Studies of new methods for preparing, fabricating, and containing such compounds, and for measurement of properties.

460. Salt Fabrication - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; LANL Contact D. H. W. Carstens, (505) 667-5849/FTS 843-5849

- Development and evaluation of fabrication processes for lithium tritide deuteride.

- Use of hot pressing and machining to improve part shape versatility, density, and surface quality.

- Conduct of component integrity studies involving radiation induced growth and outgassing.

461. Slip Casting of Ceramics - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; LANL Contact G. F. Hurley, (505) 667-9498/FTS 843-9498

- Slip casting of many ceramics including alumina, magnesia, and thoria.

- Use of colloidal chemistry and powder characterization theory along with materials engineering.

462. Whisker Growth Technology - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; LANL Contact P. D. Shalek, (505) 667-6863

- Growth of long VLS silicon carbide whiskers for spinning and weaving development and ultimate composite reinforcement.

463. New Hot Processing Technology - DOE Contact A. E. Evans, (301) 353-3098/ FTS 233-3098; LANL Contact H. Casey, (505) 667-4365/FTS 843-4365

- Use of hot pressing techniques to consolidate bodies of materials such as Al_2O_3, ZrO_2, UO_2, B_4C, copper, aluminum, and carbon for application such as armor, ceramic components for nuclear reactor meltdown experiments, nuclear shielding, and filters.

464. Glass and Ceramic Coatings - DOE Contact A. E. Evans, (301) 353-3098/ FTS 233-3098; LANL Contact R. E. Honnell, (505) 667-5432

- Fabrication of ceramic-metal seals, insulating coatings, and metallurgy.

465. Cold Pressing, Cold Isostatic Pressing and Sintering - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; LANL Contact G. F. Hurley, (505) 667-9498/ FTS 843-9498

- Use of cold pressing and cold isostatic pressing to consolidate ceramic and metal powders in support of laboratory programs.

466. Plasma-Flame Spraying Technology - DOE Contact A. E. Evans, (301) 353-3098/ FTS 233-3098; LANL Contact H. Casey, (505) 667-4365/FTS 843-4365

- Fabrication of free-standing shapes, and metallic and ceramic coatings by plasma spraying.

467. Rapid Solidification Technology - DOE Contact A. E. Evans, (301) 353-3098/ FTS 233-3098; LANL Contact H. Casey, (505) 667-4365/FTS 843-4365

- Development of RSR technologies such as melt spinning, splat cooling, and rapid solidification plasma spraying.

- Alloy development, microstructural analysis, properties testing, process development, modeling.

468. Superplastic Forming - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; LANL Contact H. Casey, (505) 667-4365/FTS 843-4365

- Investigation of superplastic forming of titanium and uranium alloys.

- Evaluation of fine grained U-6 wt% Nb (2m grain size) in biaxial forming.

469. Microwave Sintering/Processing - DOE Contact A. E. Evans, (301) 353-3098/ FTS 233-3098; LANL Contact J. D. Katz, (505) 667-1424/FTS 843-1424

- Investigating techniques of bonding and sintering ceramics such as Al_2O_3, B_4C and TiB_2.
- Use of 2.45 GHz microwaves which couple directly to the area in which the heat is needed.
- Investigation of the control of the heating and its effect on microstructure.

470. Predictions of Super Strong Polymers - DOE Contact Iran Thomas, (301) 353-3427/ FTS 233-3427; LANL Contact Flonnie Dowell, (505) 667-8765/FTS 843-8765

- First-principles mathematical models have been developed to predict (with the aid of computer-based modeling) new molecular structures most likely to form super strong polymers.
- Candidate molecules are being chemically synthesized and will be experimentally characterized.

471. High Energy Storage Material - DOE Contact C. B. Hillard, (301) 353-3687; LANL Contact D. V. Duchane, (505) 667-6887

- Development of vinyl fluoride/tufluoroethylene copolymer with improved dielectric properties for energy storage.

472. Synthesis of Ceramic Coatings - DOE Contact A. E. Evans, (301) 353-3098/ FTS 233-3098; LANL C. P. Scherer, (505) 665-3202

- Synthesis of ceramic coatings via sol gel techniques.

473. Laser Surface Treatment of Materials - DOE Contact A. E. Evans, (301)(353-3098/ FTS 233-3098; LANL Contact D. V. Duchane, (505) 667-6887/FTS 843-6887

- Laser treatment of metallic surfaces to modify properties such as coefficient of friction and corrosion resistance.

Materials Structure or Composition

474. Actinide Surface Properties - DOE Contact A. E. Evans, (301) 353-3098/ FTS 233-3098; LANL Contact D. C. Christensen, (505) 667-2556/FTS 843-2556

- Characterization of actinide metal, alloy and compound surfaces using the techniques of x-ray photoelectron spectroscopy, Auger analysis, ellipsometry and Fourier-transform infrared spectroscopy.

- Studies of surface reactions, chemisorption, attack by hydrogen, nature of associated catalytic processes.

475. Neutron Diffraction of Pu and Pu Alloys - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; LANL Contact A. C. Lawson, (505) 667-8844/ FTS 843-8844

- Neutron diffraction studies of plutonium and its alloys conducted at the Manual Lugan, Jr., Neutron Scattering Center (Los Alamos) and the Intense Pulsed Neutron Source (Argonne).

- Time-of-flight technique used to measure diffraction at cryogenic and elevated temperatures.

476. Surface, Material and Analytical Studies - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3912; LANL Contact W. C. Danen, (505) 667-4686

- Studies of surface and interfacial structures and properties, explosive dynamics, and laser based isotopic analysis.

- Use of techniques such as Low Energy Electron Diffraction (LEED), Auger and Loss Spectroscopies, Ion-Scattering Spectroscopy (ISS), Ultraviolet Photoelectron Spectroscopy (UPS), Synchrotron Radiation, and MeV-ion-beam scattering.

Materials Properties, Behavior, Characterization or Testing

477. Mechanical Properties of Plutonium and Its Alloys - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; LANL Contact M. Stevens, (505) 667-4414/ FTS 843-4414

- Study relationship of mechanical properties of Pu and Pu alloys to their microstructures.

- Use of optical and electron microscopy, X-ray, electron, and neutron diffraction.

478. Phase Transformations in Pu and Pu Alloys - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; LANL Contact M. Stevens, (505) 667-4414/ FTS 843-4414

- Investigation of mechanisms, crystallography, and kinetics of transformations in plutonium and alloys using pressure and temperature dilatometry, optical metallography, and X-ray diffraction.

479. Isobaric Expansion of Actinides - DOE Contact A. E. Evans, (301) 353-3098/ FTS 233-3098; LANL Contact R. Mulford, (505) 667-3543/FTS 843-3543

- Study of P-V relationships in liquid actinide elements by isobaric expansion.

480. Plutonium Shock Deformation - DOE Contact A. E. Evans, (301) 353-3098/ FTS 233-3098; LANL Contact M. J. Reisfeld, (505) 667-1375/FTS 843-1375

- Plutonium alloys subjected to shock deformation, recovered and examined to determine effects of shock on microstructures and mechanical properties.

481. Non-Destructive Evaluation - DOE Contact A. E. Evans, (301) 353-3098/ FTS 233-3098; LANL Contact M. Mathieson, (505) 667-6404/FTS 843-6404

- Development of nondestructive evaluation technology that produces qualitative estimates of material properties.

- Flash radiography, cine radiography, ultrasonic in-process probing, and tomographic techniques to enhance radiography.

482. Powder Characterization - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; LANL Contact G. J. Vogt, (505) 667-5813

- Characterization of particle size, surface area, morphology, pore size and zeta potential.

- Powders of thoria, silicon nitride, magnesia, alumina, tungsten, tungsten carbide, and copper.

483. Shock Deformation in Actinide Materials - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; LANL Contact M. Stevens, (505) 667-4414/ FTS 843-4414

- Characterization of shock effects in uranium, plutonium and plutonium alloys through use of soft recovery techniques.

484. Dynamic Mechanical Properties of Weapons Materials - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; LANL Contact P. Armstrong, (505) 667-4889

- Dynamic stress-strain and fracture behavior of potential earth penetrator materials.

485. Dynamic Testing of Materials for Hyper-Velocity Projectiles - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; LANL Contact G. T. Gray, III, (505) 667-5452/FTS 843-5452

- Microstructural characterization of soft-recovered shock-loaded materials.
- Dynamic and quasi-static mechanical testing.

486. Mechanical Properties - DOE Contact R. J. Gottschall, (301) 353-3428/ FTS 233-3428; LANL Contact M. G. Stout, (505) 667-4665/FTS 843-4665

- Multiaxial testing of metal and alloys.
- Prediction of texture development and its effects.

487. Radiation Damage in High-Temperature Superconductors - DOE Contact R. J. Gottschall, (301) 353-3428/FTS 233-3428; LANL Contact K. E. Sickafus, (505) 667-3457/FTS 843-3457

- Irradiation testing of HTSC's using various particles.
- Interpretation of damage response in terms of microstructural and physical properties.

488. Structural and Superconducting Ceramics - DOE Contact R. J. Gottschall, (301) 353-3428; LANL Contact J. J. Petrovic, (505) 667-0125/FTS 843-0125

- Interfacial and irradiation effects in structural and superconducting ceramics.

Device or Component Fabrication, Behavior or Testing

489. Radiochemistry Detector Coatings - DOE Contact A. E. Evans, (301) 353-3098/ FTS 233-3098; LANL Contact D. V. Duchane, (505) 667-6887/FTS 843-6887

- Physical vapor deposition of coatings for radiochemical detectors.

490. Target Fabrication - DOE Contact C. B. Hilland, (301) 353-3687/FTS 233-3687; LANL Contact D. V. Duchane, (505) 667-6887/FTS 843-6887; KMS Fusion, Inc., Contact Timothy Henderson, (313) 769-8500, ext. 302; LLNL Contact W. Hatcher, (415) 422-1100

- Hydrocarbon polymer applied by plasma polymerization to glass microspheres.
- Micromachining, plasma etching, plasma polymerization, laser ablation.
- Targets filled with deuterium/tritium gas.

491. Filament Winder - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; LANL Contact E. Eaton, (505) 667-5261/FTS 843-5261

- Four-axis computer-programmed winding machine.
- Winding envelopes to 4 ft. diameter, 10 ft. long.
- Winds helixes, cones, spheres, closed-end vessels of glass, kevlar, carbon, tungsten, and alumina fibers.

492. Polymeric Laser Rods - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; LANL Contact D. V. Duchane, (505) 667-6887/FTS 843-6887

- Development of polymeric-host dye-laser rods.
- *In situ* polymerization of dye/monomer mixture.
- Inexpensive "disposal" laser rods.

493. High Energy Density Joining Process Development - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; LANL Contact H. Casey, (505) 667-4365/ FTS 843-4365

- Development of microcomputer technology and signal analysis for process control and multiaxis, programmable component manipulation for high-voltage electron beam welding.
- Operation of a high-voltage electron beam welder for fabrication of products in the fissile material area.
- Investigation of real-time diagnostics of laser welding efficiency.

- Study of plasma effects on laser welding efficiency.

- Correlation of photodiode, acoustic, light-spectral and electron current measurements with high speed cinematography and resultant weld geometry.

494. Arc Welding Process Development - DOE Contact A. E. Evans, (301) 353-3098/ FTS 233-3098; LANL Contact H. Casey, (505) 667-4365/FTS 843-4365

- Video monitoring and Varistraint testing established as techniques to investigate crack susceptibility of gas-tungsten-arc welds.

495. Solid State Bonding - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; LANL Contact H. Casey, (505) 667-4365/FTS 843-4365

- Evaluating aluminum solid-state bonding for seamless ICF targets.

- Evaluation of bond load modulation and ion bombardment cleaning.

- Investigation of bonding technique optimization.

OFFICE OF FOSSIL ENERGY

	FY 1989
Office of Fossil Energy - Grand Total	$7,070,000
Office of Technical Coordination	$6,970,000
Fossil Energy AR&TD Materials Program	$6,970,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$2,009,000
Fundamental Study of Aluminizing and Chromizing Processes	0
Development of Iron Aluminides	333,000
Development and Evaluation of Advanced Austenitic Alloys	260,000
Evaluation of the Fabricability of Advanced Austenitic Alloys	144,000
Consolidation of Rapidly Solidified Aluminide Metal Powders	175,000
Investigation of Electrospark Deposited Coatings for Protection of Materials in Sulfidizing Atmospheres	50,000
Vapor-Liquid-Solid SiC Whisker Process Development	200,000
Sol-Gel Synthesis of Ceramics	75,000
Fabrication of Fiber-Reinforced Composites by Chemical Vapor Infiltration	190,000
Characterization of Fiber-CVD Matrix Interfacial Bonds	140,000
Microwave Sintering of Ceramics	200,000
Development of Advanced Fiber Reinforced Ceramics	192,000
Modeling of Fibrous Preforms for CVD Infiltration	50,000
Materials Structure and Composition	$ 300,000
Analytical Characterization of Coal Surfaces and Interfaces	300,000
Materials Properties, Behavior, Characterization or Testing	$2,914,000
Transfer Model Predicting Thermomechanical Behavior of Refractory Linings to Industry	65,000
Mechanical Properties and Microstructural Stability of Advanced Austenitic Alloys	125,000
Investigation of the Weldability of Ductile Aluminides	75,000
Corrosion Studies of Iron Aluminides	50,000

OFFICE OF FOSSIL ENERGY (Continued)

	FY 1989
Materials Properties, Behavior, Characterization or Testing (continued)	
Fireside Corrosion Tests of Candidate Advanced Austenitic Alloys, Coatings, and Claddings	15,000
Microstructural Studies of Advanced Austenitic Steels	35,000
Joining Techniques for Advanced Austenitic Alloys	37,000
Corrosion and Mechanical Properties of Alloys in FBC and Mixed-Gas Environments	320,000
Development of Surface Treatments and Modifications to Produce Corrosion-Resistant Oxide Scales	195,000
Investigation of the Effects of Microalloy Constituents, Surface Treatment, and Oxidation Conditions on Development and Breakdown of Protective Oxide Scales	110,000
Investigation of the Effects of Microalloy Constituents, Surface Treatment, and Oxidation Conditions on Development and Breakdown of Protective Oxide Scales	50,000
Investigation of the Effects of Microalloy Constituents, Surface Treatment, and Oxidation Conditions on Development and Breakdown of Protective Oxide Scales	139,000
Molten Salt-Induced Corrosion of Iron Aluminides	32,000
A Study of Erosive Particle Rebound Parameters	122,000
Studies of Materials Erosion in Coal Conversion and Utilization Systems	250,000
In-Situ Scanning Electron Microscopy Studies of Erosion and Erosion-Corrosion	195,000
Solid Particle Erosion in Turbulent Flows Past Tube Banks	0
Study of Particle Rebound Characteristics and Material Erosion at High Temperatures	110,000
Development of Nondestructive Evaluation Techniques and the Effect of Flaws on the Fracture Behavior of Structural Ceramics	315,000
Joining of Silicon Carbide Reinforced Ceramics	175,000
Nondestructive Evaluation of Advanced Ceramic Composite Materials	175,000
Structural Reliability and Damage Tolerance of Ceramic Composites	150,000

OFFICE OF FOSSIL ENERGY (Continued)

	FY 1989
Materials Properties, Behavior, Characterization or Testing (continued)	
Mechanical Properties of Ceramic Fiber-Ceramic Matrix Composites	74,000
Ceramic Catalyst Materials	100,000
Device or Component Fabrication, Behavior or Testing	$1,302,000
Materials and Components in Fossil Energy Applications (Newsletter)	110,000
Assessment of Potential Applications of Ceramic Composites in Gas Turbines	0
Mechanisms of Galling and Abrasive Wear	50,000
Fabrication of Commercial-Scale Fiber-Reinforced Hot-Gas Filters by Chemical Vapor Deposition	149,000
Development of Ceramic Membranes for Gas Separation	130,000
Investigation of the Mechanical Properties of CVD Infiltrated Ceramic Composite Tubular Components	0
Material Data Base Development for Refractories	78,000
Advanced Materials and Electrochemical Processes in High-Temperature Solid Electrolytes	250,000
Gas Separations Using Inorganic Membranes	200,000
Ceramic Fiber-Ceramic Matrix Hot Gas Filters	200,000
Identification of Materials for Hot-Gas Filter Tubesheets	135,000
Instrumentation and Facilities	$ 445,000
Management of the Fossil Energy AR&TD Materials Program	350,000
Coal Conversion and Utilization Plant Support Services	45,000
Assessment of Fossil Energy Materials Research Needs	50,000
Assessment of the Potential for Transfer of AR&TD Materials Program Technologies to Oil, Gas, and Shale Industries	0

OFFICE OF FOSSIL ENERGY (Continued)

	FY 1989
Office of Coal Technology	$ 100,000
Division of Coal Conversion	$ 0
Instrumentation and Facilities	$ 0
Materials Technical Support for the Great Plains Coal Gasification Plant	0
Division of Clean Coal Technology	$ 100,000
Instrumentation and Facilities	$ 100,000
Materials Technical Support for the Clean Coal Program	100,000

OFFICE OF FOSSIL ENERGY

The mission of the Fossil Energy Program is to develop technologies that will increase domestic production of oil and gas or that will permit the Nation to shift from oil or gas to more abundant coal. Specifically, the Fossil Energy role is to develop technologies to support the following objectives:

- Provide a capability to convert coal to liquid and gaseous fuels;
- Increase domestic production of coal, oil, and gas;
- Ensure that current and new facilities that burn coal can do so in an economically viable and environmentally acceptable manner; and
- Allow more efficient and more economically attractive utilization of fossil energy resources.

The Fossil Energy activity includes fourteen major programs, which are grouped under seven program offices. One of these seven is the Advanced Research and Technology Development Program of the Office of Technical Coordination, which is the central point of contact for inquiries from universities concerning the Fossil Energy program.

Project execution and technical monitoring are administered in five energy technology centers and selected national laboratories.

Office of Technical Coordination

Fossil Energy AR&TD Materials Program

The objectives of the Advanced Research and Technology Development program are to assess and identify long-range advanced research needs in coal processing, fossil fuels utilization and extraction, materials, components, and instrumentation; to provide oversight of ongoing advanced research in fossil energy so as to ensure balance and proper priorities; to initiate and fund projects involving new, exploratory concepts or goal-oriented basic research; to manage the Materials Research and University Coal Research programs; and to provide policies for, and overview of, Fossil Energy-supported university activities. The Advanced Research and Technology Development program also is designed to provide an effective communications channel between the Fossil Energy program and academic institutions; to encourage these institutions to become involved in programs related to the DOE Fossil Energy mission; and to manage programs concerned with providing an adequate technical base for development of commercial construction materials and instrumentation for Fossil Energy pilot plants and demonstration plants.

The program supports workshops to identify research needs in all fossil energy technologies and manages selected training programs for faculty and students at Energy Technology Centers.

Materials Preparation, Synthesis, Deposition, Growth or Forming

496. Fundamental Study of Aluminizing and Chromizing Processes - DOE Contacts J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/ FTS 626-0735; Ohio State University Contact R. A. Rapp, (614) 292-6178

- The purpose of this work is to conduct a study of aluminizing and chromizing of iron-base alloys which will lead to a fundamental understanding of these processes.

497. Development of Iron Aluminides - DOE Contacts J. P. Carr, (301) 353-6519/ FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; Oak Ridge National Laboratory Contact C. G. McKamey, (615) 574-6917/FTS 624-6917

- The objective of this project is to develop low-cost and 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 conversion systems.

498. Development and Evaluation of Advanced Austenitic Alloys - DOE Contacts J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/ FTS 626-0735; Oak Ridge National Laboratory Contact R. W. Swindeman, (615) 574-5108/FTS 624-5108

- Alloys based on modifications to four groups of alloys will be developed on the basis of attributes required for advanced steam cycle superheater service. The four alloy groups studied include modified type 316 stainless steel, modified type 310 stainless steel, modified high nickel (alloy 800H) steels, and aluminum-containing steels.

499. Evaluation of the Fabricability of Advanced Austenitic Alloys - DOE Contacts J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/ FTS 626-0735; Babcock & Wilcox Contact S. E. LeBeau, (216) 821-9110

- The purpose of this work is to evaluate the fabricability, weldability, and surface treatments of advanced austenitic tubing for superheater applications.

500. Consolidation of Rapidly Solidified Aluminide Metal Powders - DOE Contacts J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/ FTS 626-0735; Idaho National Engineering Laboratory Contacts J. E. Flinn and R. N. Wright, FTS 583-8127

- The purpose of this project is to determine the most effective means of, and associated parameters for, consolidating rapidly solidified nickel-iron aluminide powders.

501. Investigation of Electrospark Deposited Coatings for Protection of Materials in Sulfidizing Atmospheres - DOE Contacts J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; Westinghouse Hanford Company Contact R. N. Johnson, (509) 376-0715

- 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.

502. Vapor-Liquid-Solid SiC Whisker Process Development - DOE Contacts J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; Los Alamos National Laboratory Contact P. D. Shalek, (505) 667-6863/FTS 843-6863

- The purpose of this study is to optimize an existing Los Alamos whisker growth process to produce alpha-phase silicon nitride (alpha-Si_3N_4) whiskers and beta-phase silicon carbide (beta-SiC) whiskers of uniform size, optimum strength, and in quantities suitable for composite use.

503. Sol-Gel Synthesis of Ceramics - DOE Contacts J. P. Carr, (301) 353-6519/ FTS 233-6509 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; Idaho National Engineering Laboratory Contact R. M. Neilson, FTS 583-8274

- The purpose of this activity is to investigate techniques for fabricating sol-gel derived films of $YBa_2Cu_3O_{7-x}$ based superconducting ceramics.

504. Fabrication of Fiber-Reinforced Composites by Chemical Vapor Infiltration (CVI) - DOE Contacts J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; Oak Ridge National Laboratory Contacts D. P. Stinton, (615) 574-4556/FTS 624-4556

- The purpose of this task is to develop a ceramic composite having higher than normal toughness and strength yet retaining the typical ceramic attributes of refractoriness and high resistance to abrasion and corrosion.

505. Characterization of Fiber-CVD Matrix Interfacial Bonds - DOE Contacts J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; Oak Ridge National Laboratory Contact R. A. Lowden, (615) 574-7714/ FTS 624-7714

- The purpose of this task is to optimize the strength and toughness of fiber-reinforced ceramic composites by tailoring the strength of the bonds between the fiber and the matrix.

506. Microwave Sintering of Ceramics - DOE Contacts J. P. Carr, (301) 353-6519/ FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; Oak Ridge National Laboratory Contacts M. A. Janney and H. D. Kimrey, (615) 574-4281/ FTS 624-4281

- The purpose of this activity is to conduct research and development on the microwave processing of new ceramics. The heating and sintering of yttria-stabilized zirconia, the electrolyte for the monolithic fuel cell design, is being studied.

507. Development of Advanced Fiber Reinforced Ceramics - DOE Contacts J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; Georgia Institute of Technology Contact T. L. Starr, (404) 894-3678

- 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.

508. Modeling of Fibrous Preforms for CVD Infiltration - DOE Contacts J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; Georgia Institute of Technology Contact T. L. Starr, (404) 894-3678

- 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.

Materials Structure and Composition

509. Analytical Characterization of Coal Surfaces and Interfaces - DOE Contacts J. D. Hickerson, FTS 723-5721 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; Oak Ridge National Laboratory Contact E. L. Fuller, (615) 574-4959/FTS 624-4959

- The objective of this task is to provide analytical characterization of coal surfaces and interfaces between coal and various included minerals for the purpose of assisting the Pittsburgh Energy Technology Center in its research on coal characterization and cleaning.

Materials Properties, Behavior, Characterization or Testing

510. Transfer Model Predicting Thermomechanical Behavior of Refractory Linings to Industry - DOE Contacts J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; Tennessee Center for Research and Development Contact B. J. George, (615) 675-9505

- The purpose of this activity is to develop user-friendly and intelligent computer-based software for the prediction of thermomechanical behavior of refractory lining systems.

511. Mechanical Properties and Microstructural Stability of Advanced Austenitic Alloys - DOE Contacts J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; Cornell University Contact Che-Yu Li, (607) 256-4349

- The purpose of this project is to rank the strengths and metallurgical stabilities of advanced austenitic alloys at temperatures ranging from 650° to 760°C.

512. Investigation of the Weldability of Ductile Aluminides - DOE Contacts J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; Colorado School of Mines Contact G. R. Edwards, (303) 273-3773

- The purpose of this project is to study the weldability of nickel-iron aluminides.

513. Corrosion Studies of Iron Aluminides - DOE Contacts J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; University of Tennessee Contact R. A. Buchanan, (615) 974-4858

- The objective of this project is to investigate the aqueous corrosion of iron aluminides based on Fe_3Al.

514. Fireside Corrosion Tests of Candidate Advanced Austenitic Alloys, Coatings, and Claddings - DOE Contacts J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; 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.

515. Microstructural Studies of Advanced Austenitic Steels - DOE Contacts J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; University of Southern California Contact J. A. Todd, (213) 743-4966

- The purpose of this project is to develop a thorough understanding of the metallurgical factors contributing to degradation of austenitic alloys in advanced steam power boilers under long-term, high-temperature operating conditions.

516. Joining Techniques for Advanced Austenitic Alloys - DOE Contacts J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; University of Tennessee Contact C. D. Lundin, (615) 874-5310

- 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.

517. Corrosion and Mechanical Properties of Alloys in FBC and Mixed-Gas Environments - DOE Contacts J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; Argonne National Laboratory Contact K. Natesan, (312) 972-5103/FTS 972-5103

- The purposes of this task are to: (1) develop corrosion information in the temperature range 400° to 750°C in mixed-gas atmospheres containing O, S, and Cl by use of internally cooled tube specimens of selected commercial materials, and (2) evaluate mechanisms of the formation and breakaway behavior of protective scales on base metals and weldments exposed to atmospheres containing O, S, and Cl.

518. Development of Surface Treatments and Modifications to Produce Corrosion-Resistant Oxide Scales - DOE Contacts J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; Oak Ridge National Laboratory Contact J. H. DeVan, (615) 574-4451/FTS 624-4451

- The purpose of this task is to develop protective oxide scales on Cr_2O_3- and Al_2O_3-forming iron-based alloys in mixed oxidant (O_2, SO_2, H_2S, H_2O) environments for coal-related applications at 600° to 800°C.

519. Investigation of the Effects of Microalloy Constituents, Surface Treatment, and Oxidation Conditions on Development and Breakdown of Protective Oxide Scales - DOE Contacts J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; Battelle Columbus Laboratories Contact I. G. Wright, (614) 424-4377

- The objective of this program is to gain an improved understanding of the effects of alloying constituents present at low levels on the development and mode of breakdown of protective oxide scales in conditions representing those encountered in combustion and gasification processes.

520. Investigation of the Effects of Microalloy Constituents, Surface Treatment, and Oxidation Conditions on Development and Breakdown of Protective Oxide Scales - DOE Contacts J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; Case Western Reserve University Contact K. M. Vedula, (216) 368-4211

- The focus of the current program is to obtain a better understanding of the effects of reactive element additions on the protectiveness of oxide scales formed in sulfidizing/oxidizing atmospheres.

521. Investigation of the Effects of Microalloy Constituents, Surface Treatment, and Oxidation Conditions on Development and Breakdown of Protective Oxide Scales - DOE Contacts J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; Universal Energy Systems, Inc., Contact V. Srinivasan, (513) 426-6900

- The main objective of this program is to develop a comprehensive basic understanding of the effects of additions of microalloy constituents and the surface conditions on the nucleation, growth and breakdown of protective oxide scales in the mixed oxidant environments relevant to coal utilization and conversion technologies.

522. Molten Salt-Induced Corrosion of Iron Aluminides - DOE Contacts J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; University of Cincinnati (Contract No. DE-AC05-84OR21400, Martin Marietta Energy Systems, Inc. Subcontract No. 19X-SD169V) Contact R. Y. Lin, (513) 556-3116

- The purpose of this project is to evaluate the molten salt-induced hot corrosion of nickel iron and iron aluminides.

523. A Study of Erosive Particle Rebound Parameters - DOE Contacts J. P. Carr, (301) 353-6519; FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; University of Notre Dame Contact T. H. Kosel, (219) 239-5642

- This research project is designed to provide a systematic investigation of the effects of materials properties and experimental variables on the rebound directions and velocities of erodent particles.

524. Studies of Materials Erosion in Coal Conversion and Utilization Systems - DOE Contacts J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; Lawrence Berkeley Laboratory Contact A. V. Levy, (415) 486-5822

- The erosion of materials surfaces by small solid particles carried in gas and liquid streams is being investigated. The materials are tested over a range of conditions that simulate portions of the operating environments of containment surfaces in coal gasification, liquefaction, and fluidized-bed combustion processes.

525. In-Situ Scanning Electron Microscopy Studies of Erosion and Erosion-Corrosion - DOE Contacts J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; Oak Ridge National Laboratory Contact J. R. Keiser, (615) 574-4453/FTS 624-4453

- This project involves the evaluation of erosion and erosion-corrosion of alloys using microscopic techniques.

526. Solid Particle Erosion in Turbulent Flows Past Tube Banks - DOE Contacts J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; University of California, Berkeley Contact J. A. C. Humphrey, (415) 642-6460

- The purpose of this investigation is to improve the understanding of erosion processes in gas streams.

527. Study of Particle Rebound Characteristics and Material Erosion at High Temperatures - DOE Contacts J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; University of Cincinnati Contact W. Tabakoff, (513) 475-2849

- The purpose of this effort is to investigate the erosion processes and fluid mechanics phenomena that occur in fluidized-bed combustors, coal-fired boilers, cyclones, pumps, turbines, valves, and other coal combustion systems.

528. Development of Nondestructive Evaluation Techniques and the Effect of Flaws on the Fracture Behavior of Structural Ceramics - DOE Contacts J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; Argonne National Laboratory Contact J. P. Singh, (312) 972-5132/FTS 972-5132

- 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 NDE techniques.

529. Joining of Silicon Carbide Reinforced Ceramics - DOE Contacts J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; Idaho National Engineering Laboratory Contact B. H. Rabin, FTS 583-0058

- The purpose of this project is to identify and to develop techniques for joining silicon carbide fiber-reinforced composite materials.

530. Nondestructive Evaluation of Advanced Ceramic Composite Materials - DOE Contacts J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; Idaho National Engineering Laboratory Contact J. B. Walter, FTS 583-0033

- The purpose of this project is to develop an effective capability for nondestructive evaluation of ceramic fiber reinforced ceramic composites.

531. Structural Reliability and Damage Tolerance of Ceramic Composites - DOE Contact J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/ FTS 626-0735; National Institute of Standards and Technology Contact E. R. Fuller, (301) 921-2901

- The objective of this study is to characterize the high temperature failure mechanisms and factors that influence their operation with an aim toward improving the properties of structural ceramics, especially silicon carbide and silicon nitride based materials, for use in coal conversion applications.

532. Mechanical Properties of Ceramic Fiber-Ceramic Matrix Composites - DOE Contacts J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/ FTS 626-0735; North Carolina A&T State University Contact J. Sankar, (919) 334-7620

- The purpose of this project is to expand the mechanical properties data base for composites fabricated by forced chemical vapor infiltration (CVI).

533. Ceramic Catalyst Materials - DOE Contacts J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; Sandia National Laboratory Contact D. H. Doughty, FTS 844-1933

- This project involves investigation of the role of ceramic materials properties in the activity and selectivity of novel catalytic materials.

Device or Component Fabrication, Behavior or Testing

534. *Materials and Components in Fossil Energy Applications* (Newsletter) - DOE Contacts J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/ FTS 626-0735; Battelle-Columbus Laboratories Contact I. G. Wright (BCL), (614) 424-4377

- The purpose of this task is to publish a periodic newsletter to address current developments in materials and components in fossil energy applications.

535. Assessment of Potential Applications of Ceramic Composites in Gas Turbines - DOE Contacts J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; Babcock & Wilcox Contact W. P. Parks, (804) 522-6196

- The purpose of this work is to review the materials requirements for direct coal-fired gas turbines or gas turbines for coal gasification combined cycle systems, to assess the state of technology for materials to meet those requirements, and to identify areas and components that require additional materials research and development and for which structural ceramic composites have potential applications.

536. Mechanisms of Galling and Abrasive Wear - DOE Contacts J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; National Institute of Standards and Technology Contact L. K. Ives, (301) 975-6013

- This project is directed to developing an understanding of the wear mechanisms of materials associated with valves in coal conversion systems.

537. Fabrication of Commercial-Scale Fiber-Reinforced Hot-Gas Filters by Chemical Vapor Deposition - DOE Contact J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; 3M Company Contact T. Kafka, (612) 736-1689

- The purpose of this project is to scale-up the chemical vapor infiltration (CVI) process developed at Oak Ridge National Laboratory (ORNL) for fabricating ceramic fiber-ceramic matrix composites. The goal is to use this scaled-up CVI process to produce composite filters.

538. Development of Ceramic Membranes for Gas Separation - DOE Contacts J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; Oak Ridge Gaseous Diffusion Plant Contact D. E. Fain, (615) 574-9932/FTS 624-9932

- 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.

539. Investigation of the Mechanical Properties of CVD Infiltrated Ceramic Composite Tubular Components - DOE Contacts J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; Virginia Polytechnic Institute and State University Contacts K. L. Reifsnider and W. W. Stinchcomb, (703) 961-5316

- 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.

540. Material Data Base Development for Refractories - DOE Contacts J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; Massachusetts Institute of Technology Contact Oral Buyukozturk, (617) 253-7186

- The objective of this task is to study the failure mechanisms of refractory-brick-lined coal gasification vessels under transient temperature loadings.

541. Advanced Materials and Electrochemical Processes in High-Temperature Solid Electrolytes - DOE Contacts J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; Pacific Northwest Laboratory Contact J. L. Bates, (509) 375-2579

- The objective of this research is (1) to identify, develop, and demonstrate advanced materials for use as alternative electrodes and current interconnections in solid oxide fuel cells.

542. Gas Separations Using Inorganic Membranes - DOE Contacts L. A. Jarr, FTS 923-4555 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; Oak Ridge National Laboratory Contact B. Z. Egan, (615) 574-6868/FTS 624-6868

- The objective of this project is to explore the applicability of inorganic membranes to separate gases at high temperatures and/or in hostile process environments encountered in fossil energy conversion processes such as coal gasification.

543. Ceramic Fiber-Ceramic Matrix Hot Gas Filters - DOE Contacts N. Holcombe, 5TS 923-4829 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; Oak Ridge National Laboratory Contact D. P. Stinton, (615) 574-4556/FTS 624-4556

- This task will develop ceramic fiber-ceramic matrix materials and fabrication techniques suitable for production of hot-gas cleanup filters.

544. Identification of Materials for Hot-Gas Filter Tubesheets - DOE Contacts V. Kothari, FTS 923-4505 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; Oak Ridge National Laboratory Contact R. W. Swindeman, (615) 574-5108/FTS 624-5108

- The objective of this work is to assess current tubesheet designs and blowback manifold materials for ceramic crossflow and ceramic candle filters.

Instrumentation and Facilities

545. Management of the Fossil Energy AR&TD Materials Program - DOE Contacts J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/ FTS 626-0735; Oak Ridge National Laboratory Contact R. R. Judkins, P. T. Carlson and D. N. Braski, (615) 574-4572/FTS 624-4572

- 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.

546. Coal Conversion and Utilization Plant Support Services - DOE Contacts J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; Oak Ridge National Laboratory Contact J. R. Keiser, (615) 574-4453/FTS 624-4453

- This task will provide screening data on the susceptibility to corrosion and stress-corrosion cracking of potential materials of construction for coal conversion and utilization plants.

547. Assessment of Fossil Energy Materials Research Needs - DOE Contacts J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735 National Institute of Standards and Technology Contact S. J. Dapkunas, (301) 975-6119

- The purpose of this activity is to identify long-range materials research and development needs and opportunities as they impact evolving fossil energy technologies.

548. Assessment of the Potential for Transfer of AR&TD Materials Program Technologies to Oil, Gas, and Shale Industries - DOE Contacts J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; Oak Ridge National Engineering Laboratory Contact P. T. Carlson, FTS 574-5135

- The purpose of this assessment is to maximize the benefit of research on the AR&TD Materials Program, to enhance Department of Energy (DOE) research and development coordination efforts, and to provide possible materials technologies that could significantly benefit the oil, gas, and shale (OGS) industries.

Office of Coal Technology

The Office of Coal Technology is responsible for management of cooperative agreements with industry to foster clean coal technology; for the conduct of research and development programs for coal combustion and conversion, embodying retrofit or near-or mid-term applications such as fluidized-bed combustion and surface coal gasification; and for environmental, health and safety technology integral to such coal combustion and conversion systems.

Division of Coal Conversion

Instrumentation and Facilities

549. Materials Technical Support for the Great Plains Coal Gasification Plant - DOE Contacts W. Miller, FTS 923-4827 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; Oak Ridge National Laboratory Contact R. R. Judkins, (615) 574-4572/FTS 624-4572

- This task provided materials technical support services to the Great Plains Coal Gasification Plant.

Division of Clean Coal Technology

Instrumentation and Facilities

550. Materials Technical Support for the Clean Coal Program - DOE Contacts R. Santore, FTS 723-6131 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; Oak Ridge National Laboratory Contacts R. R. Judkins, (615) 574-4572/FTS 624-4572 and J. R. Keiser, (615) 574-4453/FTS 624-4453

- This task is to provide materials technical support services to the projects on the Clean Coal Program which are being managed by the DOE-Pittsburgh Energy Technology Center (PETC).

PARAGRAPH DESCRIPTIONS

OFFICE OF ENERGY UTILIZATION RESEARCH*

This office supports generic research of a long-term, high-risk, high-payoff nature aimed at stimulating innovation in conservation technology. The research is both broadly based and multi-sectoral, providing a technology base for the other conservation programs.

Energy Conversion and Utilization Technologies Division**

The mission of ECUT is to support generic, long-term, high-risk directed basic and applied research and exploratory development of new or improved concepts to produce a technology base which private industry can use in producing products that use energy more efficiently. Materials related research in the ECUT Division is found in two programs, the Materials Program*** and the Tribology Program****. The Tribology Program is managed by Argonne National Laboratory (ANL) and the Materials Program out of DOE Headquarters with assistance from several National Laboratories. The goal of both projects is to develop innovative concepts to a point where they can be taken over for further development by private industry or other government programs. The materials work in the Materials Program is in the areas of intermetallic compounds, tough ceramics and composites, biodegradable plastics, recovery and reuse of plastic scrap, corrosion resistant alloys and coatings, materials processing and reliability, superconductors, and thermal insulations. Materials research in the Tribology Program is in the areas of wear of lubricated solids, the friction and wear of ceramics, and tribological surface modifications and coatings. The DOE contact is Stanley M. Wolf, (202) 586-1514 for the Materials Program and David Mello, (202) 586-9345 for the Tribology Program.

*Discontinued after April 1, 1990.

**After April 1, 1990, reorganized into the Advanced Industrial Concepts Division and the Office of Advanced Transportation Materials.

***After April 1, 1990, the Advanced Industrial Materials Program.

****After April 1, 1990, the Transportation Tribology Program.

Materials Preparation, Synthesis, Deposition, Growth or Forming

1. Solid Lubricants Deposited From the Gas Phase FY 1989
$75,000

DOE Contact: D. Mello, (202) 586-9345
The Pennsylvania State University (NIST Grant No. 60NANB5DO548) Contact: E. E. Klaus, (814) 865-2574

This is an investigation of the feasibility of depositing (from the gas phase) hydrocarbon and solid lubricant films onto metal and ceramic substrates. The objective is to assess the viability of the gas phase deposition approach for lubrication of heat engines and industrial machinery and for metal working. The deposition rates and the compositions and structures of the films are determined as functions of the vapor pressures of the lubricant precursors and oxygen in the gas phase, gas flow rate, and substrate temperature. The films are then tested for friction and wear characteristics at high temperatures. Initial efforts were concerned with the development of a vapor delivery system and deposition of films from mineral oil vapors onto iron-, nickel- and copper-based alloys substrates held at temperatures up to 900°C. Current efforts are focused on ceramic substrates doped with small amounts of metal surface-contaminants. Significant decreases in friction for both metal and ceramic/metal-doped substrates have been achieved. The method has also been successfully tested in an experimental engine cylinder kit by Detroit Diesel Allison Division of G.M.

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

2. Engineered Tribological Surfaces FY 1989
$755,000

DOE Contact: D. Mello, (202) 586-9345
ANL (Contract No. W-31-109-ENG-38) Contact: Fred Nichols, (312) 972-8292

This project is concerned with the development and understanding of surface modification processes to improve the frictional behavior of sliding surfaces. The activities in the project currently focus on high-temperature applications in oxidizing environments prototypical of upper cylinder-wall regions in LHR engine designs. The activities involve development efforts in ion-enhanced deposition (IAD) of lubricous coatings, ion beam mixing of metals with the potential to form lubricous compounds at elevated temperatures, and ion implantation of lubricous compounds into near-surface regions. An advanced ion-beam-assisted deposition system has been designed and constructed and IAD coatings of Ag on Al_2O_3 and B_2O_2 on steel were prepared and shown to have outstanding adherence and friction properties.

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

3. Surface Roughness Wear Model for Ceramics — FY 1989 — $75,000

DOE Contact: D. Mello, (202) 586-9345
SKF-MRC, Inc. (Contract No. DE-AC02-87CE90001) Contact: John McCool, (215) 889-1300

This project conducted at SKF-MRC, Inc., with support from ORNL and ANL, has resulted in the development of a PC-based software package (Ruffian) which predicts wear and load-bearing area, and aids in surface finish selection for ceramic bearings. The program was validated in FY 1989 based on testing support from ORNL and ANL. The computer software development work has also led to the ability to estimate frictional flash temperatures. Work in FY89 focused on surface-modified materials. The Ruffian code has been transferred to industry. A new version for coated materials has been prepared.

Keywords: Friction, Wear, Surface Topology, Surface Microstructure, Ceramics, Modeling

4. Microporous Ceramics — FY 1989 — $75,000

DOE Contact: Stanley M. Wolf, (202) 586-1514
LBL Contact: Arlon Hunt, (415) 486-5370

The objective of this research project is the development and production of controlled porosity materials with tailored thermal, optical, and physical characteristics. This effort is a combined program of analytical studies and experimental measurement of the particle creation and assembly process. In addition, the properties of the finished material will be determined and related to the preparation technique.

Keywords: Thermal Insulation, Sol-Gel, Processing

5. Chemical Vapor Deposition of Ceramic Composites FY 1989
$925,000

DOE Contact: Stanley M. Wolf, (202) 586-1514
ORNL Contact: Peter Angelini, (615) 574-4565
SNL-L Contact: Mark Allendorf, (415) 294-2895
Thermoelectron Technologies Contact: Nancy Scoville, (617) 647-1343

The objective of this effort is to explore novel ceramic matrix composites produced by simultaneous chemical vapor deposition (CVD) of a dispersoid phase and a matrix phase. The basic mechanisms which control the toughness, strength, thermal expansion, and thermal conductivity of the composite coatings are investigated by varying the quantity, composition, and morphologies of the two phases.

The ultimate objective is to utilize the CVD process to fabricate ceramic matrix composites, stable in air at 2500°F with 30 ksi fracture strength and 10 MPa $\sqrt{m}$ fracture toughness and thus develop a single step process for fabrication of ceramic composites which are stable in air at high temperatures, and will have numerous applications in automotive and gas turbine engines, chemical processing and waste heat energy.

Keywords: Structural Ceramics and Composites, Chemical Vapor Deposition, Coatings

6. Thin-Wall Hollow Ceramic Spheres from Slurries FY 1989
$600,000

DOE Contact: Stanley M. Wolf, (202) 586-1514
ORNL Contact: David L. McElroy, (615) 574-5976
Georgia Institute of Technology Contact: J. Cochran, (404) 894-6104

This effort is investigating the development of processes for economically fabricating hollow thin-wall spheres from conventional ceramic powders using dispersions and is assessing their potential use. Initially successful production of spheres of Al_2O_3 and $Al_2O_3Cr_2O_3$ was followed by experimental assessment of the structural and thermal insulation potential for these unique low density materials using both simulated models and experimental measurements. Georgia Tech will continue to assess the structural capability of the spheres and, together with ORNL, evaluate the feasibility of using opacifiers to reduce high temperature thermal conductivity.

A commercial company, Ceramic Filler Inc., is operating a pilot plant in Atlanta, Georgia, and a production facility (capacity 800 tons/year) in South Carolina.

Transfer of this technology will bring a potential payoff of a high temperature insulating material with less cost, higher thermal efficiency, and without ecological and health dangers.

Keywords: Structural Ceramics, High Temperature Service, Insulation

7. The Role of Inert Gas Entrapped in Rapidly Solidified Materials — FY 1989 $365,000

DOE Contact: Stanley M. Wolf, (202) 586-1514
INEL Contact: John Flinn, (208) 526-8127
SNLL Contact: W. G. Wolfer, (415) 294-2307

This investigation seeks to determine property modifications, including enhanced microstructural stability and strengthening, for rapidly solidified materials containing entrapped inert gases. The approach is both experimental and theoretical with initial work on nickel-base alloys.

It has been determined that rapid crystallization during powder atomization provides a supersaturation of vacancies in the form of nanosized clusters that are stabilized by internal oxidation to 0.9 T_m and responsible for the observed high temperature strengthening.

The applicability of rapid solidification processing to superalloys will be investigated in FY90.

Keywords: Gases in Metals, Rapid Solidification

8. Biobased Materials - Composites — FY 1989 $130,000

DOE Contact: Stanley M. Wolf, (202) 586-1514
SERI Contact: Helena Chum, (303) 231-7249
University of Wisconsin Contact: Ray Young, (608) 262-0873
U.S. Forest Products Laboratory Contact: Roger Rowell, (608) 264-5816
University of Southern Mississippi Contact: Lon Mathias, (601) 266-4868
Virginia Polytechnic Institute & State University Contact: Wolfgang Glasser, (703) 231-4403

The overall objective of this effort is to develop cost-effective and environmentally compatible materials for composites and other materials for the automotive industry that incorporate high levels of inexpensive renewable polymers, but have strength properties of synthetic materials and have good overall properties, including low cost. Current work is emphasizing assessing chemical modifications of wood and wood components from inexpensive wood fractionation routes to produce materials for the automotive industry. Renewable materials are lightweight, corrosion resistant and have sound deadening properties. These properties make them well-suited for automotive applications. Strength properties, principally impact strength, need to be improved.

The approach involves tailoring of plastics properties with the design of specific chemical modifications of the wood materials. Some modifications impart thermoplasticity directly; others improve physical properties such as dimensional stability. Approaches that use non-woven technologies and wood fibers as reinforcing agents for composites are investigated. The non-woven mats can be molded into specific shapes that lead to parts consolidation and avoid multiple stamping operations used to fabricate these parts from steel.

Keywords: Composites, Biodegradable Plastics, Natural/Synthetic Resins

9. <u>Microwave-Driven Spray Drying</u> — <u>FY 1989</u> $290,000

DOE Contact: Stanley M. Wolf, (202) 586-1514
LANL Contacts: F. Gac, (505) 667-5126

The objective of this effort is to develop a generic micro-driven spray drying process for the aerosol preparation of fine, homogeneous powders in complex metal oxide systems. Microwave powder shall be coupled directly to the mist of aqueous or organic solutions of metal compounds, and will heat the mist to drive off the solvent leaving a fine powder of a complex metal compound. Given sufficiently high evaporation rates, a very homogeneous powder will result directly from solutions of metal nitrates, chlorides, etc. Although the focus will be on the synthesis of complex metal oxide powders, the process is conceivably applicable to any application that utilizes spray drying.

Keywords: Microwave Processing, Spray Drying, Powder Synthesis

10. <u>Additives for High-Temperature Liquid Lubricants</u> — <u>FY 1989</u> $55,000

DOE Contact: D. Mello, (202) 586-9345
JPL Contact: Emil Lawton, (818) 354-2982

This project will evaluate the feasibility of chelating macrocyclic compounds as lubricant additives for reduction of friction and wear at high temperatures. Control of friction and wear at high temperature is essential for the realization of energy efficiency in the advanced heat engines.

The basic thrust will be to synthesize at least six precursor dinitrile compounds to be evaluated as lubricant additives. These compounds may react *in situ* with the sliding contact surfaces forming lubricating films. In this study the compatibility of the proposed compounds with ceramic surfaces and lubricant additives that are commonly used in lubricating oils will be determined. The physical properties, and thermal and oxidative stability of these compounds will also be determined. The effect of molecular structure, as well as the mechanism of action of these molecules will be investigated. The start of this project has been delayed due to problems in negotiation of the inter-agency agreement.

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

11. IAD of Tin and Cr_2O_3 — FY 1989 $100,000

DOE Contact: D. Mello, (202) 586-9345
NRL (Contract No. DE-AI02-88CE90024) Contact: Fred Smidt, (202) 767-4800

The objective of this project is to determine the mechanism by which IAD produces beneficial modifications of tribological coatings and to establish the necessary correlations between processing and tribological properties such as friction, wear and adhesion. General principles for producing the improved coatings will then be defined for the application of these coatings to advanced energy systems.

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

12. Self-Lubricating Ceramic Surfaces — FY 1989 $100,000

DOE Contact: D. Mello, (202) 586-9345
Universal Energy Systems (Contract No. DE-AC02-88CE90026) Contact: Rabi Bhattacharya, (513) 426-6900

This project seeks to establish optimum conditions for ion implantation and ion-beam mixing of suitable additives into the surfaces of bulk ZrO_2 and Al_2O_3 as well as into coatings of ZrO_2, Al_2O_3, Cr_3C_2 and TiN, for obtaining self-lubricating low friction and wear characteristics. The additives chosen are BaF_2/CaF_2 + Ag or Sn, MoS_2, WS_2 and TaS_2. Initially, ion implantation and subsequent annealing are being performed to synthesize these additives in the near-surface region. Ion beam mixing of thin films of these additives at room temperature and elevated temperature is being investigated and results will be compared with that of direct ion implantation. Detailed characterization using SEM, TEM and RBS techniques will be performed on treated surfaces before and after tribological evaluation of the surfaces.

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

13. Surface Laser Treatment of Partially Stabilized Zirconia (PSZ) FY 1989
$75,000

DOE Contact: D. Mello, (202) 586-9345
Illinois Institute or Technology Contact: Victor Aronov, (312) 567-3035

This project examines the role of phase-transformation-induced surface stresses in the wear of partially-stabilized zirconia. A series of specimens with different phase compositions are subjected to laser-scanning heat treatments and the resulting microstructural alterations are being compared to wear tests. This project is concluding in FY 1989.

Keywords: Surface Modification, Laser, Zirconia, Friction, Wear, Microstructure

14. Ultra Low Wear Materials for Energy Conservation FY 1989
$49,000

DOE Contact: D. Mello, (202) 586-9345
Burton Technologies, Inc. (Contract No. DE-AC02-88CE90027) Contact: R. A. Burton, (919) 839-8287

A new effort to evaluate a low-wear, vitreous-carbon material was funded in FY89. Initial results demonstrated wear rates lower than many ceramics and low, steady friction coefficients. The glassy carbon had none of the environmental sensitivity normally experienced by carbon-based materials like graphite when used in sliding dry air. Test specimens would be fabricated by Burton Technologies and provided to ORNL for testing in a high-speed sliding machine constructed to impose severe sliding conditions such as might be encountered in mechanical face seals and engine components. Burton Technologies will also conduct mechanical face-seal simulator tests in their laboratory. Correlations between these two testing geometries will be drawn. The behavior of the glassy carbon will be compared to that of metals and ceramics subjected to the same severe conditions. This work should open up new applications for the vitreous-carbon materials.

Keywords: Ceramics, Alloys, Friction, Wear

Materials Structures and Composition

15. Modeling of Ordered Intermetallic Alloys FY 1989
$538,000

DOE Contact: Stanley M. Wolf, (202) 586-1514
LANL Contact: P. Jeffrey Hay, (505) 667-3663, FTS 843-363
Yale University Contact: John Hack, (203) 432-4256
Virginia Polytechnic Institute Contact: Diane Farkas, (703) 961-4742

The ultimate objective of this effort is the development of the mathematical models and research software for use in the design of materials for energy technology applications.

During FY 1989 emphasis was shifted from modeling the Ni-Al systems to modeling and confirmation laboratory testing of $MoSi_2$. To date, modeling efforts have related the role of boron at grain boundaries in Ni_3Al and found agreement with subsequent experiment.

$MoSi_2$ represents an attractive material for high temperature applications (high melting point, oxidation resistance, ductile above 900°C), but brittle behavior at low temperature limits usefulness and provides a good field for improvement when addressed by a combination of modeling and experiment.

Keywords: Intermetallic Alloys, Modeling of Materials

16. Materials-by-Design (MBD) - New Ordered Intermetallic Alloys — FY 1989 $379,000

DOE Contact: Stanley M. Wolf, (202) 586-1514
ORNL Contacts: Peter Angelini, (615) 574-4565 and D. M. Nicholson, (615) 574-5873
Imperial College (U.K.) Contact: D. G. Pettifor, 011-411-589-5111, ext. 5756

This project contains two major interacting, cooperative efforts. The first develops and uses theoretical tools useful for the design of ductile high-temperature intermetallics. This theoretical effort attempts to determine alloy additions which ductilize intermetallics currently being developed. In addition, survey calculations are used to indicate other candidates for ductile alloys.

The Materials-by-Design theoretical work uses structure maps, dislocation theory, the tight-binding-bond method, embedded atom method, simulation mathematical models, and first principles local density calculations to arrive at a theoretical design for new ductile ordered intermetallic alloys. Close collaboration with the second (experimental alloy design) group is maintained.

The ultimate objective of the experimental alloy design group is to provide input and to verify, by critical experiments, the predictions made by the theoretical MBD calculations. Binary and ternary ordered intermetallic alloys have been prepared, and their phase relationship and their mechanical behavior characterized for comparison theory.

The theoretical embedded-atom calculations performed at LANL predict that (1) grain boundaries in NiAl are intrinsically brittle, (2) boron will segregate to the grain boundaries in NiAl, and (3) boron will not strengthen the grain boundaries in NiAl. Verification experiments at ORNL have confirmed predictions (1) and (2), but contrary to prediction (3), it has been found that boron does, in fact, strengthen grain boundaries in NiAl and is very effective in suppressing intergranular fracture.

Keywords: Modeling Intermetallic Alloys

17. Polymer Decomposition Expert Systems FY 1989
$100,000

DOE Contact: Stanley M. Wolf, (202) 586-1514
ORNL Contact: W. E. Thiessen, (615) 574-4973

The purpose of this work was to develop an expert system computer program to predict potential reaction pathways for the conversion of waste polymers and polymer mixtures into useful materials.

The ability of the expert system for chemistry to predict reaction pathways was enhanced by employing mechanistic principles. Careful employment of chemical constraints was used to limit the number of suggested degradation pathways, while still permitting the computer program to "invent" new chemistry.

During FY89 work was principally directed toward the construction of routines capable of descriptions from general representations of polymers of interest, such descriptions as would permit reliable predictions of potential reactions. Some new polymer reaction paths were discovered.

Keywords: Expert Systems, Polymer Decomposition

18. Thermosetting Resins with Reversible Crosslinks FY 1989
$165,000

DOE Contact: Stanley M. Wolf, (202) 586-1514
Polytechnic of New York Contact: Giuliana Tesoro, (718) 643-5244

The objective of this effort is to determine if it is possible to develop thermosetting resins with "reversible crosslinks." If so, it may be possible to produce plastics with the strengths, toughness, temperature capabilities, and corrosion resistances typical of thermoset resins but which can be easily reprocessed like a thermoplastic. This process would allow easier recycling, thereby reducing the need for virgin plastics made from natural oil or gas as well as easing the repair of lightweight automotive structural parts.

In the initial phase of the project, the feasibility of the approach was demonstrated for an epoxy resin, crosslinked with disulfide-containing reagents, solubilized by reduction after curing, and thereafter crosslinked by oxidation or by reaction with bifunctional compounds. This sequence has been accomplished for commercial epoxy resins of higher molecular weight and of higher functionality. Evaluation of the thermal and mechanical properties of the crosslinked resins has shown that they are similar to, and, in some instances, superior to those of products crosslinked with commercial curing agents.

Experimental polyimides containing disulfide bonds have been prepared and it has been shown that, as in the case of epoxy resins, it is possible to solubilize cured resins by reduction, and to set the soluble products in a subsequent step.

Keywords: Thermoset Resins, Recycling Plastics

19. Biobased Materials - Packaging Plastics — FY 1989 $140,000

DOE Contact: Stanley M. Wolf, (202) 586-1514
SERI Contact: Helena Chum, (303) 231-7249
Michigan Biotechnology Institute Contact: Ramani Narayan, (517) 349-2970

Research in this area will attempt to develop cost-effective and environmentally degradable packaging plastics that incorporate high levels of inexpensive renewable polymers, but have strength properties of synthetic thermoplastics.

During FY 1989 assessments were made of the suitability of starch/polystyrene graft copolymers for compatibilizing starch and polystyrene plastics at low concentration levels of the grafts, while maintaining the physical properties of the synthetic plastics in the resulting ternary alloys (starch, polystyrene, and graft copolymer).

Keywords: Packaging, Plastics, Copolymers

20. Innovative Approaches to the Chemical Recycling of Plastics — FY 1989 $435,000

DOE Contact: Stanley M. Wolf, (202) 586-1514
SERI Contacts: Helena Chum, (303) 231-7249 and Robert Evans, (303) 231-1384

This research activity is aimed at developing cost-effective and environmentally benign processes for recovering mixed plastics from various sources, such as auto-shredder waste, carpet waste, and other source-separated mixed plastic streams.

Current effort is directed at the identification of experimental conditions for the chemical recovery of a high proportion of monomeric and other high-value components from plastics mixtures using advanced thermal processes.

The SERI molecular-beam mass spectrometer is being used to detect real time products of these processes and establish conditions that will accomplish the ultimate objective of small-scale experiments.

Keywords: Plastics Recycling, Pyrolysis

21. Recycling of Sheet Molding Compounds — FY 1989 $165,000

DOE Contact: Stanley M. Wolf, (202) 586-1514
Stevens Institute of Technology Contact: K. E. Gonsalves, (201) 420-5779

The ultimate objective of this project is the development of final flow sheets and the assessment of the technical and economical feasibility of the proposed recycling process.

As a first step model polymers for recycling from a given class of commercially significant polymeric materials were selected. Thermoset composites (SMC) are widely used in the automotive industry (and elsewhere), so this class of materials was chosen.

In order to establish the parameters essential for economically converting discarded thermoset composites (such as SMC) to useful products, two basic types of operations are necessary: mechanical operations (chopping, grinding and filtration); and chemical processes (solvent extraction, hydrolysis, separation). These were studied in detail.

Technical collaboration with General Motors, manufacturer of SMC based automotive components, and Ashland Chemical Co., sole supplier of the basic SMC ingredients package to GM, was established. Thus, SMC sheets, already compression molded, and polyester resins for PHASE ALPHA SMC were obtained from both GM and Ashland.

Within the next 5 to 10 years junkyards will be covered with SMC automobiles and trucks that cannot be scrapped and recycled in a manner similar to those made from metals. This study could reduce the bulk of the material for dumping and provide economic recovery of useful raw materials.

Keywords: Plastics Recycling

22. Laser Deposition of Thin Films for High Temperature Superconductors — FY 1989 $110,000

DOE Contact: Stanley M. Wolf, (202) 586-1514
ORNL Contact: Peter Angelini, (615) 574-4565
NCSU Contact: J. Narayan, (919) 737-7874

The purpose of this research is the development of laser deposition methods for films and coatings of high temperature superconductor composites, wires and tapes.

During FY89 work concentrated on production of thin films and composites of 123-YBaCuO with silver and the development of microstructures capable of high critical current density and superior mechanical properties.

Keywords: Laser Deposition, Thin Films, HTSC

23. Microwave Sintering and Joining of Advanced Ceramics (HTSC Materials, Zirconia-Toughened Alumina, ZTA and Microwave Joining of Ceramics)

FY 1989
$600,000

DOE Contact: Stanley M. Wolf, (202) 586-1514
ORNL Contacts: H. E. or D. J. Kim, (615) 574-1926 (HTSC Materials), H. D. Kimrey, (615) 576-5183 (ZTA)
QuesTech, Inc., Contact: D. Palaith, (703) 760-1299*

In both HTSC Materials studies and in the ZTA research area a major objective was to evaluate the effectiveness of microwave sintering as opposed to conventional sintering techniques. HTSC activities were aimed at developing a technically superior, cost effective method for manufacturing high temperature superconductors. Densification behavior and superconducting properties of both microwave and conventionally sintered superconductors using powders from commercial industry and in-house sources were studied. Densification was very different for different powders but only slightly affected by microwave versus conventional sintering. Superconducting properties showed some differences but not major improvement from microwave sintering.

The objective of ZTA sintering research was to assess microwave effects on the kinetics of grain growth in alumina in order to understand the controlling parameters and then to develop a method for fabricating high toughness ZTA from low cost materials. To date it has been found that kinetics of grain growth are much higher for microwave heating than conventional heating; rate of grain growth, for microwave at 1500°C was the same as that for conventional heating at 1700°C. Found densification of alumina with 20 wt % zirconia occurred 300-400°C lower for microwave sintering compared with conventional sintering.

In microwave joining of ceramics the objective was to demonstrate the applicability of the technique to materials of industrial interest and under conditions relevant to industrial processing, and develop application projects in collaboration with industry.

A single-mode, tunable rectangular cavity has been integrated with a hydraulic press, IR pyrometer, forward and reflected power probes, and *in situ* acoustic NDE. A separate apparatus using a cylindrical resonant cavity and a frequency sweeper was used to measure dielectric properties of candidate materials.

*Current address: Technology Assessment and Transfer, Inc., (301) 261-8373.

Theoretical feasibility was demonstrated. An experimental system was constructed which verified the microwave heating model. Alumina-glass-alumina joints were made. Mullite-to-mullite joints were made without surface preparation or interlayer. These demonstrated that the joints are stronger than the base material. Novel instrumentation for dielectric properties and *in situ* NDE was developed. The capability to perform experiments in nitrogen or inert gas environment was added. Current focus is on applying the technique to alumina (ECUT funding) and proprietary materials submitted by industry (corporate sponsorship).

Keywords: Microwave, Sintering, HTSC, Zirconia, Alumina, Ceramic Joining

24. Molecular Beam Epitaxy (MBE) Synthesis of Superconducting Materials

FY 1989
$300,000

DOE Contact: Stanley M. Wolf, (202) 586-1514
ORNL Contact: Rodney McKee, (615) 574-5144

This research project is devoted to defining the fundamental crystal growth requirements that will lead to the development of a processing technology for growth of atomically flat, single crystal films of $YBa_2Cu_3O_7$ on practical substrates. This could allow large, 3 to 8 inch single crystal materials that could be used in further High Temperature Superconductor R&D activities or in immediate commercial development.

Keywords: Superconductor Films, Molecular Beam Epitaxy

25. High Strength Zirconia Fibers

FY 1989
$60,000

DOE Contact: Stanley M. Wolf, (202) 586-1514
ORNL Contact: Peter Angelini, (615) 574-4565
CWRU Contact: A. H. Heuer, (216) 368-3868

The ultimate objective of this research is to provide improved oxide, single crystal reinforcement for advanced, high temperature structural composites.

Bulk single crystals of Y_2O_3 stabilized ZrO_2 of various compositions were tested in compression in various orientations at elevated temperatures. Information obtained was used to guide growth of optimum fibers by laser float-zone melting.

It was determined that 4.5 m/o Y_2O_3 partially stabilized ZrO_2 single crystals have flow stresses in excess of 700 MPa at 1400°C.

Solid solution strengthened ZrO_2, fully stabilized, single crystals, show a maximum in yield stress at 1400°C at 21 m/o Y_2O_3.

Keywords: Zirconia Fibers

26. Biomimetic Thin Film Ceramic Coatings — FY 1989 $20,000

DOE Contact: Stanley M. Wolf, (202) 586-1514
PNL Contact: Gary McVay, (509) 375-3762

The objective of this research is to develop energy-conserving, novel processing methods (mimicking natural or biological processes) for the nucleation and growth of ceramic oxide thin films onto metal, ceramic, and polymer surfaces from aqueous solutions.

This project is developing a new process for the formation of thin film materials. Mineral deposition from aqueous solutions is controlled by organized organic functional groups attached to the underlying substrate by appropriate coupling agents. Such derivatization eliminates dependence of the thin film growth process on the native substrate characteristics and allows a generalized scheme for thin film deposition to be developed.

The process under development closely follows the methods used by biological systems to grow hard (ceramic) tissue. As such, the process is very energy efficient. In addition, the devices developed from this unique process will contribute significantly to more efficient energy utilization. Applications will focus on protective coatings, sensors, and catalysts. Examples of the most realistic applications follow:

1. Protective coatings for corrosion or abrasion resistance.

2. Built-in or remote, industrial sensors (corrosion detectors or in-line chemical sensors for process control).

3. Catalytic surfaces for chemical and energy processes (hydrogenation, polymerization, cracking, or coal liquefaction).

4. Thin film coatings on radiant tiles or industrial gas burners.

Keywords: Mineral Deposition, Ceramic Coatings

27. Market Impact of HTSC Technology in Selected Applications — FY 1989 $150,000

DOE Contact: Stanley M. Wolf, (202) 586-1514
ANL Contact: E. J. Daniels, (708) 972-5279

The initial objective of this market survey was to estimate the potential for energy conservation through use of HTSC technology in the following four market applications: magnetic separation, motors, heat pumps, and transportation.

It has been determined that the total potential for energy conservation in the four application areas is approximately four quads per year, but due to cost considerations, market penetration would be limited, and the energy savings from HTSC technology is estimated at one-half to one quad per year.

Keywords: HTSC Market Survey, Estimates

28. Ceramic-Metal Joining — FY 1989 $100,000

DOE Contact: Stanley M. Wolf, (202) 586-1514
ORNL Contact: Peter Angelini, (615) 574-4565

The purpose of this task was to develop new high temperature, high strength, oxidation resistant alloys for brazing of structural ceramics by establishing a systematic framework for braze alloy development that does not rely entirely on trial-and-error experimentation.

The approach taken involved a combination of measuring the thermodynamic properties of model Ti-containing melts, analyzing the microstructures produced by reaction of these melts with selected oxide ceramics, and studying reaction kinetics. Correlations were made by braze alloy thermodynamic properties, joint microstructures, and joint properties.

Keywords: Ceramic-Metal Joining

Materials Properties, Characterization, Behavior or Testing

29. Friction and Wear Research and Development — FY 1989 $423,000

DOE Contact: D. Mello, (202) 586-9345
ORNL (Contract No. DE-AC05-840R21400) Contact: Peter Blau, (615) 574-1514

A major mechanism for transition from the mild to the severe wear mode in the alumina-silicon carbide composite is the formation and propagation of cracks in the alumina matrix. The whiskers in the composite provide a potential toughening mechanism as compared to the whisker-free matrix by interacting with cracks of sufficient length which form during severe wear. Additional toughening by the incorporation of a zirconia-rich precipitate in the alumina matrix has been demonstrated and should operate even for very short cracks which may form during mild wear. Possible improvement in the wear and friction performance provided by the additional increase in fracture toughness will be investigated by ORNL.

Friction and wear of ceramics at elevated temperature is of particular interest since this is the temperature range in which the use of ceramics is most advantageous. Previous results at ORNL for unlubricated sliding of the Al_2O_3-SiC composite at a temperature of 425°C indicated that severe wear occurs at applied normal forces of 2 to 8 N, and sliding-friction coefficients are in the range of 0.8 to 1.3. These tests did not compensate for stress variation during the test or examine the sliding distance to mild-to-severe transition. Further high-temperature sliding-wear tests of the composite will be done at ORNL in the newly acquired High Temperature Tribology Test System, which is capable of positively controlled atmospheres and temperatures as high as 1000°C. Sliding distance to transition as a function of applied stress will be determined for unlubricated sliding. In addition, tests will be performed at elevated temperatures with experimental high-temperature lubricants to investigate the lubricated wear performance of the composite at elevated temperature.

The "friction microprobe" is envisioned as a unique friction research tool to be developed at ORNL under the ECUT Tribology Program. It will be capable of measuring the friction coefficients of individual micrometer-sized constituent phases on the bearing surfaces of engineering materials including metals, ceramics, composites, coatings, and burnished debris deposits. Its use may lead to the development of a practical mixtures rule for tailoring the frictional characteristics of materials through the use of proportional blending combined with processing to produce specific phase orientations on the contact surface.

ORNL will extend the evaluation of whisker composite materials to include tests using high-temperature liquid and solid lubricants. The relationship between surface lubricating layers and wear mechanisms will be studied in the alumina-silicon carbide whisker composite to see if it is suitable for high-temperature lubricated applications.

A study of the friction and wear behavior of nickel aluminide alloys was initiated at ORNL in FY 1988 and will be continued in FY 1989.

ORNL will investigate the use of SiC/Si_3N_4 composite for high-temperature applications.

Keywords: Ceramics, Friction, Wear

30. Ordered Intermetallic Alloys for High Temperatures FY 1989
$680,000

DOE Contact: Stanley M. Wolf, (202) 586-1514
ORNL Contacts: Peter Angelini, (615) 574-4565 and C. T. Liu, (615) 574-4459

The ultimate objectives of this research project are to develop low-density, high-strength ordered intermetallic alloys for high-temperature structural use in advanced energy conversion systems and heat engines, and then transfer the technology to the U.S. materials industry to help competitive ability in world markets.

Both macroalloying and microalloying processes are being employed to improve metallurgical and mechanical properties or ordered intermetallic alloys based on NiAl and Ti_5Si_3. The selection of alloying additions is based on physical metallurgy principles, structural maps developed recently, and some empirical correlations. Emphasis is being placed on improving tensile ductility at ambient temperatures.

Both microalloying and macroalloying processes are used to improve the ductility and strength of stoichiometric NiAl. The grain boundaries are intrinsically brittle. Boron has a strong tendency to segregate to the grain boundaries and completely suppress intergranular fracture. However, there is no attendant improvement in tensile ductility because boron is an extremely potent solid-solution strengthener in NiAl. Both strength and ductility of NiAl can be substantially improved by certain alloying elements which refine microstructure through precipitation of ductile particles. More than 100 percent increase in high-temperature strength and room-temperature ductility has been achieved through alloy additions. This is a major advance in alloy design of NiAl aluminide.

Compositions of a eutectic alloy of Ti_5Si_3 and Ti_3Al have been identified and successfully prepared by drop casting. Hot forging of this material has substantially refined the microstructure and produced a stable two phase structure of Ti_5S_3 and Ti_3Al. The hot fabricability of Ti_5Si_3/Ti_3Al alloys is found to be better than that of binary Ti_3Al.

A complete evaluation of fabrication and mechanical properties of Al_2O_3 fiber-reinforced Ni_3Al composites was carried out to determine the optimum matrix-fiber combination and fabrication procedures for producing Ni_3Al-Al_2O_3 composites of near full density. The results indicate that Al_2O_3 fibers do not strengthen the NiAl alloy matrix at elevated temperatures. Composite alloys using ceramic particles in place of the Al_2O_3 fibers will be produced. It is anticipated that many carbides, oxides and nitrides may also be considered for use in the Ni_3Al matrix.

Work with industry on technology transfer identified a need for a high-yield, creep resistant, castable alloy which has been developed through alloy modification by addition of molybdenum and reduction of boron to 50 ppm. Weld repair of castings was identified as another requirement. Filler metal containing lower boron has been found suitable for weld repair of castings.

Keywords: Ordered Intermetallics and Their Composites, Technology Transfer

31. Ordered Intermetallic Alloys for Corrosion Resistance (FeAl Development)

FY 1989
$250,000

DOE Contact: Stanley M. Wolf, (202) 586-1514
ORNL Contacts: Peter Angelini, (615) 574-4565 and C. T. Liu, (615) 574-4459

An initial objective in this area was the identification of an FeAl composition with the best combination of room temperature ductility, and corrosion resistance in oxidizing molten nitrate salt environments.

A binary base composition of FeAl was selected on the basis of tensile strength results, creep strength, fabricability and corrosion resistance. Minor alloying additions brought a room temperature tensile ductility greater than 10 percent. (This represents a five-fold increase in ductility compared to the pure binary aluminide.) FeAl compositions with excellent corrosion resistance in molten nitrate salts were also identified.

Future activities will include; alloy design to improve creep strength, while maintaining ductility; evaluation of resistance of FeAl compositions to high-temperature oxidation; a weldability study; and finally, scale-up to industrial size "heats" and further interactions with industry.

Keywords: Corrosion Resistance, Iron Aluminide

32. Characterization of SiC Whisker - $MoSi_2$ Composites for Elevated Temperature Applications

FY 1989
$100,000

DOE Contact: Stanley M. Wolf, (202) 586-1514
LANL Contact: J. J. Petrovic, (505) 667-0125

SiC whisker-$MoSi_2$ matrix composites are being examined for potential elevated temperature structural applications in oxidizing environments.

Significant improvement in high temperature yield strength has occurred as a result of solid solution alloying of the matrix. At 1500°C, composite yield strengths were 8-10 higher than pure $MoSi_2$, reaching values of 80 MPa in air testing. High temperature ductility and oxidation resistance were retained in the composites.

In FY90, project emphasis will shift to lowering the brittle-to-ductile transition of $MoSi_2$ by a Materials-by-Design approach, and the development of high toughness partially stabilized ZrO_2-$MoSi_2$ matrix composites. Technology transfer interactions with U.S. industrial organizations will continue.

$MoSi_2$ based composites constitute a new class oxidation-resistant high temperature materials which represent an alternative to structural ceramics.

Keywords: Intermetallic Alloy Composites, Whiskers

33. Electrochemically Conducting Polymers — FY 1989 $250,000

DOE Contact: Stanley M. Wolf, (202) 586-1514
LANL Contact: S. Gottesfeld, (505) 667-0853

The ultimate objective of this project is the development of electrochemical techniques for the synthesis and analysis of conducting polymers. The composition, morphology, and stability of conducting polymer films will be optimized for a range of energy conversion and utilization applications, including high energy density batteries, corrosion resistant conductive coatings, and electrochromic films for variable opacity windows.

Keywords: Conducting, Polymers, Film Deposition

Device or Component Fabrication, Behavior or Testing

34. Development of a Wear Model for Lubricated Sliding of Ceramics — FY 1989 $115,000

DOE Contact: D. Mello, (202) 586-9345
Georgia Institute of Technology (ORNL Subcontract 780219X-15) Contact: Ward Winer, (404) 894-3270

Investigating the effect of lubricant compositions on the wear of several advanced ceramics, including partially stabilized zirconia, silicon nitride, silicon carbide, sialon, and possibly a superconducting ceramic compound. Wear tests include rolling-element EHD tests and pin-on-disc tests under lubricated conditions and temperatures up to 150°C. Test results are being applied to the development of wear model based on ceramic-lubricant/additive interactions.

Keywords: Ceramics, Erosion, Wear, Friction, Lubrication

35. Lubrication Research and Development FY 1989
$760,000

DOE Contact: D. Mello, (202) 586-9345
National Institute for Standards and Technology: Gaithersburg (Interagency Agreement OR-21350) Contact: Stephen Hsu, (301) 921-2113

Base oils are composed of many organic molecular structures that may function independently, synergistically, or antagonistically to affect the performance of the lubricants. Furthermore, lubricating oil additives respond differently in different base oils, due to the interactions between the additives and the base oil constituents. The approach of this investigation is to separate the lubricating base oils into their major fractions and subfractions, to identify the molecular structures and chemical composition of the fractions and subfractions and to characterize the tribological performance of these compound classes in friction, wear and oxidation tests. Additives then will be tested with the fractions to identify what causes synergism and what causes antagonism.

Ceramic materials are being used increasingly in various applications requiring wear resistance under severe environmental conditions. Data obtained at NBS and those reported in the literature indicate that the wear rate and the friction coefficient of ceramics are generally too high for achieving material conservation or energy conservation. In order to successfully utilize ceramics, lubricants must be developed to control friction and wear. The purpose of this project is to identify what reacts with ceramics and to understand the basic lubrication processes of ceramics at low temperature. This activity will involve studying the reactions between different ceramics, such as silicon nitride, silicon carbide and alumina, with synthetic base oils and additives. Specifically, the tribochemical reactions leading to lubricating film formation, as well as the effect of ceramic surfaces on the oxidative and thermal stability of lubricant chemical structure and reaction kinetics, will be determined. The information generated in this project would allow lubricants to be designed for future systems that utilize ceramic components.

Ceramic coatings are being considered as thermal barrier insulating layers on the inside surfaces of the cylinder walls of LHR engines. The critical factor in determining the success of these engines lies in the control of friction and wear at the contact between the ceramic coatings and the piston ring. Ceramic coatings are also being considered for other critical areas such as the valve seats. Yet, there are no reliable test methods available for evaluating the friction, wear and ultimate life of these coatings. The purpose of this project is to develop a test procedure for evaluating the performance of ceramic coatings for tribological applications. This research will be conducted in close cooperation with Caterpillar and Cummins Engine. The ceramic coatings will be selected based on the present knowledge and experience of these two companies, acquired in the development of the LHR engine. Initially, the ball-on-three-flat test procedure that was developed at NBS for the ECUT Tribology Program will be used. The tests will be in close cooperation with the industry participants. The results of the research will be evaluated to gain an understanding of the behavior of ceramic coatings as well as for developing new performance test procedures.

Successful implementation of advanced engine designs, such as the low-heat-rejection (LHR) engine, is hindered by the lack of stable lubricants and additives for high temperature operations. The lubricant temperature in conventional engines is less than 200°C. The temperature requirements for future advanced engines exceeds 400°C. The elevated temperatures encountered in the LHR engines require development of lubricants that can withstand severe thermal and oxidative environments. An effective lubrication for these systems also requires friction and wear control as well as deposit control. The purpose of this project is to develop the necessary knowledge base for the selection and formulation of future lubricants, including the base oil and the additives.

Previous research at NBS has led to the development of several important test methods for the evaluation of high temperature performance of lubricants, as well as performance data on various synthetic base fluids and additives. During FY89 these test methods will be used to identify the key structural and chemical requirements for stable lubricants. This project will be coordinated with the efforts at Cummins Engine and AKZO Chemical, who are involved in the development of a lubricant for the LHR engine.

Keywords: Metals, Oils, Friction, Wear, Engines

36. Energy-Efficient Gear-Lubrication Model — FY 1989 $50,000

DOE Contact: D. Mello, (202) 586-9345
Northwestern University (NBS Subcontract No. 60NANBD0547) Contact: Herbert Cheng, (312) 491-7062

The main objectives in this activity conducted at Northwestern University include modeling of friction and wear in the partial elastohydrodynamic lubrication regime, calculations of power loss and wear loss in spur gears and experimental validation of the friction and wear models. This work is expected to aid the development of new lubricants for more energy-efficient power transmissions. Initial project work has led to the development and preliminary experimental validation of a model for predicting gear friction and resultant power loss. In FY 1989, validation of this model will be completed and a model for predicting wear in spur gears will be developed and experimentally validated.

Keywords: Gears, Oils, Frictions, Wear, Engines

37. Wear Mechanism Modeling FY 1989
$70,000

DOE Contact: D. Mello, (202) 586-9345
Cambridge University Contact: M. F. Ashby, 0-223-33-2-2622

One of the facts of life in tribology is that various investigators employ different wear/friction test geometries and conduct tests at different pressures and speeds, with little or no effort to correlate between the different tests. Often different wear mechanisms occur under different conditions, and the situation can be very complicated. A recent technique published by Lim and Ashby uses normalized coordinates to correlate, in a surprisingly consistent manner, an extremely large and varied data base on steel-on-steel studies. This project, begun in FY89, extends the treatment to include arbitrary combinations of wear/friction pairs with differing material properties. During FY89, a consistent technique is being developed for calculating both bulk and flash temperatures due to frictional heating and fitting to various experimental results gave a rather consistent model.

Keywords: Metals, Ceramics, Friction, Wear, Engines

38. Advanced Laser Fluorescence Measurements of Lubricant Film Behavior in a Diesel Engine FY 1989
$65,000

DOE Contact: D. Mello, (202) 586-9345
MIT Contact: John Heywood, (617) 253-2243

Recently at MIT, a novel laser fluorescence technique was developed which measures oil film thickness between the cylinder liner and the piston rings in a reciprocating diesel engine. The laser diagnostic engine study provides *in situ* real time lubricant measurements, while much advanced fundamental research is based on bench experiments. It is known that some tribochemical reactions occur under instantaneous conditions, which can be best addressed with *in situ* engine experiments. With a coordinated approach, the proposed engine study may be used to validate concurrent bench experiments. The principal objectives of the proposed study are: (1) to demonstrate the laser fluorescence diagnostics in determining the lubricant film behavior between the piston and the liner in an operating engine, and (2) to use this technique to measure and then develop models for lubricant behavior under various engine operational conditions as well as different surface material and lubricant environments, particularly those applicable to high temperature operations.

Keywords: Metals, Oils, Friction, Wear, Engines, Laser Fluorescence, Films

39. Effect of Cycle-to-Cycle Variations on Instantaneous Friction Torque FY 1989
$50,000

DOE Contact: D. Mello, (202) 586-9345
Wayne State University (ANL Subcontract No. 73072401) Contact: Naeim Henein, (313) 577-3887

A project involving a new technique to evaluate instantaneous friction torque (IFT) in an operating, reciprocating internal-combustion engine, was begun at Wayne State University in mid-FY 1989. This project is jointly funded by NSF and the ECUT Tribology Program with the bulk of the work supported by NSF in a 3-year grant to Wayne State. The tribology program is only supporting research on "The Effect of Cycle-to-Cycle Variations (CCV) on the Accuracy of the Instantaneous Friction Torque Determined by the (P-W) Method." The method itself is being developed in the NSF-funded project. The ECUT-supported work includes and has the prime objective of conducting in-engine testing of surface-modified components developed in an ECUT Tribology project at ANL.

Initial activities in this project involved a careful and quantitative evaluation of commercially available instrumentation for the measurement of angular velocity, pressure and torque. Based on this evaluation, optimal instrumentation was selected, acquired and installed in the experimental engine. The project will be conducted in three phases over a period of three years.

Keywords: Friction, Torque, Engines, Combustion, Modeling

40. Novel Thin Film Acoustic Wave Sensors FY 1989
$290,000

DOE Contact: Stanley M. Wolf, (202) 586-1514
SNLA Contact: G. C. Frye, (505) 844-0787

This project will attempt to develop a new class of chemical sensors that can be used as process monitors to improve process energy efficiency.

Sol-gel chemistry and surface modification techniques are used to develop oxide coatings with controlled pore sizes and tailored chemical properties. These films provide chemical selectivity based on both molecular size and chemical interactions.

Keywords: Acoustic Wave Sensors, Coatings, Sol-Gel Processing

41. Development of High-Temperature Superconducting Magnets for High-Efficiency Motors (Pulsed Laser Deposition of Conductors for HTSC Motor Solenoids and Applications for High T_c Superconducting Magnets) FY 1989
$75,000

DOE Contact: Stanley M. Wolf, (202) 586-1514
ORNL Contacts: Peter Angelini, (615) 574-4565, D. H. Lowndes, (615) 574-6306 and R. Feenstra, (615) 574-4341

The major objectives of this project are the development of pulsed laser deposition methods which will continuously deposit HTSC films on practical substrates followed by the transfer of the technology to the electric motor industry.

Pulsed laser deposition conditions have been found that result in high J_c (>1 MA/cm^2), high T_c(~92°K) $YBa_2Cu_3O_{7-x}$ films formed on single crystal substrates. Rapid, low temperature post deposition oxidation, resulting in fully oxidized $YBa_2Cu_3O_{7-x}$ films, has been demonstrated and investigations of the influence of substrate polycrystallinity and substrate surface preparation on film morphology are underway.

As part of this research effort, potential applications for HTSC magnets for motors, heat pumps, etc., are being identified and general design requirements for magnets in these applications are being developed.

Keywords: HTSC Films, Superconducting Magnets, Motor

42. Bulk Ceramic BiSrCaCuO and TlBaCaCuO Superconductors for Trapped-Flux Permanent Magnets FY 1989
$290,000

DOE Contact: Stanley M. Wolf, (202) 586-1514
PNL Contact: Larry R. Pederson, (509) 375-2731
Boeing Aerospace Contact: Thomas Luhman, (206) 234-2683

A preliminary goal of this project is the design and demonstration of a trapped-flux permanent magnetic device using bulk, polycrystalline superconducting ceramics in the BiSrCaCuO and/or TlBaCaCuO systems that have critical current densities of at least 10^5 A/cm^2 at 77°K. Subsequently it is intended to improve the critical properties of bulk, polycrystalline superconducting ceramics so that they can be utilized in practical devices, including motors, generators, and switches.

Freeze-drying and aerosol pyrolysis processes will be used to prepare phase-pure, homogeneous, fine-grained, superconducting ceramics. The BiSrCaCuO and TlBaCaCuO systems were selected because of their high critical temperatures. Critical current densities in a magnetic field will be enhanced by doping the grain boundaries so that they become superconducting by a proximity effect, and by introducing secondary phase precipitates to act as flux pinning centers.

Keywords: Superconducting Magnets

43. Electrochemical Methods for *In-Situ* Repair and Reinforcement of Metallic Coatings

FY 1989
$20,000

DOE Contact: Stanley M. Wolf, (202) 586-1514
ORNL Contact: Peter Angelini, (615) 574-4565
University of Florida Contact: Ellis D. Verink, (904) 392-8163

The initial objective of this research was to assess the feasibility of anodizing diffused aluminum coatings on ferrous alloy substrates (immersed in molten nitrite/nitrate baths at temperatures in the range of 600°C), from the standpoint of determining whether the aluminum oxide produced by anodizing could be employed to repair and/or reinforce diffused aluminum coatings by sealing off surface imperfections.

Ferrous alloy substrates, coated with diffused aluminum coatings, were examined metallographically, and then anodized in a molten nitrite/nitrate bath, and then re-examined to determine whether new aluminum oxide films were formed.

It was found that new oxide forms in imperfections in the coating, and to some extent over the surface at large. The surface configuration has the characteristic, microscopic "roughness" associated with the pack cementation process. Viewing at 5000X showed a distinctive distribution of new oxide which suggests that the tiny inter-particulate volumes are accessible to, and become filled with new aluminum oxide. Tagged oxygen techniques are now being used to elucidate the details of the process further.

Keywords: Anodized Aluminum Coatings, Corrosion Repair

OFFICE OF BUILDINGS AND COMMUNITY SYSTEMS

The Office of Buildings and Community Systems works to increase the energy efficiency of the buildings sector through performance of R&D on building systems, building equipment, and community energy systems. In addition, the Office carries out the statutory requirements of appliance standards and labeling, building energy performance standards, and residential conservation service, and Federal energy management program. 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;
- improve the energy efficiency of advanced electric heat pump and refrigeration systems, and of light systems; and
- develop new planning techniques and systems that will decrease the energy consumption of communities.

<u>Building Systems Division</u>

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 develop and improve existing insulating materials; to develop and verify analytical models that are useful to building designers and researchers for predicting the thermal performance characteristics of materials; to develop methods for measuring the thermal performance characteristics; and to 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

44. Unguarded Thin Heater Tester

FY 1989
$150,000

DOE Contact: Peter Scofield, (202) 586-9193
ORNL Contact: David McElroy, (615) 574-5976

Materials under investigation include mineral fiberboard, and powered insulations. Most existing insulation test equipment has been designed to provide data on steady-state conditions. In actual use, however, insulating materials experience a continually changing thermal environment. The research is designed to (a) validate the device through comparisons with guarded hot plates, and (b) study transient processes in insulation materials. A series of technical presentations and reports, detailing the equipment and the results of a variety of test series, is planned.

Keywords: Building Insulation, Heat Transfer, Nondestructive Evaluation

45. Variable R/Switchable Surface Analysis

FY 1989
$30,000

DOE Contact: Peter Scofield, (202) 586-9193
ORNL Contact: David McElroy, (615) 574-5976

This project involves technical and economic evaluation of feasibility of using switchable radiation control materials for building envelope surfaces. Potential new materials as well as those now available will be analyzed. This task uses simulations to determine the energy savings possible by varying R-values in envelope systems, and will consider both a variety of approaches to the question and the likelihood of, and barriers to, their acceptance by code groups and mainstream builders.

Keywords: Active Thermal Insulation, Switchable Emittance, Energy Savings Calculation

46. Energy Savings with Advanced Building Materials

FY 1989
$100,000

DOE Contact: Peter Scofield, (202) 586-9193
LBL Contact: Ron Kammerud, (415) 486-6620

This project is for the identification and quantification of the energy saving potentials of commercial buildings using advanced materials. The four generic classes of materials being analyzed are: high R-value (>100) insulations, variable (switchable) R-value insulations, selective surface coatings and switchable emissivity films. The results of this analysis will be used as a guide for the allocation of program resources and to establish technical performance objectives for the development of new advanced materials.

Keywords: Active Thermal Insulation, Switchable Emittance, Energy Savings Calculation

47. Recommended R-Levels - ZIP Program FY 1989 $30,000

DOE Contact: Peter Scofield, (202) 586-9193
NIST Contact: Steve Petersen, (301) 975-6136

This effort has two parts. First to provide minimum recommended R-values for residences for inclusion in the DOE Insulation Fact Sheet. These values are based on climate, insulation costs, and space heating and cooling costs. The second is to update the ZIP computer program used to provide the recommendations, to include slab floors, basement walls, cathedral ceilings, ductwork and water heaters. This Fact Sheet and the ZIP program Version 1.0 is available for use by the energy conservation community.

Keywords: Recommended R-Values, Computer Program, Economic Analysis

48. CFC Foam Characterization FY 1989 $70,000

DOE Contact: Peter Scofield, (202) 586-9193
NIST Contact: H. Fanney, (301) 975-5864

The relationship between thermal conductivity, temperature and time for existing CFC blown foam insulation materials is being determined. The project will examine five foam insulation products that were blown with CFC-11, CFC-22 and CFC-113 using the one-meter Guarded Hot Plate that has an uncertainty of 1 percent. The resulting data will provide a basis to model the aging behavior and to validate available models for the new foam products. The accuracy of the heat flow meter apparatus (ASTM C518, R-Matic) is being assessed using existing standard reference materials with R-values in the range of R-1 and R-7 per inch.

Keywords: Foam Insulation, Test Procedures

49. Foam Insulation Research FY 1989
$85,000

DOE Contact: Peter Scofield, (202) 586-9193
MIT Contact: Leon Glicksman, (617) 253-2233

Freon-blown rigid urethane foam insulation is being investigated to determine the degree to which the effective thermal conductivity decreases with time. Various types of reflective flakes are also being investigated for their effectiveness in lowering the thermal conductivity of foam insulations.

Keywords: Foam Insulation, Heat Transfer, Radiation

50. Development of Non-CFC Foam Insulations FY 1989
$75,000

DOE Contact: Peter Scofield, (202) 586-9193
ORNL Contact: David McElroy, (615) 574-5976

This a three year joint project with the rigid foam industry and EPA for the development of alternative blowing agents to be used as drop in replacements for the CFC blowing agents currently being used in the manufacture of foam insulation products. Prototype rigid foam boards with five different blends of HCFC-123 and 141b will be manufactured by industry and sent to ORNL for testing and evaluation both in the laboratory and in outdoor test facilities. Tests will be conducted to determine mechanical and thermal properties and aging characteristics.

Keywords: CFC, Foam Insulation, Insulation Sheating, Roofs

51. Evacuated Powder Panel Insulation FY 1989
$100,000

DOE Contact: Peter Scofield, (202) 586-9193
ORNL Contact: David McElroy, (615) 574-5976

This project is for the development of an advanced technology super insulation concept. A layer powder is sandwiched between two films and a soft vacuum is drawn on the powder filler. Current technology produces a R-20 per inch panel. The thermal performance of the panel in a cooler application is being evaluated, and various powders and encasing films are being characterized.

Keywords: Insulation, Vacuum, Heat Transfer

OFFICE OF INDUSTRIAL PROGRAMS

This office supports cost-shared research and development for industrial energy conservation technologies that offer large potential for saving scarce fuels. It also encourages the private sector to implement and deploy such technologies as they are developed. Materials research is done in support of the technologies under development, to develop materials with lower embodied energy and to provide materials for use in equipment/systems which can improve energy efficiency.

Improved Energy Productivity Division

This division conducts research and creates new energy conserving processes for ore reduction, metals production, and basic shape processing; sensing and control instrumentation; separation processes; and new coatings.

Materials Preparation, Synthesis, Deposition, Growth or Forming

52. Composite Cathode Material Development — FY 1989 $185,000

DOE Contact: M. J. McMonigle, (202) 586-2082
Great Lakes Contact: L. A. Joo, (615) 543-3111

This is a long term project involving testing and analysis of composite materials for cathode applications. During FY 1989, the emphasis was on finite element analysis of TiB_2-graphite samples and engineering calculations for a commercial cell heat balance in order to optimize shapes and structures.

Keywords: Composites, Cathode

53. Cerox Inert Anode Material — FY 1989 $12,000

DOE Contact: M. J. McMonigle, (202) 586-2082
EL TECH Contact: Tom Gilligan, (216) 357-4066

The addition of CeO_2 to molten cryolite produces a coating on oxygen evolving electrodes. The factors controlling the in situ formation of the coating, the coating characteristics, and the coating stability have been evaluated. Metal purity and voltage drops will be determined for commercial aluminum reduction cell operating conditions.

Keywords: Coatings, Anode, Ceramics

Materials Properties, Behavior, Characterization or Testing

54. Expand and Control Inert Electrode Cell Operating Conditions — FY 1989 $740,000

DOE Contact: M. J. McMonigle, (202) 586-2082
PNL Contact: Larry Morgan, (509) 375-3874

Cermets of Ni-Fe spinels with copper additions have been tested. Operating conditions have been identified that provide 99.8 aluminum and low anode wear rates. Confirmation tests and characterization of cermet bath interface are in progress.

Keywords: Ceramics, Cryolite, Material Science, Aluminum

Waste Energy Reduction Division

Waste Energy Reduction is concerned with the efficient conversion of fuel to a more useful energy form and with the utilization of energy embodied in waste products—solids, liquids, and gases. This division conducts research to develop advanced waste energy recovery technologies for the industrial sector.

Materials Preparation, Synthesis, Deposition, Growth or Forming

55. Microwave Sintering of β-Alumina for Use in the Sodium Heat Engine — FY 1989 $ 0

DOE Contact: J. Eustis, (202) 586-2098
ORNL Contact: W. Snyder, (615) 574-2178

This project is developing the alcohol metal thermal energy cell (AMTEC) using β-Alumina. In an effort to improve toughness of the material, sintering using 20 Giga Hertz microwave radiation is being investigated. A preliminary study has indicated feasibility.

Keywords: Structural Ceramics

Materials Properties, Behavior, Characterization or Testing

56. Advanced Heat Exchanger Material Technology Development — FY 1989 $770,000

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

This project conducts research to develop improved ceramic materials and fabrication processes and to expand the materials data base 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 synthetic-exhaust streams, conducting scale-up studies on the carbo-thermic production of β-SiC powder, and developing advanced wet forming techniques for monolithic ceramic components.

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

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

FY 1989
$300,000

DOE Contact: S. Richlen, (202) 586-2078
Babcock & Wilcox Contact: J. Bower, (804) 522-5742

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

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

58. National Laboratory Support to Assessment of Strength Limiting Flaws in Ceramic Heat Exchanger Components

FY 1989
$120,000

DOE Contact: S. Richlen, (202) 586-2078
Idaho National Engineering Laboratory Contact: W. Reuter, (208) 526-1708

This project supports the B&W study on strength limiting flaws by the development of advanced NDE, test methods, and other key technologies. Currently the project is studying the application of Moire Interferometry to measure stress of components under test.

Keywords: Structural Ceramics, NDE, Structure

59. Ceramic Fiber Residue Measurement — FY 1989 $59,000

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. Currently a test protocol is being written.

Keywords: Ceramic Composites, Whiskers

Device or Component Fabrication, Behavior or Testing

60. Ceramic Composite Heat Exchanger for the Chemical Industry — FY 1989 $923,000

DOE Contact: S. Richlen, (202) 586-2078
Babcock & Wilcox Contact: D. Hindman, (804) 522-5825

The second phase of this project which addressed critical problems of the material and design has been completed. Alumina fiber in a zirconia or alumina oxide matrix has been selected as most promising material. Currently, the field test host site has been selected and final design is being conducted.

Keywords: Ceramic Composites, Structure

61. HiPHES System Design Study for Energy Production from Hazardous Wastes — FY 1989 $ 0

DOE Contact: S. Richlen, (202) 586-2078
Solar Turbines Contact: M. Ward, (619) 544-2553

This project has completed the first phase of a three-phase effort to develop high pressure heat exchange systems for recovery of energy from hazardous wastes. A preliminary design of an advanced heat exchange processes based on the use of ceramic composites has been developed. Research on critical material and design needs will now begin.

Keywords: Ceramic Composites, Heat Exchangers

62. HiPHES System Design Study for an Advanced Reformer FY 1989
$ 0

DOE Contact: S. Richlen, (202) 586-2078
Stone & Webster Engineering Corp. Contact: P. Koppell, (617) 589-5293

This project has completed the first 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 processes based on the use of ceramics has been developed. Research on critical material and design needs will now begin.

Keywords: Composites, Heat Exchangers

63. Ceramic Components for Stationary Gas Turbines in Cogeneration Service FY 1989
$175,000

DOE Contact: W. Parks, (202) 586-2093
Battelle Contact: D. Anson, (614) 424-5823

This project capitalizes on ceramic development done in the automotive gas turbine and the HiPHES programs to upgrade components of stationary gas turbines used in cogeneration service. The initial performance assessment for the project has been started.

Keywords: Structural Ceramics, Ceramic Composites

OFFICE OF TRANSPORTATION SYSTEMS

The Office of Transportation Systems has established a number of programs to conserve energy used for transportation and to shift transportation energy demand to non-petroleum fuels.

The Heat Engine Propulsion program is underway to provide industry with proof-of-concepts for advanced gas turbine and Stirling engine technologies that demonstrate improvements in fuel efficiency and to develop technology for heavy-duty diesel operation under uncooled minimum friction conditions, including waste heat utilization.

The Advanced Materials Development program's objective is to establish an industrial technology base capable of providing reliable and cost-effective structural ceramics for application to advanced heat engines. Project management responsibility for the Heat Engine Highway Vehicle Systems project (gas turbine diesel and Stirling engines) has been delegated to the NASA Lewis Research Center. Project management of the Ceramic Technology for Advanced Heat Engines project (Advanced Materials Development program) has been assigned to the Oak Ridge National Laboratory (ORNL).

The success of these advanced heat engine systems depends strongly on the development of new or improved materials. Ceramic materials are needed for the hot-flow-path components of the advanced gas turbine and the minimum friction adiabatic (uncooled) diesel engines, to meet operating temperature and manufacturing cost requirements. The Stirling engine requires low-cost iron-based alloys capable of operating at high temperatures while exposed to high-pressure hydrogen. Material technology development programs are underway for each of these heat engine systems. The generic ceramic technology program consists of three general topics: materials and processing; data base and life prediction; and design methodology. To support the advanced material work conducted under this and other research programs, a High Temperature Materials Laboratory (HTML) has been constructed at ORNL.

Key elements of each program are organized and described briefly in the following. Robert B. Schulz is the DOE contact, (202) 586-8051, for overall coordination in the following Office of Transportation Systems material projects.

Materials Preparation, Synthesis, Deposition, Growth or Forming

64. Silicon Carbide Powder Synthesis (WBS No. 1112) FY 1989
$15,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. Ray Johnson, (615) 576-6832
Carborundum Contact: Harry A. Lawler, (716) 278-6345

The objective of this task was to develop a volume scalable process to produce high purity, high surface area sinterable silicon carbide powder.

Phase I verified the technical feasibility of the gas phase synthesis route, identified the best silicon feedstock (methyl trichlorosilane), and optimized the production process at the bench scale. Powders produced compared favorably with commercially available alternatives. In addition, a theoretical model was developed to assist in understanding the synthesis process and has been utilized to optimize operating conditions for the scale-up of the process. Phase II studies were designed to extend prior production to pilot plant rates.

Keywords: Silicon Carbide, Powder Synthesis, Sintering

65. Turbomilling of SiC (WBS No. 1116) FY 1989
$172,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: T. N. Tiegs, (615) 574-5173
Southern Illinois University Contact: Dale E. Wittmer, (618) 536-2396

First, a small feasibility study was conducted to investigate the use of a unique turbomilling process in the preparation of SiC whisker-toughened ceramic composites. Due to the early success of the feasibility study, the scope of this project was expanded to evaluate the effect of turbomilling variables and the beneficiation of SiC whiskers, examine the dispersion/homogenization of SiC whisker/alumina composites and SiC whisker/silicon nitride, and investigate loadings for reducing aspect ratios in the absence of coarse grinding particulate.

Keywords: Alumina, Silicon Carbide, Silicon Nitride, Turbomilling, Whiskers

66. TiB$_2$ Whiskers (WBS No. 1117) FY 1989
$ 0

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: R. L. Beatty, (615) 574-4536
Keramont Contact: J. C. Withers, (602) 746-9442

The scope of this work is to produce TiB_2 whiskers, TiB_2-coated alpha-SiC whiskers, consolidate SiC matrix composites, and test in air above 1200 °C. The development of TiB_2 whisker production is being investigated using a well-developed research plan. The parameters which are believed to be most important for the growth of the whiskers are the type of substrate, type of catalyst, raw materials, temperature of whisker growth, and whisker furnace design. The physical and chemical properties of the whiskers, and particularly their diameter, are dependent on parameters such as gas concentration, gas flow velocity, raw material purity, etc. Parameters necessary for the consolidation of the composites will be extrapolated to the composite powder to account for the presence of the TiB_2 whiskers.

Keywords: Synthesis and Characterization, Testing, Titanium Diboride, Whiskers

67. Powder Characterization (WBS No. 1118) FY 1989
$110,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. Ray Johnson, (615) 576-6832
National Institute of Standards and Technology (NIST) Contact: S. Malghan, (301) 975-2000

The objective of this effort is to develop a fundamental understanding of surface chemical changes which take place when silicon nitride powder is attrition milled in an aqueous environment.

A step-wise analysis of the underlying mechanisms controlling the material properties, and detailed characterization of the materials and their environments will be carried out. The following research is proposed:

- Characterization of the milled suspensions for physical, chemical, and surface chemical parameters to develop basic understanding of the resulting powder properties;

- An understanding of the role of milling fluids in controlling the post-milling surface chemical properties and size distribution of the powders;

- Define pertinent process variables and their influence in milling and deagglomeration;

- Develop mathematical models for simulation and control of powder production by attrition milling; and
- Evaluate resulting powders by sintering aid addition, consolidation, densification, and mechanical testing.

Keywords: Powder Characterization, Powder Processing, Silicon Nitride

68. Sintered Silicon Nitride (WBS No. 1121) FY 1989
$200,000

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

The program is concentrating on sintering compositions in the Si_3N_4-Y_2O_3-SiO_2 system using a two-step sintering method where the N_2 gas pressure is raised to 7-8 MPa during the second step of the process. During the sintering, dissociation reactions are suppressed by the use of high nitrogen pressure and cover powder of suitable composition over the specimen. Variables to be studied include sintering process parameters, source of starting powders, milling media and time, and specimen composition. Room temperature modulus of rupture, high temperature stress rupture, oxidation resistance, and fracture toughness have been determined.

Current efforts involve a study of "green body" forming to minimize/ eliminate agglomerate formation which leads to pore development in sintered specimens. Processes such as slip casting with and without pressure will be evaluated. In addition, specimens containing the apatite phase rather than yttrium pyrosilicate should be explored with the molybdenum silicide particles distributed in the matrix.

This task also includes technical support for sintering of silicon nitride via on-site personnel assignment to conduct high nitrogen pressure experiments.

Keywords: Sintering, Silicon Nitride, Testing

69. Si_3N_4 Powder Synthesis (WBS No. 1123) FY 1989
$ 0

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. Ray Johnson, (615) 576-6832
Ford Contact: G. M. Crosbie, 313-574-1208

The goal is to achieve major improvements in the quantitative understanding of how to produce sinterable Si_3N_4 powders having highly controlled particle size, shape, surface area, impurity content, and phase content. Of interest to the present powder needs is a silicon nitride powder of high cation and anion purity without carbon residue. The process study has been directed towards a modification of the low temperature reaction of $SiCl_4$ vapor with liquid NH_3.

A pilot plant design for the "vapor-chloride - liquid ammonia" direct reaction was designed, additional process development including the "liquid-chloride - liquid ammonia" direct reaction completed, runs to test product stability campaigned, sintering tests performed, and a new analytical method developed and reported on.

The goal for the next phase of the project was to test for unique properties of the ceramics sintered from low carbon powders before committing to a pilot plant of the 110L scale previously designed. In view of powder quantities needed to allow tests of the ceramics, the major task was to design and implement a scaled-up version of the silicon nitride synthesis processing equipment to produce greater amounts of powders with high cation and anion purity and low carbon residue.

Keywords: Silicon Nitride, Synthesis and Characterization

70. Microwave Sintering (WBS No. 1124) — FY 1989, $300,000

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

The objective of this effort is to identify those aspects of microwave processing of silicon nitride that might 1) accelerate densification, 2) permit sintering to high density using much lower levels of sintering aids, 3) lower the sintering temperature, or 4) produce unique microstructures.

The sintering and heat treatment of silicon nitride are being examined using a 200kW, 28 GHz furnace. Types of experiments to be performed include the following:

- Annealing of dense silicon nitride (and/or sialon) parts to examine the effects of microwave heating on grain growth and grain boundary recrystallization;

- Development of a microwave furnace dilatometer to provide the capability to monitor the densification of silicon nitride at all stages in the sintering process;

- Sintering of conventional silicon nitride compositions to establish a baseline of densification rates and microstructural states for microwave-sintered materials;

- Sintering of silicon nitride with reduced levels of sintering aids to produce a dense sintered body with superior properties at elevated temperatures; and

- Investigation of reaction-bonded (RBSN) and sintered reaction-bonded (SRBSN) silicon nitride using microwave heating.

Keywords: Microwave Sintering, Silicon Nitride

71. Advanced Processing (WBS No. 1141) — FY 1989 $2,701,000

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.

A silicon nitride-4% yttria composition consolidated by glass encapsulated HIPing will be used. Baseline data shall be generated from an initial process route involving injection molding. Tensile test bars will be fabricated using colloidal techniques - injection molding and colloidal consolidation. Critical flaw populations will be identified using NDE and fractographic analysis. Measured tensile strength will be correlated with flaw populations and process parameters. Flaws will be minimized through innovative improvements in process methods and controls.

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

72. Improved Processing (WBS No. 1142) — FY 1989 $355,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. Ray Johnson, (615) 576-6832
ORNL Contact: R. L. Beatty, (615) 574-4536

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. An effort is being made to develop processes that can be scaled most readily to high production rates. Simplicity of processing and high predictability of product quality are dominant issues. The studies are intended to generate processing schedules and procedures as well as protocols for characterization of raw and in-process materials. The principal material of interest in this work is silicon nitride. Gel-casting, a method developed at ORNL, was the process chosen for initial consideration.

Production of tensile and other specimens of Al_2O_3 has demonstrated the potential for process predictability and dimensional control. One or more collaborative agreements with industrial companies to develop the process for silicon nitride will be initiated in FY 1990.

Keywords: Powder Processing

73. Advanced Processing (WBS No. 1143) FY 1989
$2,701,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: R. L. Beatty, (615) 574-4536
GTE Contact: L. J. Bowen, (617) 466-2536

The purpose of this task is to develop the powder, process improvements, and controls needed to enable the reproducible fabrication of silicon nitride ceramics which demonstrate program goals for strength and Weibull modulus.

The material to be utilized is nominally designated PY6, a ceramic prepared from high-quality silicon nitride and yttrium oxide powders. A baseline process examined during the first year of the program will be modified using process improvements and tighter process controls which are demonstrated in parallel development activities. These improvements and controls will be incorporated into the evolving process as they are developed. Determination of the utility of any particular process improvement or process control will be made by monitoring the change in strength and Weibull modulus of uniaxial tensile specimens compared to the baseline process.

Keywords: Processing, Processing Controls, Silicon Nitride, Testing

74. Processing Science for Reliable Structural Ceramics Based on Silicon Nitride (WBS No. 1144) FY 1989
$166,000

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

The objective of this effort is to obtain a basic understanding of relevant problems associated with forming powder compacts from slurries which will densify to produce reliable structural ceramics.

The overall approach of this research is to obtain fundamental relations between slurry rheology, particle packing mechanics, consolidated body rheology, strain recovery, and powder compact integrity. It is expected that this understanding will lead to a definition of the colloidal and rheological requirements to reliably process advanced ceramics with improved property reliability and to new slurry consolidation methods.

Keywords: Powder Processing

75. Dispersion Toughened Si_3N_4 (WBS No. 1221) FY 1989
$480,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. Ray Johnson, (615) 576-6832
Garrett Ceramic Components Division Contact: H. C. Yeh, (213) 618-7449

For Phase I, the approach was to develop a silicon nitride matrix composite with SiC whiskers dispersed in the matrix using standard powder processing specifications in place at Garrett, and sintering and/or HIPing for final consolidation. Elastic modulus, four-point bend strength, density, thermal expansion, thermal conductivity, and fracture toughness were determined. In addition, a low cost, near-net-shape process was developed.

The objective of Phase II of this program is to maximize the toughness in a high strength, high temperature SiC whisker/Si_3N_4 matrix material system that can be formed to shape by slip casting and densified by a method amenable to complex shape mass production. The ASEA glass encapsulation hot isostatic pressing (HIP) technique shall be used for densification throughout the program. Following selection of a SiC whisker as the reinforcement in GN-10 Si_3N_4 matrix, process optimization and property evaluation studies will commence.

Keywords: Silicon Carbide, Composites, Silicon Nitride, Sintering, Hot Isostatic Pressing, Whiskers, Testing, Physical/Mechanical Properties

76. Dispersion Toughened Si_3N_4 (WBS No. 1223) FY 1989
$160,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: M. A. Janney, (615) 574-4281
GTE Contact: S. T. Buljan, (617) 890-8460

For Phase I, the approach was to closely examine toughening of Si_3N_4 through introduction of refractory, particulate, or whisker dispersoids. The initial phase development was based on a commercial Si_3N_4 material, GTE AY6, and additions of SiC and TiC whisker or particulate dispersoids. For the purposes of screening, the composites were densified by hot pressing. Mechanical and physical properties of consolidated composites were then evaluated and their microstructure thoroughly examined in order to define property-microstructure relationships and establish design parameters for further material modification. The most promising candidate developed in Phase I would serve as a basis for development of the near-net-shape fabrication process.

For Phase II, UBE, Toyo Soda Si_3N_4, and American Matrix, Tokai, and Tateho SiC whiskers will be evaluated as alternative precursor materials for composite preparation. Additional effort will be devoted to optimization of the process for near-net-shape part fabrication through optimization of binders and the compounding step of the process, injection molding, and densification parameters.

Keywords: Silicon Nitride, Composites, Sintering, Whiskers, Physical/Mechanical Properties

77. <u>Composite Development (WBS No. 1224)</u> <u>FY 1989</u> $421,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: P. F. Becher, (615) 574-5157
Norton Contact: N. D. Corbin, (508) 393-5829

The objective of Phase I of this task was the development of fully dense Si_3N_4 matrix SiC whisker composites prepared by an RBSN approach with sintering aids, followed by high pressure HIPing. The emphasis of this study was on utilizing the (Hot Isostatic Pressure) HIP process which has the potential for producing near-net-shaped complex geometries.

Baseline composite processing procedures (mixing, nitriding, HIP) that routinely result in a uniform microstructure that is fully dense and contains up to 40 v/o SiC whiskers have been applied. Whiskers from domestic and foreign suppliers were evaluated. Of all the parameters evaluated to date, those which most affect fracture toughness appear to be composition related. CVD coatings have been applied to SiC whiskers and evaluation of pcoatings is continuing.

For Phase II, studies are being conducted to tailor the whisker/matrix interface and determine the optimum whisker morphology for fracture toughness improvements. The effect of forming on whisker orientation, fracture toughness, and shape distortion is also being addressed. The primary goal is to develop a composite with a fracture toughness of >10 MPa $\sqrt{m}$ and capable of operating up to 1400°C.

Keywords: Composites, Silicon Carbide, Silicon Nitride, Hot Isostatic Pressing, Sintering, Fracture Toughness

78. Advanced Composites (WBS No. 1225) FY 1989
$127,000

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

The goal of this project is to obtain dense silicon nitride composites containing silicon carbide whiskers by transient liquid phase sintering. The systems SiAlON, SiAlON-Garnet ($Y_3Al_5O_{12}$) and SiAlON-Cordierite ($Mg_2Al_4Si_5O_{18}$) were selected for this study. Mixtures of the starting materials form a sufficient amount of liquid to aid densification at the sintering temperatures. After sintering, the liquid can be crystallized by heat treatment.

Keywords: Composites, Silicon Nitride, Silicon Carbide, Sintering, SiAlON

79. Dispersion Toughened Oxide Composites (WBS No. 1231) FY 1989
$360,000

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

This work involves development and characterization of SiC whisker-reinforced oxide composites for improved mechanical performance. Although most of the early work dealt with alumina as the matrix, a new effort in SiC whisker reinforced-SiAlON has been initiated. Emphasis in the new systems will be on pressureless sintering and control of the whisker-matrix interface properties. In addition, studies of whisker growth processes which will attempt to improve the mechanical properties of SiC whiskers by reducing their flaw sizes have been initiated.

Keywords: Composites, Alumina, Silicon Carbide, SiAlON

80. Transformation Toughened Ceramics Processing (WBS No. 1232) FY 1989
$ 0

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. Ray Johnson, (615) 576-6832
Norton Contact: Giulio A. Rossi, (508) 393-6600

During Phase I, emphasis was on production of improved zirconia toughened ceramics for advanced engine applications. The scope included powder synthesis and characterization of the sintered ceramics. Materials made from three powder sources were evaluated: a rapid solidification from-the-melt powder, and two chemically-derived powders. Rapidly solidified powders showed better performance than chemically-derived powders.

For Phase IIA of this program, the main effort for the Y-TZP materials has been to study the low-temperature degradation and understand how it is affected by microstructure and composition. In the case of the Ce-ZTA ceramics, the main goal is to optimize the mechanical properties.

Keywords: Composites, Zirconia, Sintering, Alumina, Synthesis and Characterization

81. Development of Toughened Ceramics (WBS No. 1237) FY 1989
$167,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. Ray Johnson, (615) 576-6832
Ceramatec Contact: R. A. Cutler, (801) 486-5071

Phase I of this project involved the development of layered ceramic composites which incorporate zirconia as a second phase to achieve improved strength and toughness at temperatures of up to 1000 °C. The work also addressed processing methods for fabricating these layered composites via sintering.

Results from Phase I have shown that it is possible to increase the strength of Al_2O_3-ZrO_2 ceramics by incorporating transformation-induced residual stresses in sintered specimens consisting of three layers.

Phase II objectives include: 1) to increase the use temperature of three-layer composites by substituting HfO_2 for ZrO_2; 2) develop aqueous and nonaqueous slip casting techniques for three-layer composites in order to obtain better layer uniformity and to maximize residual compressive stress by optimizing the outer layer thickness; 3) superimpose temperature stresses on transformation-induced stresses in three-layer composites; and 4) demonstrate improved thermal shock resistance and damage resistance in optimized composites.

Ceramatec has developed layered DTA composites which incorporate zirconia or hafnia as a second phase to achieve improved strength and toughness at temperatures of up to 1000 °C. Slip casting methods were developed to produce three-layer composites with room temperature strengths in excess of 1200 MPa, and 600 MPa at 1000 °C.

Keywords: Composites, Sintering, Alumina, Zirconia, Toughened Ceramics

82. Low Expansion Ceramics (WBS No. 1242) FY 1989
$277,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. Ray Johnson, (615) 576-6832
Virginia Polytechnic Institute and State University Contact: J. J. Brown, (703) 961-6640

A major objective of this research is to investigate selected oxide systems for the development of a low expansion, high thermal shock resistant ceramic. Specifically, it is the goal of this study to develop an isotropic, ultra-low thermal expansion ceramic which can be used above 1200°C and which is relatively inexpensive, and to determine conditions necessary for synthesis, densification, and characterization of these systems.

The research program includes synthesis, property characterization, and fabrication of candidate low thermal expansion ceramics from four systems based on beta-eucryptite, silica, mullite, and zircon. At the present time, encouraging results have been obtained for the development of improved thermal shock resistant beta-eucryptite and zircon (NZP) compositions.

Keywords: Structural Ceramics, Aluminum Phosphate, Silica, Mullite, Zirconia, Ultra-low Expansion, Beta-eucryptite

Materials Properties, Behavior, Characterization or Testing

83. Ceramic Component Design Technology FY 1989
$100,000

DOE Contact: Saunders B. Kramer, (202) 586-8012
NASA Contact: John Gyekenyesi, (216) 433-3210

The advanced finite element and probability codes required to design, analyze and optimize ceramic components are being developed. Enhancement of the CARES code to include the design methods for whisker toughened ceramics was begun in 1989.

Keywords: Probabilistic Computer Codes, Ceramic Component Design

84. Microstructural Modeling of Cracks (WBS No. 2111) FY 1989
$86,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. Ray Johnson, (615) 576-6832
University of Tennessee Contact: J. A. M. Boulet, (615) 974-2171

A goal of this research is to develop mathematical procedures by which existing design methodology for brittle fracture could accurately account for the influence of non-planar crack faces on fracture of cracks with realistic geometry under arbitrary stress states.

Existing models all consider the crack faces to be smooth and planar, but examination of fresh fracture surfaces by microscopy often indicates rough, irregular surfaces. In this study, the effect of protrusion interference on fracture of cracks with realistic geometry under arbitrary stress states is being examined.

Keywords: Predictive Behavior Modeling, Structural Ceramics

85. Adherence of Coatings (WBS No. 2212) FY 1989
$22,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. Ray Johnson, (615) 576-6832
ORNL Contact: C. J. McHargue, (615) 574-4344

Financial support is provided for a graduate research assistantship in the Department of Materials Science and Engineering at the University of Tennessee to conduct studies on adherence of coatings deposited on substrates subjected to ion beam mixing.

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

86. Dynamic Interfaces (WBS No. 2221) FY 1989
$188,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. Ray Johnson, (615) 576-6832
Battelle Contact: K. F. Dufrane, (614) 424-4618

The objective of this study is to develop an understanding of the friction and wear processes of ceramic interfaces based on experimental data. The supporting experiments are conducted at temperatures to 650°C under reciprocating sliding conditions reproducing the loads, speeds, and environment of the ring/cylinder interface of advanced internal combustion engines. The test specimens are carefully characterized before and after testing to provide detailed input into the model.

Current efforts for a second phase are addressing the performance of advanced toughened monolithic ceramics, thermal-spray coatings, surface modifications, and high temperature lubricants. The test rig developed in this program has been shown to give results similar to actual engine tests by the major diesel engine producers, but the rig tests are much quicker and cheaper.

Keywords: Dynamic Interfaces, Wear, Structural Ceramics, Coatings and Films, Predictive Behavior Modeling, Monolithics, Adiabatic Diesels, Friction, Lubrication

87. Advanced Statistics Calculations (WBS No. 2313) FY 1989
$191,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. Ray Johnson, (615) 576-6832
GE Contact: C. A. Johnson, (518) 387-6421

The design and application of reliable load-bearing structural components from ceramic materials requires a detailed understanding of the statistical nature of fracture in brittle materials. The overall objective is to advance the current understanding of fracture statistics, especially in the following areas:

- Optimum testing plans and data analysis techniques;
- Consequences of time-dependent crack growth on the evolution of initial flaw distributions; and
- Confidence and tolerance bounds on predictions that use the Weibull distribution and function.

The studies are being carried out largely by analytical and computer simulation techniques. Actual fracture data are then used as appropriate to confirm and demonstrate the resulting data analysis techniques.

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

88. Microstructural Analysis (WBS No. 3111) FY 1989
$50,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. Ray Johnson, (615) 576-6832
National Institute of Standards and Technology (NIST) Contact: S. M. Wiederhorn, (301) 975-2000

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. Scanning and transmission electron microscopy are used to characterize damage accumulation in the creep specimens.

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

89. Physical Properties (WBS No. 3112) FY 1989
$99,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. Ray Johnson, (615) 576-6832
ORNL Contact: D. L. McElroy, (615) 574-5976

This study is required because the thermal conductivities of the ceramics of interest are generally not known at high temperatures, and the theory has not been sufficiently developed to yield reliable predictions. The influences of second phase type, content, shape, and of parallel energy transport by photons are of particular importance. The role of photon transport at high temperatures and the influence of second phase additions are under investigation. A study of the effects of Cr_2O_3 and Fe_2O_3 additions on the thermal conductivity of Al_2O_3 has been completed. The thermal conductivities of low expansion oxide solid solutions have been determined.

Keywords: Alumina, Structural Ceramics, Thermal Conductivity

90. Microstructural Characterization of Silicon Carbide and Silicon Nitride Ceramics for Advanced Heat Engines (WBS No. 3114) FY 1989
$200,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. Ray Johnson, (615) 576-6832
ORNL Contact: T. A. Nolan, (615) 574-0811

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

A second major objective is to relate those microstructural observations to available mechanical test data produced by other participants in the ATTAP and Ceramic Technology programs. Ceramic specimens from foreign sources are also characterized to provide comparative information on microstructural properties.

Keywords: Silicon Carbide, Silicon Nitride, Microstructure, Chemical Analysis, Mechanical Properties

91. Project Data Base (WBS No. 3117)

FY 1989
$100,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. Ray Johnson, (615) 576-6832
ORNL Contact: B. L. Keyes, (615) 574-5113

This task involves efforts to develop and maintain a computer data base of mechanical property data generated in the Ceramic Technology for Advanced Heat Engines program. The data base system is currently composed of a loosely-connected framework of commercially available programs. However, data can be easily transferred by electronic means to a variety of other programs. Techniques have been developed that allow data as compiled on a variety of computers using several different software programs to be transferred directly into the data base electronically with no manual transcription of the data. Several techniques for data output in useful formats (tabular and graphical) have also been developed. The system has been designed to provide maximum flexibility to allow the addition of other data as the data base grows.

Reports containing mechanical properties and material characterization information on silicon nitride, silicon carbide, zirconia-based, and transformation-toughened ceramics have been issued.

Keywords: Database, Mechanical Properties, Structural Ceramics

92. Characterization of Transformation-Toughened Ceramics (WBS No. 3211)

FY 1989
$100,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. Ray Johnson, (615) 576-6832
AMTL Contact: Jeffrey J. Swab, (617) 923-5410

The main objective is to determine the effect of time-at-temperature on transformation toughened zirconias, especially tetragonal zirconia polycrystals (TZP) at engine operating temperatures (1000-1200°C). A preliminary study of the degradation of mechanical properties at low temperatures (200-400°C) in yttria-doped zirconias has also been initiated.

Due to the inherent problems of TZPs at low and high temperatures, evaluation and characterization of these materials are currently being phased out. The next generation of promising materials, composite ceramics toughened by fibers, whiskers, or particulates, will be studied instead. Following an initial screening, selected composite ceramics will be evaluated in detail using a similar evaluation matrix.

Keywords: Alumina, Transformation Toughened Zirconia, High Temperature Service, Engines, Fracture, Mechanical Properties

93. Fracture Behavior of Toughened Ceramics (WBS No. 3213) FY 1989 $220,000

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

Analytical modeling and experimental studies have been aimed at providing fundamental insights into the processes responsible for toughness and time-dependent strength degradation of materials such as silicon carbide, silicon nitride, partially-stabilized zirconia, and dispersion-toughened and whisker-reinforced oxides. Particular emphasis is being given to understanding the effect of environment, temperature, and compositional and microstructural characteristics upon these mechanisms. In addition, fundamental insight into the slow crack growth behavior associated with these materials is being obtained.

Keywords: Toughened Ceramics, Whiskers, Fracture, Flexure Test, Matrix, Alumina

94. Cyclic Fatigue of Toughened Ceramics (WBS No. 3214) FY 1989 $220,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. Ray Johnson, (615) 576-6832
ORNL Contact: K. C. Liu, (615) 574-5116

Using the special tensile testing system designed, fabricated, and tested at ORNL, elevated temperature tensile and fatigue tests are being performed on candidate monolithic ceramic materials such as silicon nitride. Based on test data, a number of important observations and new findings have been made. Studies of cyclic fatigue behavior at 1200°C show that silicon nitride may be strain hardened slightly, such that increasing the load via multiple step loading with intermittent cycling resulted in increased fatigue life under certain conditions. Examinations of the fracture surfaces have shown that all fractures were initiated at internal flaws, suggesting that the equipment and test methods are reliable and the data are indicative of material performance.

Keywords: Cyclic Fatigue, Toughened Ceramics, Tensile Testing, Silicon Nitride

95. Tensile Stress Rupture Development (WBS No. 3215)

FY 1989
$315,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. Ray 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 tests on candidate structural ceramics. Existing data requirements specify that tensile creep-rupture data be developed in the range of 1260°C to 1371°C. These data bases are to be generated using cylindrical bar specimens of materials such as silicon nitride with the tests conducted in an air environment. Ten standard uniaxial level arm creep frames were modified to incorporate the specimen load train with a self-aligning feature and closed-loop control capability. Proper design of the furnace to produce a uniform temperature zone at the required temperature while minimizing specimen grip temperature was mandatory. A laser interference fringe technique is employed for creep measurements.

Keywords: Silicon Nitride, Tensile Testing

96. Rotor Materials Data Base (WBS No. 3216)

FY 1989
$300,000

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

The goal of this research program is to systematically study the tensile strength of a silicon nitride and a silicon carbide ceramic as a function of temperature and time in an air environment. Initial tests were aimed at measuring the statistical parameters characterizing the strength distribution of three sample types. The resulting data will then be used to examine the applicability of current statistical models as well as sample geometries for determining the strength distribution.

Next, stress rupture data will be generated by measuring fatigue life at a constant stress. The time-dependent deformation will also be monitored during testing so that the extent of high-temperature creep may be ascertained. Tested samples will be thoroughly characterized using established ceramographic, SEM, and TEM techniques. A major goal of this effort will be to better understand the microstructural aspects of high-temperature failure.

The resulting stress rupture data will be used to examine the applicability of a generalized fatigue-life (slow crack growth) model. If necessary, model refinements will be implemented to account for both crack blunting and creep damage effects. Once a satisfactory model is developed, separate stress-rupture (confirmatory) experiments will be performed to examine the model's predictive capability.

Keywords: Creep, Engines, High Temperature Service, Structural Ceramics, Tensile Testing, Predictive Behavior Modeling

97. Toughened Ceramics Life Prediction (WBS No. 3217) FY 1989 $324,000

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

The objective of this effort is to determine the behavior of toughened ceramics, especially SiC whisker-toughened Si_3N_4, as a function of time and temperature as the basis for developing a life prediction methodology. The room temperature and elevated temperature strength and reliability, the fracture toughness, slow crack growth, and the creep behavior will be determined for the as-manufactured material. The same properties will be evaluated after long-time exposure to various high temperature isothermal and cyclic environments.

A second major effort will be to better understand the relationship between microstructure and mechanical behavior for a limited number of materials. These results will provide input for parallel materials development and design methodology development. Resultant design codes will be verified.

Keywords: Creep, Fracture Toughness, Life Prediction, Silicon Nitride

98. Life Prediction Methodology (WBS No. 3222) FY 1989 $586,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: C. R. Brinkman, (615) 574-5106
Allison Gas Turbine Division Contact: D. L. Vaccari, (313) 230-4313

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 subject 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: Life Prediction, Nondestructive Evaluation, Structural Ceramics

99. Life Prediction Methodology (WBS No. 3223) FY 1989 $1,621,000

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

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

Keywords: Life Prediction, Nondestructive Evaluation, Structural Ceramics

100. Ceramic Durability Evaluation AGT FY 1989 $80,000

DOE Contact: Saunders B. Kramer, (202) 586-8012
NASA Contact: Sunil Dutta, (216) 433-3282
Garrett Turbine Engine Contact: L. Lindberg, (602) 231-4001

The objective of the program is to evaluate commercially available structural and glass ceramic material specimens exposed to combustion products at temperatures up to 2500°F for periods up to 3,500 hours. In 1989, Kyocera SN-251 silicon nitride and Carborundum TiB_2 and silicon carbide were tested.

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

101. Environmental Effects in Toughened Ceramics (WBS No. 3314) FY 1989
$690,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: Victor J. Tennery, (615) 574-5123
University of Dayton Contact: N. L. Hecht, (513) 229-4341

The objective of this task is to characterize the mechanical behavior and environmental degradation processes operative in candidate AGT ceramics using flexural and uniaxial tensile testing and extensive pre- and post-test characterization of physical properties and microstructure.

Flexural strength is being measured over a wide range of stressing rates, temperatures, and atmospheric conditions to quantitatively determine relevant fatigue parameters.

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

102. LHR Diesel Coupon Tests (WBS No. 3315) FY 1989
$150,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. Ray Johnson, (615) 576-6832
ORNL Contact: C. R. Brinkman, (615) 574-5106

The objective of this effort is to subject a number of candidate advanced ceramic materials and metal-ceramic joints to diesel "adiabatic" engine environments where the effects of a number of variables (e.g., temperature, fuel type, and engine operating conditions) can be determined.

Following characterization (i.e., dimensions, weight, density, and a quality assurance inspection for defects), small rectangular test bars of candidate ceramic material are inserted into a single-cylinder diesel engine combustion chamber. Engine insertion periods typically average up to 1000 hours. After exposure, the specimens are removed and examined for four-point bend rupture testing and the results compared to the unexposed material database. Engine operating conditions are varied to impose thermal transients, and specimen temperatures are monitored.

Keywords: Diesel Engines, Structural Ceramics, Testing

103. High Temperature Tensile Testing (WBS No. 3412) FY 1989
$225,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. Ray Johnson, (615) 576-6832
North Carolina A&T State University Contact: V. Sarma Avva, (919) 334-7620

The objective of this task is to test and evaluate advanced ceramic materials at temperatures up to 1500°C in uniaxial tension. Testing may include fast fracture strengths and stepped static fatigue strength along with analysis of fracture surfaces by scanning electron microscopy.

GTE SNW 1000 Si_3N_4 tensile samples were tested using the ORNL self-aligning grip system at three stressing rates. Fractography indicated that fracture was transgranular at room temperature and the fracture origins were normally porosities and occasionally inclusions. Dynamic fatigue was not observed in SNW 1000 Si_3N_4.

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

104. Standard Tensile Test Development (WBS No. 3413) FY 1989
$220,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. Ray Johnson, (615) 576-6832
National Institute of Standards and Technology (NIST) Contact: S. M. Wiederhorn, (301) 975-2000

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.

Two inexpensive techniques for tensile testing have been developed at NIST. These techniques are being used to test materials intended for heat engines. The results obtained by high temperature tensile testing will be compared with those obtained by compressive and flexural testing. Data obtained from these studies will be compared with various theories of creep and creep rupture that have been developed to date. Based on the data obtained from these studies, a methodology for high temperature design will be recommended.

Keywords: Creep, Structural Ceramics, Tensile Testing

105. Fracture Toughness Determination of Thin Coatings (WBS No. 3414) FY 1989 $69,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: W. C. Oliver, (615) 576-7245
Vanderbilt Contact: James J. Wert, (615) 322-7311

The long-range goal of this project will be to develop the scientific base and technology required to obtain the fracture toughness of a material from ultra-low load indentation experiments using the mechanical properties microprobe.

First, a thorough literature search on the subject of indentation fracture was performed. Then, a system to conduct high load indentation experiments monitoring load and displacement, and to establish the effect of visible fracture events on such data was built. Experiments on silicon, sapphire, and zirconia have been performed.

Keywords: Fracture Toughness, Structural Ceramics

106. Non-Destructive Evaluation (WBS No. 3511) FY 1989 $435,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. Ray 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 in ceramics that affect the structural performance. High-frequency ultrasonics and radiography are being used to detect, size, and locate critical flaws and to nondestructively measure the elastic properties of the host material.

Keywords: NDE, Radiography, Structural Ceramics, Ultrasonics

107. NDE of Advanced Ceramics by Synchrotron Computer Tomography (WBS No. 3513) FY 1989 $ 0

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. Ray Johnson, (615) 576-6832
Radiation Science Contact: Allen S. Krieger, 508-494-0335

Synchrotron radiation was used to obtain computed tomography (CT) scans of ceramic specimens with resolution an order of magnitude finer than that which can be achieved with electron impact X-ray tubes or radioactive sources. Initial effort was devoted to a demonstration of the resolution, sensitivity, and maximum attainable thickness capabilities that can be achieved with currently available X-ray energy and intensity.

Keywords: Computed Tomography, Nondestructive Evaluation

108. Ceramic Component NDE Technology

FY 1989
$100,000

DOE Contact: Saunders B. Kramer, (202) 586-8012
NASA Contact: Alex Vary, (216) 433-6019

The objective is to identify and develop NDE techniques for ceramic heat engine components. The NDE methods under study are X-ray, radiography, ultrasonics, scanning laser acoustic microscopy and thermo-acoustic microscopy.

Keywords: Ceramics, NDE, X-ray, Ultrasonics

109. Computed Tomography (WBS No. 3515)

FY 1989
$110,000

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

The objectives of this program are to: 1) develop necessary techniques for reliable use of polychromatic X-ray computed tomography to characterize structural ceramics relative to density distributions, presence of voids, inclusions, and cracks; and 2) develop calibration methods for CT scanners for ceramic materials.

Argonne is using 1) an available medical CT scanner which has had extensive software modifications for ceramic applications; 2) commercially prepared ceramics (Si_3N_4, SiC, Al_2O_3, and ZrO_2), and compounds tailored for specific mass and electron density; and 3) available international attenuation coefficient tables. There are two distinct parts to the approach: 1) development of a calibration phantom, and 2) corrections for streak artifacts.

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

110. Nuclear Magnetic Resonance Imaging (WBS No. 3516) FY 1989 $216,000

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

The objectives of this program are to 1) establish the feasibility of using NMR imaging systems to map organic B/P distributions in injection-molded green ceramics, 2) examine the potential for NMR spectroscopy to determine if there are any chemical variations within and/or between batches of organic binder which impact process reliability, and 3) determine the sensitivity of NMR imaging methods to injection molding process variables as manifested in distribution of the organic.

Argonne has demonstrated that NMR imaging with appropriate techniques, field gradient strength, and with correct back projection imaging algorithms, polymeric binders can be imaged at room temperature. In addition, with appropriate filler fluids, NMR imaging can be used to detect defects in partially densified ceramics. A 2-T superconducting-magnet NMR imaging system has been used to evaluate the feasibility of imaging B/P directly. Green state test specimens were made by mixing various wt. % binder with Si_3N_4 powder.

Keywords: Binder, Nuclear Magnetic Resonance, Silicon Nitride

111. Powder Characterization (WBS No. 3517) FY 1989 $360,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. Ray Johnson, (615) 576-6832
ORNL Contact: O. O. Omatete, (615) 576-7199

Objectives for this effort include: 1) identification, characterization, and modification of those aspects of the chemistry and physics of a ceramic powder and of the powder/solvent interface that control processing; 2) development of standard methods of analysis for achieving (1), and 3) development of procedures for writing specifications for ceramic powders that include any of the methods of analysis developed during this project.

The approach is a combination of basic science and applied engineering. ORNL and three universities are participating in the project. There are three distinct elements:

- A round-robin characterization of electrophoretic mobility and acid-base character in aqueous suspension to be conducted by all participants;

- Gas chromatography of Si_3N_4 surfaces and electrophoretic studies of slurries for gel casting to be performed by ORNL, and special projects to be performed at each university which are described in project summaries for WBS Nos. 3518, 3519, and 3520.

- Adaptation and verification of analytical procedures developed during the project to determine their usefulness in the research laboratory or in industrial practice.

Keywords: Powder Characterization

112. Spectroscopic Characterization (WBS No. 3518) FY 1989 $81,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: M. A. Janney, (615) 574-4281
University of Wisconsin Contact: M. A. Anderson, (608) 202-2470

This is one of three companion tasks to develop an understanding of the critical characterization parameters for powders to be used as the starting materials for high-performance ceramics. The objective of this particular effort is to perform a thorough spectroscopic analysis and characterization of selected ceramic powders and/or whiskers in non-aqueous suspension. The spectroscopic studies will be supported by other surfaces studies such as adsorption isotherm determination, calorimetry, and light scattering, etc., to confirm and amplify the data generated in the spectroscopic studies.

Keywords: Powder Characterization, Spectroscopy

113. Surface Adsorption (WBS No. 3519) FY 1989 $81,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: M. A. Janney, (615) 574-4281
Rutgers University Contact: D. J. Shanefield, (201) 932-2226

This is one of three companion tasks to develop an understanding of the critical characterization parameters for powders to be used as the starting materials for high-performance ceramics. The purpose of this effort is to conduct a study of the basic mechanisms of adsorption from non-aqueous solvents onto ceramic surfaces, and the modification of those surfaces to make them uniformly processable. Adsorption studies on both monomers and polymers will be considered. Various gas-phase treatments that might be applied to the ceramic powders to make their surfaces more uniform may also be pursued.

Keywords: Powder Characterization, Surface Modification

114. Thermodynamics of Surfaces (WBS No. 3520) FY 1989
$81,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: M. A. Janney, (615) 574-4281
Pennsylvania State University Contact: J. H. Adair, (814) 863-0857

This is one of three companion tasks to develop an understanding of the critical characterization parameters for powders to be used as the starting materials for high-performance ceramics. The objective of this task is to determine the thermodynamic nature of the ceramic powder surface in non-aqueous powder suspension. The methods take the form of the Drago analysis for non-aqueous solvents or may use some other formalism such as that used in chromatographic studies. The result that one may reasonably expect from such a study is a set of classification categories for ceramic powders, binders, dispersants, etc., that will guide ceramic process engineers in their selection of processing aids for a particular ceramic powder.

Keywords: Powder Characterization, Thermodynamics

Technology Transfer and Management Coordination

115. Management and Coordination (WBS No. 111) FY 1989
$900,000

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

116. International Exchange Agreement (IEA) Annex II Management and Support (WBS No. 4115) FY 1989
$379,000

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

The purpose of this effort is to assist and encourage international cooperation in the development of voluntary standard methods for determining mechanical, physical, and structural properties of advanced ceramic materials. There are four tasks in the Annex II agreement, "Cooperative Program on Ceramics for Advanced Heat Engines and Other

Conservation Applications," 1) technical information exchange, 2) ceramic powder characterization, 3) ceramic chemistry, and 4) ceramic material property measurements. Participants in Annex II include the United States, the Federal Republic of Germany, and Sweden.

A follow-on task, Subtask 5, which involves mechanical properties characterization has been proposed and agreed upon by participants.

Keywords: IEA, Powder Characterization, Mechanical Properties

117. Standard Reference Materials (WBS No. 4116) FY 1989 $130,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. Ray Johnson, (615) 576-6832
National Institute of Standards and Technology (NIST) Contact: A. L. Dragoo, (301) 975-2000

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

Device or Component Fabrication, Behavior or Testing

118. Advanced Coating Technology (WBS No. 1311) FY 1989 $175,000

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

The objective of this project is to develop an adherent coating that will prevent sodium corrosion of silicon nitride, silicon carbide, or other ceramics used as components in gas turbine engines.

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

119. Advanced Coating Technology AGT (WBS No. 1312) FY 1989
$512,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. Ray Johnson, (615) 576-6832
GTE Contact: H. J. Kim, (617) 466-2742

The objective of this project is to develop oxidation-resistant, high toughness, adherent coatings for silicon-based ceramic substrates, namely reaction bonded Si_3N_4, sintered SiC, and HIPed Si_3N_4 for use in an advanced gas turbine engine. Chemical vapor deposition (CVD) is being used to develop appropriate coating configurations to accommodate as many of the mechanical, thermal, and chemical requirements demanded of the application as possible.

A Phase II effort comprised of three major tasks: 1) optimization and modification of the coating configuration; 2) performance assessment; and 3) modeling was initiated in FY 1989.

Keywords: Coatings and Films, Chemical Vapor Deposition, Engines, Structural Ceramics, Silicon Carbide, Silicon Nitride, Adherence, Contact Stress, Modeling

120. Wear Resistant Coatings (WBS No. 1331) FY 1989
$270,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. P. Stinton, (615) 574-4556
Caterpillar Contact: C. D. Weiss, 309-578-8672

The goal of this project is to develop wear-resistant coatings for application to metallic components of low-heat-loss diesel engines, specifically, piston rings and cylinder liners. Three coating processes, plasma spraying, vapor deposition (CVD-PVD), and enameling, are being investigated to develop adherent, wear-resistant ceramic coatings. The coating systems will be screened for wear and friction at 350°C under lubricated conditions. Coatings which show promise will be optimized by adjustments to chemistry and hard particle content to meet the wear and friction goals. Optimized coatings will then be fully characterized for oxidation, adherence, uniformity, thermal shock, wear, and friction. Selected coatings will be applied to simulated engine component specimens and thermal conductivity measurements will be obtained.

Keywords: Chemical Vapor Deposition, Coatings and Films, Engines, Friction, Structural Ceramics, Wear

121. Wear Resistant Coatings (WBS No. 1332) FY 1989
$264,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. P. Stinton, (615) 574-4556
Cummins Contact: Malcolm Naylor, (812) 377-7713

The goal of this project is to develop wear-resistant coatings for application to metallic components of low-heat-loss diesel engines, specifically, piston rings and cylinder liners. Visual inspection and oxidation; friction and wear tests; thermal shock uniformity, hardness, and adherence; and electron microscopy and surface analysis will be evaluated to determine the chemical and microstructural characteristics that control the coatings' wear, adherence, and reliability. Based on a review of the data, the most promising coating systems will be selected for further evaluation.

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

122. Active Metal Brazing PSZ-Iron (WBS No. 1411) FY 1989
$220,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. Ray 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. A novel method for brazing zirconia to cast iron has already been established. Presently, this work is focused on the joining of partially stabilized zirconia and silicon nitride by brazing. Current efforts include 1) completing the initial assessment of zirconia joint strength, 2) high temperature brazing of titanium vapor-coated silicon nitride, 3) correlating braze joint microstructures with strength data to identify factors controlling joint strength, and 4) developing a method of calibrating the indentation fracture technique to determine the accuracy of residual stresses measurements in ceramic-to-metal joints.

Keywords: Metals, Structural Ceramics, Joining/Welding, Brazing, Cast Iron, Zirconia, Alumina, Silicon Nitride

123. Metal-Ceramic Joints AGT (WBS No. 1412) FY 1989
$205,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: M. L. Santella, (615) 574-4805
GTE Contact: E. M. Dunn, (617) 466-2312

The goal of this work is to demonstrate analytical tools for use in designing ceramic-to-metal joints including the strain response of joints as a function of the mechanical and physical properties of the ceramic and metal, the materials used in producing the joint, the geometry of the joint, externally imposed stresses both mechanical and thermal in nature, temperature, and the effects on joints exposed for long times at high temperature in an oxidizing (heat engine) atmosphere. The technical work involves both analytical and experimental tasks. The goal of the analytical work is a predictive model that can be used in engineering design of ceramic joints. The experimental work will involve the fabrication and testing of first small scale and later scale-up sized joints.

Keywords: Engines, Joining/Welding, Metals, Structural Ceramics, AGT, Metal-Ceramic, Physical/Mechanical Properties

124. Metal-Ceramic Joints AGT (WBS No. 1413) FY 1989
$ 0

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: M. L. Santella, (615) 574-4805
Battelle Contact: A. T. Hopper, (614) 424-4567

The objective of this project is to develop the analytical tools necessary to design reliable high strength ceramic oxide-to-ceramic oxide and ceramic oxide-to-metal joints. The technical work involves both analytical and experimental tasks. The goal of the analytical work is a predictive model that can be used in engineering design of ceramic joints. The experimental work will involve the fabrication and testing of first small scale and later scale-up sized joints.

Keywords: Engines, Joining/Welding, Metals, Structural Ceramics, Modeling, Oxides

125. Ceramic-Ceramic Joints AGT (WBS No. 1421) FY 1989
$325,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: M. L. Santella, (615) 574-4805
Norton Contact: G. A. Rossi, (508) 393-5829

The purpose of this program is to develop techniques for producing reliable ceramic-ceramic joints and analytical modeling to predict the performance of the joints under a variety of environmental and mechanical loading conditions including high temperature, oxidizing atmospheres. The ceramic materials under consideration are silicon nitride and silicon carbide. The joining approach for silicon nitride is based on the ASEA hot isostatic pressing process, while the plan is to co-sinter silicon carbide green forms together. These joining methods were selected to produce joints which exhibit the minimum possible deviation in properties from those of the parent ceramic materials. Analytical models will be experimentally verified by measurements on experimental size and scale-up joints as part of this work.

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

126. Thick Thermal Barrier Coatings — FY 1989 $25,000

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

Design and demonstration of the durability of thick thermal barrier coatings with low thermal conductance for use in low heat rejection diesel engines is the objective of the project. Zirconia-based coating systems will be developed and applied to metal engine parts for evaluation in a single cylinder engine rig.

Keywords: Coatings, Oxide Ceramics, Diesel Engines

127. Thick Thermal Barrier Coatings — FY 1989 $175,000

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

Zirconia thermal barrier coating (TBC) systems are being developed and applied to diesel engine parts for evaluation in a single cylinder engine rig.

Keywords: Coatings, Oxide Ceramics, Diesel Engines

128. Sliding Seal Materials for Diesel — FY 1989 $ 0

DOE Contact: John W. Fairbanks, (202) 586-8066
NASA Contact: Richard Barrows, (216) 433-3388
Southwest Research Institute Contact: Shannon Vinyard, (512) 684-5111

The project, completed in 1989, was conducted in three phases. During the initial year quantitative information was obtained regarding the friction and wear behavior of candidate carbides rubbing against two ceramic cylinder liner materials under conditions representative of the environment of seal rings in adiabatic diesels. The second phase effort concentrated on ion-implantation surface treatments to improve the friction and wear characteristics of the candidate materials. In the final phase, piston seals were fabricated, tested, and evaluated in a test bed single cylinder engine with a ceramic cylinder liner.

Keywords: Carbides, Tribology, Ion-Implantation, Diesel Engines

129. <u>High Temperature Solid Lubricant Coatings</u> <u>FY 1989</u>
$50,000

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

High temperature wear resistant coating systems for use in the range of 500°C in diesel engines are being developed and evaluated. Plasma sprayed wear resistant matrix coatings containing solid lubricants for reduced friction and the modification of the surface chemistry of structural ceramics for improved friction and wear are two approaches being considered.

Keywords: Wear, Coatings, Diesel Engines, Tribology

130. <u>Advanced Turbine Technology Applications Project (ATTAP, AGT-5)</u> <u>FY 1989</u>
$5,100,000

DOE Contact: Saunders B. Kramer, (202) 586-8012
NASA Contact: Paul Kerwin, (216) 433-3409;
General Motors, Allison Gas Turbine Division, Contact: Phil Haley, (317) 230-2272

The requirements of this project are to demonstrate improved fuel economy, reduced emissions and alternate fuel capability and to develop ceramic materials for most or all of the hot section components. Efforts include material characterization, process development, and component design and test. In 1989, design of a 2500°F axial turbine stage was completed. Prototype ceramic components for dimensional and properties characterization have been fabricated.

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

131. Advanced Turbine Technology Applications Project (ATTAP, AGT-101)

FY 1989
$5,100,000

DOE Contact: Saunders B. Kramer, (202) 586-8012
NASA Contact: Thomas N. Strom, (216) 433-3408
Garrett Turbine Engine Contact: Jim Kidwell, (602) 220-3463

Advanced structural ceramic materials are being applied to hot flow path components for an automotive type turbine engine designed for operation at 2500°F. The project combines an integrated design, fabrication, and test approach with component technology verification in an engine environment. Design of a 2500°F radial turbine stage has been completed. Fabrication of prototype components is underway. A study to quantify rotor impact damage has been initiated to provide design data for the turbine rotor and a flow stream particle trap.

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

OFFICE OF ENERGY STORAGE AND DISTRIBUTION

The mission of the Office of Energy Storage and Distribution is to lead a national research and development program focused on translating technical and scientific breakthroughs into options for electric energy delivery and control systems and for energy conversion. The Office manages programs in electric energy systems and energy storage and is responsible for the formulation and execution of appropriate national policies and the verification of program balance and priorities among the technologies.

Energy Storage

The Energy Storage Program supports research and development of advanced energy storage and electrochemical conversion systems that will facilitate the substitution of nuclear and renewable energy sources for oil and gas 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 three subprograms: Electrochemical Energy Storage, Battery Development, and Thermal Energy Storage.

Materials Preparation, Synthesis, Growth or Forming

132. Corrosion-Resistant Coatings for High-Temperature, High-Sulfur Activity Applications

FY 1989
$137,000

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

This research project explores electrodeposition and chemical vapor deposition techniques used to prepare corrosion-resistant coatings for high-temperature batteries. The deposition of molybdenum and Mo_2-C by electrochemical deposition in molten salt was optimized in order to obtain reproducible thicknesses and smooth surface morphology. The corrosion resistance of Mo, Mo_2-C and TiN were determined in Na-polysulfide melt. All three coatings showed behavior comparable to that of solid Mo in this melt.

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

Materials Properties, Behavior, Characterization or Testing

133. Materials Durability in the Zinc/Bromine System FY 1989 $104,000

DOE Contact: A. Landgrebe, (202) 586-1483
Sandia National Laboratory Contact: C. Arnold, (505) 844-8728

Project efforts are directed toward improving the chemical durability of polyvinyl chloride (PVC) in zinc/bromine battery environments. The durability of several PVC formulations under consideration by the Energy Research Corporation as flow frame materials has been studied. Chemical and mechanical property measurements were performed. These experiments showed that both the concentration of several additives in the PVC and the shear modules were significantly reduce after exposure to a bromine-containing electrolyte. Another potential flow frame material, Tefzel, was also evaluated under accelerated aging conditions and shown to remain essentially unchanged except for some discoloration. In contrast, all of the PVC formulations exposed to similar conditions were not only discolored but blistered and swollen as well.

Keywords: Batteries, Corrosion

134. Solid-Electrolyte Cell Research FY 1989 $150,000

DOE Contact: A. Landgrebe, (202) 586-1483
Argonne National Laboratory Contact: C. Christianson, (312) 972-7563

Efforts are directed toward developing glass-to-header seals that are mechanically stable and provide hermetic seals for use in sodium/sulfur cells. The material investigated for this purpose was a sodium-ion conducting glass (in mol%): 42 Na_2O, 8 Al_2O_3, 5 ZrO_2, and 45 SiO_2, which has a resistivity of about 220 ohm-cm at 300°C. Ceramics based on magnesium oxide were found to be ideal candidates for sealing the glass to a header.

Keywords: Ceramics, Solid-Electrolytes

135. Zinc Electrode Morphology in Acid Electrolytes FY 1989 $100,000

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

Zinc electrode morphology is studied in acidic zinc chloride and zinc bromine electrolytes to provide the fundamental information needed to improve the design and performance of zinc/halogen batteries. *In situ* studies of the formation of zincate ions in Zn/AgO cells containing 12 M potassium hydroxide were initiated. Additional studies were made in 12 M KOH with silicate, sorbitol and mixtures of both additives.

Keywords: Electrodes, Morphology

136. Zinc/Air Battery Development for Electric Vehicles FY 1989 $119,000

DOE Contact: A. Landgrebe, (202) 586-1483
Metal Air Technology Systems International Contact: R. Putt, (415) 654-1960

Demonstrated that zinc loadings greater than 100 mAh/cm^2 can be attained in a reticulated electrode structure. A process was developed for pre-plating copper substrate on a reticulated electrode structure. The process yielded a dense, uniform, and continuous zinc deposit.

Keywords: Batteries, Electrode

137. Dendritic Zinc Deposition in Flow Batteries FY 1989 $ 0

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

The extent of hydrogen evolution during zinc deposition from zinc bromine solution by periodic current, as opposed to direct current were compared. In acidic zinc electrodeposition, hydrogen evolution can be reduced by applying pulse modulation below the levels at which constant current is applied. The effects of current or potential modulation observed during this research, combined with studies of substrate orientation and surface profile effects, are expected to contribute to a better understanding of the mechanism of electrodeposition of zinc from acidic solutions.

Keywords: Corrosion, Structure, Batteries, Behavior Modeling

138. Fast Ion Conduction and Corrosion Processes in Lithium Glasses FY 1989
$50,000

DOE Contact: A. Landgrebe, (202) 586-1483
MIT Contact: H. Tuller, (617) 253-6890

Since calcium oxide is thermodynamically stable in contact with lithium, its roles in stabilizing lithium-borate-based fast ion-conduction glasses against lithium attack and decreasing lithium ion conductivity are being investigated. The ionic conductivity was examined for CaO additions ranging from 0-30 mol% for both the diborate and metaborate systems which had $(LiCl)_2/B_2O_3$ ratios of 0.15:0.25 and 0.15:0.40, respectively.

Keywords: Solid Electrolytes, Fast Ion Conductors, Corrosion

139. Polymeric Electrolytes for Ambient-Temperature Lithium Batteries FY 1989
$46,000

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

A detailed study by thermal gravimetric analysis and differential scanning calorimetry of polyethylene oxide was undertaken to determine the effects of hydration/dehydration on parameters such as T_g, maximum water uptake, amount of coordinated water, and the reversibility of hydration/dehydration of polymeric electrolytes for lithium batteries. The results show that the hydration/dehydration characteristics of the electrolyte are strongly influenced by the identity of the cation in the electrolyte.

Keywords: Polymers, Batteries

140. Exploratory Cell Research and Study of Fundamental Processes in Solid State Electrochemical Cells FY 1989
$ 0

DOE Contact: A. Landgrebe, (202) 586-1483
University of Minnesota Contact: W. Smyrl, (612) 625-0717

The enhancement and characterization of polyethylene oxide (PEO) conductivity and interfacial cell properties using newly developed methodologies have continued. Sodium/solid-polymer-electrolyte rechargeable $Na/NaCF_3SO_3PEO_8/V_6O_{13}$ cells were investigated and found to have high open-circuit voltages (OCV), good cycling capability, and specific energy of 260 Wh/kg. Stability and good reversibility were observed for up to 11 cycles. Solid-polymer-electrolyte cells based on divalent metals gave mixed results. Anion insertion/removal in electroactive polymer film electrodes was studied by impedance measurements.

Keywords: Conducting Polymers, Batteries

141. Corrosion, Passivity, and Breakdown of Alloys Used in High-Energy-Density Batteries

FY 1989
$ 0

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

Over the past year a complete investigation of the passivation behavior of iron in anhydrous propylene carbonate (PC) containing 0.5 M $LiClO_4$ was undertaken. In addition, preliminary studies of the effect of the electrolyte anion on the phenomena observed have been conducted by investigating passivation in the presence of 0.5 M $LiAsF_6$. Recent studies of iron in PC containing 0.5 M $LiAsF_6$ showed that iron pits upon modest anodic polarization, indicating that the air-formed film is not as protective in the presence of AsF_6 as in the presence of ClO_4. The reasons for this behavior is the subject of ongoing work.

Keywords: Corrosion-Aqueous, Ferrous Metals, Batteries

142. Advanced Chemistry and Materials for Fuel Cells

FY 1989
$150,000

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

Work has focused on investigating oxygen reduction in new acidic electrolytes and evaluating new fuel cell electrocatalysts. A new process was developed for making more uniform, carbon-supported platinum samples. This improved the quality of the EXAFS data. EXAFS studies were carried out on Fe-TMPP on Cabot Black Pearls Carbon.

Keywords: Fuel Cells, Catalysts, Pyrolysis

143. Electrocatalysts for Oxygen Reduction and Generation FY 1989
$205,000

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

Both *ex situ* and *in situ* Fourier transform infrared reflectance absorption spectroscopy (FTIRRAS) were used to examine monolayers of adsorbed iron and tetrasulfonated phthalocyanine (CoTSPc) on silver, highly ordered pyrolytic graphite (HOPG), and ordinary pyrolytic graphite (OPG). In addition to nitrogen-containing polymers, other polymers such as polystyrene mixed with cobalt acetate and Vulcan XC-72 carbon and heat-treated at 800°C were examined.

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

Materials Structure and Composition

144. Molten Salt Cell Research FY 1989
$350,000

DOE Contact: A. Landgrebe, (202) 586-1483
Argonne National Laboratory Contact: C. Christianson, (312) 972-7563

Experiments are underway to improve the Li-alloy/metal disulfide cell (i.e., to develop separator/electrolyte systems that are stable at high Li activities). High-temperature immobilized electrolyte (HTIE) materials are being investigated for this purpose. These materials consist of an insulator-type ceramic material (e.g., MgO) that is infiltrated by a liquid salt which is held in the pores by capillary forces. The dc conductivity was measured on HTIE separator materials in a specially designed cell and was found to be significantly lower than the conductivity of pure molten salt.

Keywords: Batteries, Solid Electrolytes

145. New Alkali-Based Battery Materials FY 1989
$205,000

DOE Contact: A. Landgrebe, (202) 586-1483
Stanford University Contact: R. Huggins, (415) 723-4110

An effort is underway to characterize high-sodium-activity alloys and low-melting-point molten salts for sodium metal chloride cells. This research seeks to improve the removal of the high-impedance solid electrolyte. A number of alloy compositions were screened for their ability to act as fast, reversible sodium-conducting electrodes. The use of a family of alkali halide ammoniate salts for sodium metal chloride cells was also investigated.

Keywords: Batteries, Chemical Vapor Deposition, Fast Ion Conductors

146. Spectroscopic Studies of Passive Films on Alkali and Alkaline Earth Metals in Nonaqueous Solvents — FY 1989 — $86,000

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

Research efforts have focused on preparing and characterizing submonolayer deposits of alkali and alkaline earth metals on metal surfaces and developing the understanding of passive surface layers in rechargeable alkali batteries. The activation of carbon dioxide induced by the presence of alkali metal atoms adsorbed on an otherwise inert substrate was examined with an array of surface analytical methods. The analytical techniques in this study included work function measurements, low energy electron diffraction, Auger electron, X-ray photoelectron XPS, high resolution electron energy loss, and thermal desorption spectroscopies.

Keywords: Surface, Structure, Vapor Deposition, Films, Batteries

147. Raman Spectroscopy of Electrode Surface in Ambient-Temperature Lithium Secondary Battery — FY 1989 — $ 0

DOE Contact: A. Landgrebe, (202) 586-1483
Jackson State University Contact: H. Tachikawa, (601) 968-2171

In situ Raman spectroscopy was applied to study lithium electrodes in propylene carbonate, 2-methyl tetrahydrofuran and acetonitrile. *In situ* Raman spectroscopic investigations of zinc electrode surfaces were also carried out in 7.0 M potassium hydroxide solutions with and without zinc oxide.

Keywords: Surface, Structure, Batteries

Device or Component Fabrication, Behavior or Testing

148. Proton-Exchange-Membrane Fuel Cells for Vehicles — FY 1989 — $1,350,000

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

Los Alamos National Laboratory conducts three major proton-exchange-membrane (PEM) fuel cell projects. These projects seek to: 1) develop better gas diffusion electrodes, 2) measure and model the mass transport properties and conductivity of proton-conducting membranes, and 3) measure the operating characteristics of single PEM fuel cells and determine the conditions providing optimal performance. In FY 1989, measurements of water drag under experimental conditions close to those of an operating PEM fuel cell were initiated. The profile of Nafion impregnated in Prototech electrodes was evaluated by employing an electron probe microanalyzer. A series of tests were also performed on the effects of ionomeric membrane thickness on the performance of single PEM cells.

Keywords: Fuel Cells, Separators, Electrodes

149. Incorporation of Phase-Change Materials in Building Materials — FY 1989 — $148,000

DOE Contact: E. Reimers, (202) 586-2826
University of Dayton Research Institute Contact: I. Salyer, (513) 229-2113

This project seeks to develop low-cost, effective PCMs that melt and freeze sharply in the temperature range 23°C to 25°C. These PCMs will be used as thermal storage building interiors and wallboard systems. Octadecane paraffin has been identified as a promising energy storage PCM for the passive solar application. Its melting point is about 23°C; it is chemically, physically, and biologically inert; its melt/freeze characteristics are well behaved with a substantial heat of fusion; it is inexpensive; and it can be incorporated into a number of different conventional building materials.

Keywords: Thermal Storage, Phase Change Materials

150. Component Stress During Freeze/Thaw Cycling of Sodium/Sulfur Cell FY 1989
$210,000

DOE Contact: A. Landgrebe, (202) 586-1483
Sandia National Laboratory Contact: J. Braithwaite, (505) 844-7749

The objective of this task is to provide developers with the understanding and methodology to improve the freeze/thaw (F/T) durability of sodium/sulfur cells. The major effort for FY 1989 focused on refining and validating a mathematical model that will accurately predict the state-of-stress for the primary components of a normally operating cell. During this time, the materials-behavior models were refined to enable calculations to be consistent with actual strain measurements. The measurement of the physical properties of sodium polysulfide/graphite composites was also completed.

Keywords: Composites, Batteries, Mathematical Modeling

151. β-Alumina Electrolyte Degradation FY 1989
$52,000

DOE Contact: A. Landgrebe, (202) 586-1483
Sandia National Laboratory Contact: E. Beauchamp, (505) 844-6039

The thrust of this project is to study mechanisms that cause the failure of β-alumina electrolyte in sodium/sulfur battery cells. Results obtained in early FY 1989 showed that, in general, the failure of the small "PB" cell can now be traced to identifiable outside factors, such as contamination, or to problems incurred during production of components.

Keywords: Electrolytes, Batteries

152. Aluminum/Air Technology Development FY 1989
$580,000

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

The air cathode materials and design for aluminum/air batteries will be optimized for long life and low cost, the aluminum alloy material and electrode geometry will be optimized for low self-discharge and high specific peak power, and the auxiliary battery systems, such as solids separation, will be designed for long life and high reliability. During FY 1989, a 12-volt (10-cell) aluminum/air battery was built which incorporates redesigned, more rugged B-300 cells. A series of six tests was conducted to complete the initial evaluation. The test variables included current density, electrolyte composition, and electrolyte concentration.

Keywords: Batteries, Electrolytes

153. Research on Slurry Zinc/Air Battery

FY 1989
$ 0

DOE Contact: A. Landgrebe, (202) 586-1483
Pinnacle Research Institute Contact: H. S. Alcazar, (408) 252-1360

The generation of slurry zinc in a charge cell and its use in a Zn/air cell were demonstrated. Dendritic zinc was deposited, under conditions requiring minimal electric energy. Discharge rates comparable to those obtained with slurries made with mixtures of zinc powder were obtained with the regenerated dendritic zinc slurry. The minimum constant current density, which is the minimal energy for deposition of suitable dendritic zinc at a given zincate concentration and temperature, was determined.

Keywords: Deposition, Battery

154. Aluminum Anode Research

FY 1989
$ 0

DOE Contact: A. Landgrebe, (202) 586-1483
SRI International Contact: D. MacDonald, (415) 859-3195

The corrosion rate and mechanism of an aluminum alloy are investigated in order to develop improved aluminum alloys for an aluminum/air battery. In FY 1989, solution-phase inhibition was investigated as a promising strategy for controlling the corrosion of aluminum. Potassium manganate (K_2MnO_4) and Na_2Sn_3 + $In(OH)_3$ were effective inhibitor systems, particularly at high discharge rates (400mA/cm^2); but, at low discharge rates only K_2MnO_4 offered a significant advantage in coulombic efficiency over the uninhibited solution.

Keywords: Batteries, Corrosion

155. Solid Polymer Electrolytes for Rechargeable Batteries

FY 1989
$97,000

DOE Contact: A. Landgrebe, (202) 586-1483
SRI International Contact: D. MacDonald, (415) 859-3195

High-conductivity polymeric electrolytes for rechargeable lithium cells are developed. In FY 1989, poly(ethyleneimine) and poly(aloxane) based polymers were successfully synthesized.

Keywords: Polymers, Electrolytes, Batteries

156. Advanced Membrane Development for the Zinc/Bromine System FY 1989
$140,000

DOE Contract: A. Landgrebe, (202) 586-1483
Sandia National Laboratory Contact: C. Arnold, (505) 844-8728

The primary emphasis of this task is to select and evaluate chemical pretreatment techniques for use on the silica-filled microporous polyethylene separators used in the zinc/bromine battery technology. Desirable changes in resistivity and permeability were produced with the uniform impregnation with sulfonated polysulfone, and an extensive range of separator performance was demonstrated. Two candidate separators, Daramic and SF-400, were impregnated with Nafion, a fully-fluorinated, sulfonic acid polymer. Several studies were completed to evaluate the effects of surface treatments and various impregnation procedures.

Keywords: Polymers, Batteries, Composites

157. Improved Chromium Platings for Sodium/Sulfur Cell Containers FY 1989
$69,000

DOE Contact: A. Landgrebe, (202) 586-1483
Sandia National Laboratory Contact: W. D. Bonivert, (415) 294-2987

The research emphasis will be on developing techniques to electroplate high-quality chromium layers onto carbon and stainless steels. In this activity, the effect of three different electrolyte compositions on deposit quality and performance was studied. These electrolytes included 1) a standard chromium-oxide/sulfuric acid electrolyte suitable for use with pulse and pulse-reverse plating techniques, 2) a commercial electrolyte formulation (M&T CF-500) that produces crack-free deposits that was modified by adding vanadium pentoxide, and 3) a second commercial electrolyte (M&T CR-110) that produces highly cracked deposits.

Keywords: Batteries, Corrosion, Electrolytes

158. Dispersed Phase-Change Material Evaluation FY 1989 $20,000

DOE Contact: E. Reimers, (202) 586-4563
A.D. Solomon Contact: A. Solomon, 1-972-57-699698 (Israel)

Researchers are constructing a mathematical model and computer program capable of predicting the transient thermal response of building materials containing PCMs as distributed aggregate. A computer model was developed that is capable of handling thermal transport and storage of both sensible and latent heat. Excellent agreement was found between experimental data and the data obtained using the computer model.

Keywords: Phase-Change Materials, Latent and Sensible Heat, Mathematical Modeling

159. Phase-Change Materials Wallboard Fabrication and Testing FY 1989 $60,000

DOE Contact: E. Reimers, (202) 586-4563
Martin Marietta Energy Systems Contact: J. Tomlinson, (615) 574-0768

A facility is being fabricated for preparing full-sized samples of PCM wallboard and for conducting dynamic thermal tests to determine comparative thermal performance. The facility for imbibing full-scale sheet-rock panels was completed. Arrangements for using an existing insulation test fixture at Oak Ridge for the dynamic tests were made.

Keywords: Phase-Change Materials

160. Effects of Dopants on Solid-State Phase-Change Materials FY 1989 $50,000

DOE Contact: E. Reimers, (202) 586-4563
University of Nevada - Reno Contact: D. Chandra, (816) 276-1283

Temperature-adjusted, organic, solid-state PCMs with solid-solid transition temperatures near room temperature are being developed. Work was continued in the identification and development of solid materials that exhibit a heat of transition as the material changes from one crystal structure to another. Glycerol was successfully used as a dopant to pentaerythritol and neopentylglycol.

Keywords: Phase-Change Materials, Composites

Electric Energy Systems

The Electric Energy Systems Program supports research and development directed toward solving mid- to long-term problems in electric energy transmission and distribution and promotes the development and integration of new materials, advanced controls, and new design concepts into the utility network. The program supports research activities in the following areas: Electric Field Effects, Reliability, and Electric Systems and Materials Research.

Materials Properties, Behavior, Characterization or Testing

161. High-Temperature Superconducting Materials Pilot Centers — FY 1989 $6,000,000

DOE Contact: R. Eaton, (202) 586-1506
Oak Ridge National Laboratory Contact: A. C. Schaffhauser, (615) 574-4826
Argonne National Laboratory Contact: E. Kaufmann, (312) 972-3606
Los Alamos National Laboratory Contact: R. Quinn, (505) 665-3030

The Pilot Centers were established at three national laboratories (Oak Ridge, Argonne, and Los Alamos) to keep the United States at the forefront of HTS technology research. The laboratories work collaboratively with industry to perform materials research. The laboratories also expedite research efforts by streamlining the process of obtaining patent rights and other intellectual property.

Keywords: Pilot Centers, Superconductors

162. Microfilamentary Superconducting Composite — FY 1989 $170,000

DOE Contact: R. Eaton, (202) 586-1506
Ames Laboratory Contact: D. K. Finnemore, (515) 294-3312

A material processing technique is being developed to make stabilized microfilamentary superconducting wires suitable for magnets that operate at 35 K and require a length-to-diameter ratio of 10,000 to 1. Tasks include filament (microfilamentary composite similar to Nb_3Sn/Cu composites) preparation, development of high current transfer at the matrix superconductor boundary, and the study of strain tolerance of the composite. Proof of principle was demonstrated for forming long, slender fibers of Bi-Sr-Ca-Cu-O by a gas fiberization technique producing amorphous fibers having a length to diameter ratio in the 1000:1 to 10,000:1 range.

Keywords: Composites, Fibers, Grain Boundaries, Superconductors

163. Practical Superconductor Development for Electric Power Applications

FY 1989
$1,359,000

DOE Contact: R. Eaton, (202) 586-1506
Argonne National Laboratory Contact: R. Weeks, (312) 972-4930

The conductor development program aims to develop improved high-temperature superconducting (HTS) wires and tapes that have higher current-carrying capacity, greater flexibility and improved chemical stability. Conductors made of HTS thin films are investigated since they have potential for higher current capacity than has been measured in bulk HTS conductors. Ceramic processing, fabrication, and joining techniques are developed from the new classes of superconducting ceramics for use as superconducting parts in electrical power devices. Through densification procedures which avoid liquid grain boundary phases, the critical current density in $YBa_2Cu_3O_7$ was increased to a minimum of 10^4 amps/cm^2.

Keywords: Superconductors, Composites, Structure, Coatings and Films

164. Practical Conductor Development for Electric Power Systems

FY 1989
$1,150,000

DOE Contact: R. Eaton, (202) 586-1506
Brookhaven National Laboratory Contact: D. Welch, (516) 282-3517

The various methods employed for fabricating composite conductors containing high-T_c oxides will be restricted to those which can be scaled up to produce long lengths of conductor. Among the candidate methods are: various coating-on-substrates methods including thermal- and plasma-spraying and the use of organic binders; powder-in-a-tube methods; and the oxidation of rapidly solidified alloys. The composite conductors are characterized metallurgically and with respect to their superconducting properties. In FY 1989 two conductor fabrication methods were established: the powder-in-a-tube method in which oxide powders are packed into appropriate tubing, reduced in size, and then reacted to form a sintered-oxide wire or tape; and coating methods, in which the oxide powders are coated onto a substrate, using a binder or other techniques such as plasma spraying.

Keywords: Composites, Coatings and Films, Superconductors

165. Thin Films Superconductors for Electric Power Systems FY 1989
$830,000

DOE Contact: R. Eaton, (202) 586-1506
Solar Energy Research Institute Contact: R. McConnell, (303) 231-1019

The approach is to conduct research into fabrication processes for thin films, to characterize the properties of the films, and to support the development of a technology base on high-temperature superconducting thin films from which private enterprise can choose options for further development and commercialization. SERI's tasks for this research include: Superconducting Thin Film Task and Materials Analysis Task. A major achievement in FY 1989 was the evaluation of 162 research proposals in response to a SERI solicitation. Two new techniques, electrodeposition and chemical vapor deposition, were the subject of preliminary studies and proposals. Melt growth techniques were explored and coatings were made on sheets and filaments, some as long as 17 cm.

Keywords: Superconductors, Coatings and Films, Polymers, Crystal Growth, Structure

166. High-Temperature Superconductor Materials and Power Device Development
FY 1989
$1,000,000

DOE Contact: R. Eaton, (202) 586-1506
Sandia National Laboratory Contact: D. Schueler, (505) 844-1068

The principal effort of the project is to increase superconductor critical current density on the high temperature ceramic superconductor by reducing or eliminating grain boundary carbonate formation. The approaches pursued are: 1) preventing it from forming in the first place by controlling the solution-precipitation process; 2) decomposing the carbonate by heating to a point above which it is stable, probably 1350°C; and 3) using compounds that contain no Ba, such as the newly discovered BiSrCaCuO, 120K superconductor. Microcracks occur in bulk superconductors during the conversion of tetragonal YBCO to superconducting orthorhombic phase. One way to eliminate these microcracks is by particle orientation, such as by sinter forging, or by reclosing them by hot isostatic pressing of the orthorhombic form. In FY 1989, research focused on process scale-up methods for chemically prepared (chem-prep) precursor powders for $YBa_2Cu_3O_7$ in a reproducible and controlled fashion, and improving high-temperature processing conditions required to convert chem-prep and mixed-oxide powders to quality ceramic samples that have the highest critical current densities.

Keywords: Superconductors, Crystal Defects and Grain Boundaries, Structure, Consolidation of Powder, Powder Synthesis and Characterization

167. Fabrication Development of High-Temperature Superconductor for Electric Utility Applications

FY 1989
$600,000

DOE Contact: R. Eaton, (202) 586-1506
Los Alamos National Laboratory Contact: G. Maestas, (505) 667-3973

The approach stresses the simultaneous development of several fabrication techniques variously based on melt texturing, vapor deposition, and powder consolidation and fabrication. These approaches specifically address the currently known problems related to superconducting transport currents; in particular, the presence of non-superconducting intergranular barriers, the inherent anisotropy of the superconducting properties and development of crystal texture, and the questions of microcracking. While focusing on Tl-Ca-Ba-Cu-O as the benchmark current material, the proposed program will maintain the flexibility to incorporate new superconducting materials as they develop to an appropriate state.

Keywords: Superconductors, Structure, Coatings and Films, Crystal Defects and Grain Boundaries, Powder Consolidation, Powder Synthesis and Characterization

168. Development of Practical Conductors Utilizing High-Temperature Oxides

FY 1989
$560,000

DOE Contract: R. Eaton, (202) 586-1506
Oak Ridge National Laboratory Contact: A. Schaffhauser, (615) 574-4826

The primary effort is toward reducing or eliminating grain boundary resistance, one of the recognized causes of the poor critical currents observed in sintered $YBa_2Cu_3O_{7-x}$. Techniques are developed for the production of high purity, homogeneous, morphologically controlled precursor powder and the fabrication of conducting high-T_c oxides in complex shapes. Integration of the results of investigations of the dependence of grain boundary resistance and critical current density on composition and processing variables and the effects of texturing in superconducting ceramics will permit the production of high-J_c superconducting materials. An aerosol reactor system for the production of highly homogeneous, submicron oxide powders has been designed and constructed. Projects have also been initiated to study the effects on grain boundary composition of sintering and heat treatment schedules and the application of elevated oxygen pressures during heat treatment.

Keywords: Superconductors, Crystal Defects and Grains, Boundaries, Structure, Consolidation of Powders, Powder Synthesis and Characterization

169. Evaluation of Polymers for Electric Insulation FY 1989
$100,000

DOE Contact: R. Eaton, (202) 586-1506
Oak Ridge National Laboratory Contact: H. McCoy, (615) 574-5115

Mechanical, electrical and thermal property tests are performed on several aged polymers suitable for use in dielectric materials. Long-term degradation and multifactor aging studies in a variety of environments (nitrogen and transformer oil) are conducted to determine mechanical creep data. Several polymers were studied over a temperature range of -196 to 200°C. A report describing the aging tendencies (to 50,000 hours) of these polymers has been completed.

Keywords: Insulators/Dielectrics - Polymeric, Creep, Fracture, Polymers

Device or Component Fabrication, Behavior or Testing

170. Films Processing Methods and Device Technology Development FY 1989
$800,000

DOE Contact: R. Eaton, (202) 586-1506
Lawrence Berkeley Laboratory Contact: N. E. Phillips, (415) 486-4896

Methods are being investigated for producing thin films of high-T_c superconductors and appropriate substrate and passivating materials to provide a basis for the fabrication of practical conductors. The film deposition techniques include reactive magnetron sputtering, pulsed laser deposition, and sol-gel processing. The critical temperatures of the films was greatly improved this year due to closer control over composition and reliable characterization.

Keywords: Superconductors, Crystal Growth, Coatings and Films

171. Device Technology Development/System Study for HTS Equipment FY 1989
$300,000

DOE Contact: R. Eaton, (202) 586-1506
Pacific Northwest Laboratories Contact: J. Currie, (509) 375-4355

This study investigated the potential impacts of HTS applications on the electric utility industry in terms of performance, cost, and market issues that will drive the acceptance of HTS technologies. A computer code has been developed to compare the performance of conventional and HTS power transformers.

Keywords: Superconductors, Transformers, Utility Industry

172. Prototype Testing of Dynamic Insulation Using Sol-Gel Zinc Oxide — FY 1989 $ 0

DOE Contact: R. Eaton, (202) 586-1506
University of Southern California Contact: T. C. Cheng, (213) 743-6938

A ZnO insulator string is fabricated and tested to determine the optimum design for electrical insulation of overhead line transmission. In FY 1989, testing of the ZnO insulator string was performed at Bonneville Power Administration. These experiments showed that the properly-functioning imbedded ZnO disks were able to keep the outer ceramic insulators dry under fog conditions.

Keywords: Insulation, Ceramics

173. Interfacial Aging Phenomena in Power Cable Insulation Systems — FY 1989 $50,000

DOE Contact: R. Eaton, (202) 586-1506
University of Connecticut Contact: M. S. Mashikian, (203) 486-5298

Chemical, electrical and physical phenomena occurring at the insulation/shield interfaces in extruded high-voltage power cables are studied to determine the factors which contribute to cable insulation aging. Transport of ionic impurities from the semiconducting layers into the insulation are monitored. To date test cells fabricated from commercial and model semiconducting shield materials have been aged through 23,000 and 15,000 hours, with electric stress of 65 V/mil and 80 V/mil respectively. Selected specimens from the 15,000 hour sample have been removed from the test and have been subjected to the analysis protocol.

Keywords: Semiconductors, Insulators/Dielectrics - Polymeric

174. Conducting Polymer Research for Electric Power Equipment Applications — FY 1989 $9,000

DOE Contact: R. Eaton, (202) 586-1506
Westinghouse Contact: E. Schoch, (412) 256-1960

State-of-the-art conducting polymer materials are assessed to determine the technical and economical feasibility of replacing traditional stress grading materials in electrical equipment with conducting polymers. In FY 1989, 32 potential applications were discussed and ranked according to technical impact and probability of success. The highest scoring applications were coatings of dielectric films in capacitors, busing coatings, and surface conductor films in gas-insulated equipment, and covers for conductors and static charge dissipating brushes in rotating machines.

Keywords: Polymers, Coatings and Films

175. Fuel Cells for Transportation - Fuel Cell Testing — FY 1989 $170,000

DOE Contact: A. Landgrebe, (202) 586-1483/FTS 896-1483
LANL Contact: S. Gottesfeld, (505) 667-0853

The objectives of this project are to measure the operating characteristics of single proton-exchange-membrane fuel cells and to determine the conditions providing optimal performance.

A performance level of 0.9 W/cm^2 has been repeatedly demonstrated with 3 atm H^2 and 5 atm air in our low Pt loading cells. Testing of single cells under a variety of experimental conditions has been continued, stressing the effects of reactant gas pressures and of contact resistances. It was demonstrated that increased air pressure results in a shift of water from cathode to anode improving the performance at both interfaces. The electrode/membrane contact was found to be associated with a resistance of the order of 0.1 ohm cm^2, apparently caused by partial microscopic delamination. Elimination of this source of resistance can lead to further improvement in cell performance.

Keywords: Fuel Cells, Proton-Exchange-Membrane

176. Fuel Cells for Transportation - Electrode Optimization — FY 1989 $240,000

DOE Contact: A. Landgrebe, (202) 586-1483/FTS 896-1483
LANL Contact: S. Gottesfeld, (505) 667-0853

The objective of this project is to develop fabrication techniques for fuel cell membrane/electrode assemblies that deliver high performance with low Pt loading.

The Pt loading in gas diffusion electrodes employed in our polymer electrolyte fuel cells has been further reduced by a factor of two, from 0.40 to 0.23 mg/cm^2, without loss of performance. This was achieved by "planarization" of the front surface of the Prototech electrode prior to application of the Pt/C catalyst. This approach resulted in more uniform contact between the catalyst and the membrane. Impedance spectra taken for operating cells have demonstrated that losses caused by dehydration of the ionomeric additive can be distinguished by this diagnostic technique from losses caused by gas transport limitations and that increased resistance of the membrane with current density can be detected.

Keywords: Fuel Cells, Platinum Catalyst

177. Fuel Cells for Transportation - Non-Pt Electrocatalysts | FY 1989 | $110,000

DOE Contact: A. Landgrebe, (202) 586-1483/FTS 896-1483
LANL Contact: S. Gottesfeld, (505) 667-0853

The objectives of this project are to evaluate the effectiveness of transition metal macrocyclic catalysts such as FeTMPP and CoTMPP for oxygen reduction in PEM fuel cells.

A series of tests was completed in our polymer electrolyte cells with cathodes employing FeTMPP and CoTMPP catalysts. It was found that the activity of such catalysts is substantially lower than that of Pt in the acidic polymer environment. This conclusion is based on careful comparison with the performance of electrodes of identical structure made by the same manufacturer and employing a Pt cathode catalyst. Considering the small loadings of Pt required to achieve high performance in our polymer electrolyte cells, we have concluded that the metal macrocyclic catalysts tested are not viable cathode catalyst replacements.

Keywords: Fuel Cells, Metal Macrocyclic Catalyst

178. Fuel Cells for Transportation - State of Water and Water Transport in Proton Exchange Membranes | FY 1989 | $110,000

DOE Contact: A. Landgrebe, (202) 586-1483/FTS 896-1483
LANL Contact: S. Gottesfeld, (505) 667-0853

The objectives of this project are to measure and model the state of water and the water transport properties of proton-conducting membranes available from industry and to use these data to improve fuel cell performance.

Measurements of water drag in polymer electrolyte cells have provided important basic parameters required for optimized cell operation and stack design. The protonic water drag for Nation 117 has been determined as 2.5 and 1.7 H_2O/H^+, at 25 and 80°C respectively, for well hydrated and well humidified membranes. The drag may be lower (1 H_2O/H^+) in some ionomer membranes of lower EW. It was demonstrated that a sufficient rate of H_2O in aerosol form can be supplied with the fuel feed stream to satisfy such water drag requirements, but better micromanagement of water within the gas diffusion electrode structure is required to take full advantage of this type of water supply.

Keywords: Fuel Cells, Polymer Electrolyte, Water Transport

179. Fuel Cells for Transportation - CO Tolerance

FY 1989
$120,000

DOE Contact: A. Landgrebe, (202) 586-1483/FTS 896-1483
LANL Contact: S. Gottesfeld, (505) 667-0853

The objectives of this project are to quantify the effects of CO on PEM fuel cell performance and to investigate the effectiveness of oxygen injection and alloy catalysts for improving CO tolerance.

The technique of *in-situ* bleeding of low levels of oxygen or air has been demonstrated to be very effective and reproducible in removing poisoning effects of 100 ppm CO in the fuel feed stream. (Patent application has been accepted.) This technique may be a key to the application of carbonaceous fuel reformates as anode feeds in polymer electrolyte fuel cells. We have shown that the technique is effective at low hydrogen stoichiometries and with H_2CO_2 fuel cell mixtures. The air bleeding approach has been by far superior to the application of any carbon-supported "CO tolerant" Pt alloy electrocatalyst, such as PtRu or PtSn, tested by us this year.

Keywords: Fuel Cells, Oxygen Bleeding

180. Fuel Cells for Transportation - Industrial Contract International Fuel Cells Inc.

FY 1989
$650,000

DOE Contact: A. Landgrebe, (202) 586-1483/FTS 896-1483
LANL Contact: S. Gottesfeld, (505) 667-0853

The objectives of this contract are to develop low cost manufacturing techniques for PEM fuel cells and to fabricate and test a 5-10 kW PEM fuel cell stack.

The subject of this work is the investigation of designs and manufacturing methods for low cost fabrication of high-efficiency, high-power-density, proton exchange membrane fuel cell power plants. The objective is to evaluate high-performance proton exchange membrane-electrode configurations for practical and economic methods of manufacture and assembly. The evaluation will include assembly of the most promising configuration together with the other necessary components and ancillaries into a proton exchange membrane fuel cell power section subsystem. The power section will be tested to determine the performance and functioning of individual components. The goal is a high performance fuel cell power section wherein the potential of all components for low cost and ease of manufacture has been evaluated based on the contractor's fuel cell power plant production experience. Work began in July 1989.

Keywords: Fuel Cells, Low Cost Fabrication

OFFICE OF SOLAR HEAT TECHNOLOGIES

The goal of the Office of Solar Heat Technologies is to provide industry with a technology base that will ensure the supply of components and systems that convert solar energy into usable thermal energy at competitive costs. The overall objective of the Office is to enhance the technical and economic feasibility of solar heat technologies for heating and cooling of buildings, agricultural and industrial applications, and generation of electricity. This involves: (a) supporting long-term, high risk research and development which industry cannot be expected to support, but which has high benefit potential; and (b) transferring research results to industry. The Office works in close cooperation with industry and institutions, including international organizations, to ensure that government-sponsored activities focus on research and development of concepts which have great potential payoff and do not duplicate efforts in the private sector. The Office balances the program among exploratory research and development; materials and components development; systems design, test and evaluation; and technology transfer activities.

Solar Buildings Technology Division

The program goal is to develop a technology base that will allow industry to develop solar energy products and designs for the buildings that are reliable and economically competitive, and can contribute significantly to national building energy requirements. The objectives are:

- In the near-term, to provide industry with the information required to improve system performance and achieve acceptable equipment service life and reliability.
- In the long-term, to develop solar energy technologies that can supply up to 80 percent of residential building space heating and hot water requirements and 60 percent of its cooling requirements, and up to 60 percent of nonresidential building heating, cooling, and daylighting energy requirements, at costs competitive with conventional technologies.

The program sponsors activities, in cooperation with the building sector, that promise to improve dramatically the efficiency, cost, and applicability of solar building technologies in the long-term while providing design data from testing and analysis of state-of-the-art materials and systems useful to industry in the near-term. R&D is conducted on new approaches for collection, conversion, storage, and delivery of solar energy using the building envelope and equipment. A "whole buildings" or systems perspective is employed by the program to ensure that the research direction and activities reflect an understanding of the interaction of new technologies with buildings and building systems.

Materials Preparation, Synthesis, Deposition, Growth or Forming

181. Electrochromic Glazings (Nickel-based) FY 1989
$285,000

DOE Contact: M. M. Jenior, (202) 586-2998, FTS 896-2998
LBL Contact: S. Selkowitz, (415) 486-5064, FTS 451-5064

The objectives of this project are to develop switching devices for regulating daylight and solar heat gain for all building glazing applications. The current focus is on electrochromic devices based on nickel oxide that can switch reversibly over a large visible transmission range (e.g., 80-10 percent), have long operating lifetimes, and are compatible with large-area, low-cost deposition processes used by industry. In FY89, electrochromic nickel films were made at LBL by both electrochemical and sputtering techniques. The properties of these films were compared to those made by industrial collaborators using similar techniques and significant differences were observed. Lithiated nickel oxide films were successfully produced with relatively high coloration efficiency, thus opening the possibility of a lithium-based nickel electrochromic device. Stable manganese oxide films were fabricated for testing as counterelectrodes. The polymer electrolyte used in previous studies was improved and new solid-state and polymeric candidate materials were identified and will be tested.

Keywords: Coatings and Films, Low Temperature Service

182. Solid State Tungsten-Based Electrochromic Films Windows FY 1989
$120,000

DOE Contact: M. M. Jenior, (202) 586-2998, FTS 896-2998
EIC Contact: R. D. Rauch, (617) 769-9450

This research is focused on the development of an all solid-state electrochromic film for windows that can provide active control of solar gains through windows by the application of a small DC current. The fabrication processes must be appropriate for large areas using standard thin film vacuum deposition techniques.

These "smart" windows will offer a means of regulating solar input to and radiation heat loss from building interiors to improve energy efficiency. Thin film laminated tungsten-based electrochromic devices with typical five-layer configurations (transparent conductor, electrochromic, ion-conducting, counterelectrode, transparent conductor layers on glass) have been fabricated and their optical and electrochemical behavior characterized. The devices exhibit reversible electrochromic switching over approximately 100 cycles. The primary focus of FY 1989 work was on appropriate materials for the various layers of solid-state films, in particular the ion-conducting, counterelectrode and transparent conductor layers, and the behavior when used with one other

Keywords: Coatings and Films, Low Temperature Service

183. Tungsten-Based Electrochomic Materials for Controlled Radiant Energy in Buildings
FY 1989
$222,000

DOE Contact: M. M. Jenior, (202) 586-2998, FTS 896-2998
Tufts University Contact: R. B. Goldner, (617) 628-5000

This project involves development and modeling of all-solid optical switching devices based on tungsten-based electrochromic films and other identified candidate materials in a generic electrochemical structure: TC/CE/IC/EC/TC (where TC = transparent conductor, CE = counterelectrode, IC = ion conductor, and EC = electrochromic layers). The approach is four-fold: to demonstrate feasibility and identify candidate materials (Phase I, completed); to improve and model each of the window layers and build prototypes (Phase II, in progress); to use these prototypes to help solve the problems associated with large area electrochromic (ec) windows development (Phase III); and to transfer the technology (Phase IV). Electrically switchable glazings can control the radiant energy transfer in buildings and other enclosed spaces (e.g., vehicles) economically and automatically, thereby significantly improving their energy efficiency. The feasibility of variable reflectivity in (poly-) crystalline films of tungsten oxide (c-WO_3) and of solid state structures operable largely in the variable reflectivity mode have also been demonstrated. Also, candidate materials for each window layer have been identified and their performance limits have been established. In FY89, the research team focused on fundamental scale-up and material problems of the ion-conducting, counterelectrode, and transparent conductor layers, and on low-temperature deposition methods.

Keywords: Coatings and Films, Transformation, Low Temperature Service

184. Holographic Diffractive Structures for Enhanced Daylighting
FY 1989
$125,000

DOE Contact: M. M. Jenior, (202) 586-2998, FTS 896-2998
Advanced Environmental Research Group Contact: R. Ian-Frese, (617) 864-4982

This project involves the development of a low-cost holographic diffractive structure (HDS) system that maximizes the utilization of sunlight for daylighting. HDSs are designed to direct and distribute sunlight into inaccessible areas (holographic solar access) or can make the energy of the sun available during the hours of the day when solar angles would otherwise be unfavorable for the practical use of solar energy. The use of holographic diffraction to provide area lighting from solar radiation would be less expensive than artificial lighting; air conditioning loads would also be reduced. The technical feasibility of using HDSs for daylighting has been demonstrated. The holograms used in the demonstration were made of silver halide emulsions on glass and plastic substrates—a process which is economically infeasible on a commercial scale. The development of a working prototype capable of achieving a 47° acceptance angle, full azimuth range, and optimal efficiency is planned. Instead of being produced in silver halide emulsion, it will be embossed on a film which will then be suspended between two plates of glass or adhered to a glass surface. In FY89, holographic diffractive structure materials were developed, installed in a scaled architectural model, and delivered to LBL for testing.

Keywords: Coatings and Films, Low Temperature Service

Materials Properties, Behavior, Characterization, or Testing

185. Desiccant Concepts — FY 1989 — $125,000

DOE Contact: J. Goldsmith, (202) 586-8779, FTS 896-8779
SERI Contact: A. Pesaran, (303) 231-7636, FTS 327-7636

The overall objectives of this research are to improve the cost performance and reliability of desiccant dehumidifiers for solar cooling applications. The specific objective of this project is to generate experimental data bases to investigate the impact of desiccant contamination due to airborne pollutants (particularly cigarette smoke) on the performance of desiccant materials. A desiccant contamination test facility was fabricated and made operational in June 1989. In the facility, 100 samples of 10 desiccant materials are exposed to humid air charged with a variety of common contaminants. Another 100 samples are exposed to clean humid air. During the duration of the 9 month experiment, samples from both clean and contaminated batches will be removed for study. The data will be used to determine the service life of desiccants and methods to mitigate the potential contaminant induced degradation.

Keywords: Polymers, Organics, Surface Phenomena, Desiccants

186. Advanced Desiccant Materials Research — FY 1989 — $100,000

DOE Contact: J. Goldsmith, (202) 586-8779, FTS 896-8779
SERI Contact: A. Czanderna, (303) 231-1240, FTS 327-1240

This project involves determining how the desired sorption performance of advanced desiccant materials can be predicted by understanding the role of their surface phenomena and materials modifications. The technological objective is to identify a next generation, low-cost material with which solar radiation or heat from another low-cost energy source is used for regenerating the water vapor sorption activity of the desiccant. In FY89, the polystyrene sulfonic acid PSSALS was identified as the most effective of several derivatives studied. This compound was tested by an industrial collaborator in a commercial desiccant cooling system. An additional industrial partner has been placed on subcontract to prepare PSSA salts under carefully controlled conditions and to produce a new hydrophilic polymer for characterization.

Keywords: Polymers, Surface Phenomena, Desiccants

187. Open-Cycle Absorption Solar Cooling — FY 1989 — $125,000

DOE Contact: J. Goldsmith, (202) 586-8779, FTS 896-8779
Arizona State University Contact: B. Wood, (602) 965-7298

The objective of the material research aspect of this project is to identify a suitable mixture of absorbent-refrigerant pairs for use in a high performance open-cycle absorption system. The combination of an open flow collector/regenerator and low cost/high performance hygroscopic salts will be explored. Candidate materials include lithium bromide, lithium chloride, and calcium chloride solutions. Experiments to determine crystallization concentrations as a function of temperature will be performed. Equations for calculating the thermophysical properties of various solutions will be developed.

Keywords: Low Temperature Service, Absorbents

188. Solar Cooling Research Facility — FY 1989 — $425,000

DOE Contact: J. Goldsmith, (202) 586-8779, FTS 896-8779
Florida Solar Energy Center Contact: S. Chandra, (305) 783-0300

The purpose of this project is to establish a comprehensive experimental and analytical capability for the study and advancement of solar cooling technologies applicable to hot, humid climates. Research will be concentrated in four areas: (1) moisture research and analysis; (2) radiant barrier systems; (3) enthalpy exchange systems; and (4) integrated systems research. The recent increase in population in hot, humid regions of the United States has significantly increased the energy demand for air conditioning in these climates, resulting in the need for research on solar cooling and dehumidification technologies. Activities will include identifying the utility and application of desiccant materials and developing innovative materials and systems. In FY 1989, high quality moisture transport data for both common and innovative building materials were collected. The combined heat and mass transfer algorithms developed in FY88 were also extended to incorporate phase change and other innovative building materials.

Keywords: Low Temperature Service, Desiccants, Absorption

189. Core Daylighting System Design FY 1989
$40,000

DOE Contact: M. M. Jenior, (202) 586-2998, FTS 896-2998
LBL Contact: S. Selkowitz, (415) 486-5064, FTS 451-5064

The objectives of this research are to identify, develop, and characterize light guide materials and systems for collecting and transmitting sunlight and daylight within buildings to reduce electric lighting requirements. In large buildings, these systems should be sufficiently efficient to transmit usable quantities of light deep within buildings. In smaller buildings, they should provide improved comfort. The optical systems should be durable, have no complex-operating elements, and should introduce no unpleasant optical effects. In FY89, work continued on the design and development of a prototypical core daylighting system using a simplified tracker for light collection, a fiber optic link to couple the collector to the light guide system, and a light distribution system within the interior space. The design of a fresnel lens with a dispersion-compensating grating was completed, and a patent application filed. Discussions were held with Canadian researchers and funding agencies to conduct a joint demonstration and field test of core daylighting systems in the U.S. and in Canada.

Keywords: Coatings and Films, Low Temperature Service

190. Advanced Evacuated Tubular Concentrator Research FY 1989
$63,000

DOE Contact: J. Goldsmith, (202) 586-8779, FTS 896-8779
University of Chicago Contact: J. O'Gallagher, (312) 702-7757

The objective of this project is to develop a manufacturable version of an advanced evacuated compound parabolic concentrator (CPC) collector that has an annual efficiency of 50 percent at temperatures up to 350°F (175°C) and is economically competitive with flat plate collectors. CPC collectors will provide a general purpose solar thermal energy source with a variety of heating and cooling applications in diverse climates and locations. The concept being developed in this project employs moderate levels of nonimaging concentration applied to an appropriately configured selective absorber integrated into an evacuated tube. During FY89, an evaluation of design concepts on the leading edge of non-imaging concentrator technology was begun. This includes an assessment of current applications of CPC technology in Japan, Europe, and Israel.

Keywords: Coatings and Films, Low Temperature Service

191. Durability Testing Methods for Optical Switching FY 1989
$100,000

DOE Contact: M. M. Jenior, (202) 586-2998, FTS 896-2998
SERI Contact: A. W. Czanderna, (303) 231-1240

The objective of this project is to identify detailed performance criteria and methodologies for durability testing of electrochromic optical switching materials and multilayer devices. Electrochromic devices can control radiant energy buildup in enclosed spaces (e.g. buildings, and vehicles) by changing their optical characteristics in response to an electrical signal. The approach to developing the testing methodologies was to contact experts in the fields of electrochromic research and solar device testing. In FY89 a draft report was prepared which presented background about electrochromic window applications, identified general evaluation criteria, listed expected performance criteria, identified and discussed methods needed for laboratory testing of prototypes, ranked the recommended evaluation methods, and made recommendations for advancing the state of the art. The draft report was distributed to experts in both government and industry. Comments on the draft will be used to improve the final version of the report.

Keywords: Coatings and Films, Component Test

Solar Thermal Technology Division

The Goal of the Solar Thermal Technology Division is to increase the use of sunlight by the design and application of solar energy concentrating systems. The concentrated energy can be used for a wide variety of applications, including electricity generation, heat for industrial processes, hazardous waste detoxification, and materials treatment. The combination of broadband energy directed in an intense (to 65,000 suns) beam can cause unique and beneficial transformations of metals, alloys, ceramics, and fibers. A major new initiative is the use of concentrated solar energy for the transformation of hazardous chemical wastes to nontoxic by-products and useful chemical feedstocks.

Materials Preparation, Synthesis, Deposition, Growth or Forming

192. Silver/Polymer Reflector Research FY 1989
$1,000,000

DOE Contact: Martin Scheve, (202) 586-8110
SERI Contact: Paul Schissel, (303) 231-1226

Research and development of silver/polymer reflector films for solar thermal systems was conducted. For solar thermal applications, the silvered films must be resistant to ultraviolet degradation, cleanable, and have specular reflectances of 90 percent or more, with a 4 mrad cone angle. Useful film lives of 5 years or longer are needed.

Solar concentrators account for about 50 percent of the installed cost of a solar thermal electricity or process heat system. Silvered polymer films offer lower cost, reduced weight, and greater design flexibility than silver on glass.

Research focused on characterization, testing, and evaluation of a variety of ultraviolet stabilized silver/polymer films.

Keywords: Polymers, Coatings and Films, Surface Characterization and Treatment, Corrosion, Radiation Effects, Reflectors, UV Degradation

Materials Properties, Behavior, Characterization or Testing

193. Sol-Gel Protective Films for Metal Solar Mirrors — FY 1989 $150,000

DOE Contact: Martin Scheve, (202) 586-8110
SNL Contact: Tom Mancini, (505) 844-8643

Front surface metal mirrors (400 series stainless steel substrates) were coated with a variety of sol-gel derived glass films for preliminary evaluation as protective coatings for silver films deposited on the stainless steel substrates. Optical measurements (hemispherical, diffuse and specular reflectance) were made to characterize changes in the mirrors resulting from the application of the sol-gel, and from environmental testing. Abrasion resistance of the films was determined by ASTM procedures. Environmental effects were determined by exposure to ambient climate (Albuquerque, NM), and by accelerated testing in acid. Two layer coating schemes were also evaluated.

The planarizing ability of sol-gel overcoats on several 400 series stainless steel substrates was investigated. Smoothing (planarizing) effects were imparted to stainless steel substrates with an initial sol-get overcoat; reflective silver films were deposited over this, and a protective sol-gel overcoat was applied to protect the silver. It was found that the specular reflectance of stainless steels could be increased from initial values of 0.36-0.90 to final values up to 0.93 by the application of planarizing sol-gel films.

Keywords: Sol-Gel, Surface Preparation and Treatment, Corrosion Resistance, Solar Concentrators

194. High Flux Effects on Materials — FY 1989 $250,000

DOE Contact: Frank Wilkins, (202) 586-1684
GTRI Contact: Joel Shutt, (404) 894-3589

Research on the beneficial effects of high solar flux on carbon fibers is being conducted. Particular investigations included the enhancement of mechanical and chemical properties of carbon fibers and carbon-carbon composites upon exposure to high intensity solar flux.

The effects of the high intensity solar flux on carbon based materials were compared with the effects produced by application of heat only. It was found that increased oxidation resistance was imparted to carbon fibers and composites by the application of intense solar flux, compared with fiber treatment at the same temperature in the absence of light flux. The technique offers the potential for substantial savings in the treatment of carbon fibers for advanced carbon-based composite applications.

Keywords: Carbon Fibers, Surface Modification, Mechanical Property Enhancement

195. Surface Transformation of Metals — FY 1989 — $600,000

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

Changes in mechanical and physical properties of alloy and transition metals when exposed to high solar flux were examined. It was found that microstructural changes could be induced in the metal surfaces by the application of intense solar flux, and mechanical properties such as hardness and wear resistance could be improved.

Surface alloying of ceramic powders on metal substrates with intense solar flux was examined. Alloy phases similar to those obtained by laser surface alloys were obtained with intense solar flux. The processing rate for metal surfaces can be much larger with the solar beam than with lasers, because the solar beam diameter is much larger.

Keywords: Surface Alloys, Surface Modification, Surface Phases

196. Materials for Applications in Regenerative Thermal Electrochemical Conversion (RTEC) Technology — FY 1989 — $100,000

DOE Contact: Frank Wilkins, (202) 586-1684
SERI Contact: Meir Carasso, (303) 231-1353

Graphite-based materials for applications in RTEC technology were identified, and prototype RTEC systems were designed and built in conjunction with Hughes Aircraft Corporation. RTEC uses intense solar flux in the regeneration cycle of ammonium/ammonium phosphate electrochemical cells.

Hughes tested a 15 W prototype RTEC systems designed by SERI. The DOE Office of Conservation will provide support for the development of RTEC systems for transportation applications in FY 1991.

Keywords: Electrochemical Systems Materials, Photoelectrochemical Systems

197. Catalysts for Solar-Assisted Water Detoxification FY 1989
$1,000,000

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

Transition metal oxide catalysts (such as titanium dioxide) use the high-energy (ultra-violet) portion of the solar spectrum in aqueous solutions to reduce toxic organic compounds to harmless chemicals. The goal of the research is to characterize the catalysts, and to augment them to use the near ultra-violet portion of the solar spectrum. The catalysts will be part of solar-assisted water decontamination systems.

Keywords: Titanium Dioxide, Water Treatment, Water Purification

OFFICE OF SOLAR ELECTRIC TECHNOLOGIES

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

198. Amorphous Silicon for Solar Cells — FY 1989 $10,500,000

DOE Contact: Morton B. Prince, (202) 586-1725
SERI Contact: Byron Stafford, (303) 231-7126

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

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

199. Polycrystalline Thin Film Materials for Solar Cells — FY 1989 $3,500,000

DOE Contact: Morton B. Prince, (202) 586-1725
SERI Contact: Kenneth Zweibel, (303) 231-7141

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

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

200. Deposition of III-V Semiconductors for High-Efficiency Solar Cells — FY 1989 $2,000,000

DOE Contact: Morton B. Prince, (202) 586-1725
SERI Contact: John Benner, (303) 231-1396
SNLA Contact: David Hasti, (505) 844-8161

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

Keywords: Semiconductors, Chemical Vapor Deposition, Solar Cells (Liquid Phase Epitaxial Growth, Molecular Beam Epitaxial Growth)

Materials Properties, Behavior, Characterization or Testing

201. Materials and Device Characterization

FY 1989
$2,900,000

DOE Contact: Morton B. Prince, (202) 586-1725
SERI 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

202. High-Efficiency Crystal Silicon Solar Cells

FY 1989
$2,000,000

DOE Contact: Morton B. Prince, (202) 586-1725
SERI Contact: John Benner, (303) 231-1396
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. This project also performs applied research upon the growth of silicon ribbons from a melt. Research centers upon understanding, from a physical perspective, exactly what happens during the growth of silicon ribbon. Questions to be answered include: what stresses do the sharp temperature gradients, inherent in high speed crystal growth impose upon the ribbon; which stress relief modes improve solar cell performance and how can they be enhanced; how can buckling be prevented; and what is an acceptable level of residual strain.

Keywords: Semiconductors, Solar Cells

OFFICE OF RENEWABLE ENERGY TECHNOLOGIES

Geothermal Technology Division (GTD)

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, GTD-sponsored materials R&D.

Materials Preparation, Synthesis, Deposition, Growth or Forming

203. Materials for Non-Metallic Heat Exchangers — FY 1989 $125,000

DOE Contact: R. LaSala, (202) 896-4198
BNL Contact: L. E. Kukacka, (516) 282-3065

This project is investigating thermally conductive polymer-based composites for use as corrosion resistant materials of construction for shell and tube heat exchangers in binary geothermal processes or for liners on carbon steel substrates. Corrosion of the brine side of tubing in shell and tube heat exchangers has been a major problem in the operation of binary 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 properties can be derived. The work consists of determinations of the effects of compositional and processing variables on the thermal properties of the composite, and measurements of the physical and mechanical properties after exposure to hot brine and isobutane/isopentane mixtures. If the goals of the program are attained, the cost of geothermal power will be reduced considerably.

Keywords: Composites, Polymers, Corrosion, Strength, Extrusion

204. Biochemical Concentration and Removal of Toxic Components from Geothermal Wastes — FY 1989 $216,000

DOE Contact: G. J. Hooper, (202) 896-1146
BNL Contact: E. T. Premuzic, (516) 282-2893

This program involves the development of biochemical processes which can be used for the concentration and subsequent removal of toxic components from geothermal waste streams. Before the large-scale development of geothermal energy can occur, environmentally and economically acceptable methods for the disposal of large quantities of potentially toxic wastes must be developed. The wastes can also provide a valuable source of strategically important metals. The work involves the identification of biosystems which efficiently select and accumulate the toxic materials of interest. This involves extra- and intra-cellular fractionation and management of natural sources, i.e., isolation, culturing, and identification of micro-organisms as well as the chemical isolation and characterization of active entities.

Keywords: Toxic Metal Removal, Absorption, Surface, Dissolution, Solidification, Industrial Waste Recovery

Materials Properties, Behavior, Characterization or Testing

205. Advanced High Temperature Geothermal Well Cements — FY 1989 $105,000

DOE Contact: R. LaSala, (202) 896-4198
BNL Contact: L. E. Kukacka, (516) 282-3065

Lightweight (<1.2 g/cc) chemically and thermal resistant well cements are needed to reduce the potential for lost circulation problems during well completion operations. Materials designed for temperatures >500°C will be needed as higher temperature resources are developed. Cements resistant to brines containing high concentrations of CO_2 at temperatures >150°C are also needed. Emphasis is being placed on high temperature rheology, phase chemistry, and the mechanical, physical, and chemical resistance properties of the cured materials.

Keywords: Cements, Material Degradation, Strength, Transformation, Bulk Characterization, Drilling

206. Corrosion in Binary Geothermal Systems — FY 1989 $3,000

DOE Contact: R. LaSala, (202) 896-4198
BNL Contact: D. van Rooyen, (516) 282-4050

This program yields corrosion data from plant tests for metals presently used in binary plants and other more potentially resistive metals and nonmetals. In operating binary processes, brine leakage into the organic working fluid side of the plants has resulted in unanticipated corrosion problems. Data are not available on the effects of salt, oxygen, and water impurities in isobutane and/or isopentane on the corrosion rates of metals. The work involves the exposure of test coupons in an operating plant. When completed, the program will yield quantitative information regarding the extent of corrosion that will occur upon contamination of the binary side of a plant, thereby allowing designers materials options.

Keywords: Alloys, Metals, Corrosion

207. Advanced High Temperature Chemical Systems for Lost Circulation Control

FY 1989
$105,000

DOE Contact: R. LaSala, (202) 896-4198
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 an advanced high temperature chemical system which when added to bentonite-based drilling fluids will produce a slurry which is 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.

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

Biofuels and Municipal Waste Technology (BMWT) Division

The goal of the BMWT program is to conduct research that will provide the technology necessary to increase the supply of domestically available feedstocks and convert those feedstocks plus wastes to liquid and gaseous fuels. Production research concentrates on feedstocks tailored for high production rates and suitability for conversion to liquid and gaseous fuels. The program includes the research necessary to recover the feedstocks and prepare them for conversion processes. Conversion technology research will reduce the wide range of organic materials to valuable energy commodities in the form of liquid and gaseous fuels including hydrogen. The thermal processes are particularly suited to producing liquid and gaseous fuels, which are mixtures of components that may require additional upgrading, while the biochemical processes that directly produce fuel, such as ethanol energy conversion processes, are adapted especially for the intended feedstock.

Materials Preparation, Synthesis, Deposition, Growth or Forming

208. Medium Temperature Solid Electrolytes: Proton Conductors FY 1989 $200,000

DOE Contact: M. Gurevich, (202) 586-6104
BNL Contact: J. Wegrzyn, (516) 282-7917
Stanford Contact: R. Huggins, (415) 723-4110

Fundamental investigations are being pursued: the synthesis and characterization of modified high temperature polymers that may serve as proton conductors and, into a non-aqueous, molten salt hydride-ion conducting electrolyte. This work is ongoing at BNL and Stanford University. BNL aims at the introduction of ionomeric substituents in various polymers found to be stable in a steam environment. Efforts at Stanford University focus on the characterization of the novel electrolyte's conductivity and stability and the identification of H_2-permeable electrodes which can serve as electrodes for "sandwich" electrochemical structures which can be used in steam electrolysis.

Keywords: Polymers, Electrolytes

209. Hydrogen Production with Photoactive Semiconductor Catalysts FY 1989 $125,000

DOE Contact: M. Gurevich, (202) 586-6104
Battelle Columbus Laboratories Contact: R. Schwerzel, (614) 424-5637

Efforts have continued in developing plasma polymerization processes for applying optically-transparent, conductive coatings on various types of semiconductor materials. Some success achieved by co-sputtering gold-teflon-polyethylene on single crystal semiconductors has not been reproducible due to non-uniformity and/or poor adhesion of the coatings. Recent experiments using polytetramethyl silanes (Poly TMS) as coatings followed by electrochemical deposition of platinum offer strong prospects for success. The platinum preferentially deposits on flawed coating areas resulting in conductive, catalytic "islands" which promise good semiconductor performance and high stability. Efforts have focused on process reproducibility and more intensive analytical efforts to physically characterize the coatings.

Successful demonstration of single-crystal semiconductor photoactive stability will permit examination of the techniques applicability to semiconductor powders use in photochemical H_2 production experiments.

Keywords: Semiconductors, Plasma Polymerization, Coatings

Materials Properties, Behavior, Characterization or Testing

210. Cold Storage of Hydrogen on Activated Carbon — FY 1989 $100,000

DOE Contact: M. Gurevich, (202) 586-6104
Syracuse University: J. Schwartz, (315) 423-2807

Studies have shown that surface-modified super-activated carbons treated to achieve high surface acidity can store up to 4 percent by weight hydrogen at 150°K and 600 psi. Efforts have focused on characterization of storage capacity and kinetics as a function of activated carbon compression, impurities, recycling. These data have been used to establish system design/performance specifications and requirements for H_2 storage system prototype fabrication.

Current efforts are directed toward the design and fabrication of a Process Development Unit capable of storing up to 1 lb. of H_2. Future efforts will optimize the adsorption process in terms of capacity, cycle times and applications.

Keywords: Hydrogen Storage, Catalysts

211. Hydrogen Production via Photoelectrolysis — FY 1989 $118,000

DOE Contact: M. Gurevich, (202) 586-6104
SERI Contact: A. Nozik, (303) 231-1953

The project focuses on the development of multiphoton photoelectrolysis devices that provide high internal photovoltages to permit the splitting of water into hydrogen and oxygen or hydrogen peroxide without the need for an external voltage supply.

One particular configuration that will be initially investigated will consist of successive layers of crystalline GaAs and $Al_xGa_{1-x}As$ semiconductors epitaxially deposited by metallorganic chemical vapor deposition (MOCVD). Each layer will be interconnected by tunnel junctions or ohmic contacts such that upon illumination photogenerated majority charge carriers combine at the interconnection, while minority charge carriers are injected into the aqueous solution at enhanced redox potentials that are sufficient to effect the decomposition of water into H_2 and O_2. In this system the incident light passes successively through each semiconductor layer, which are arranged in order of decreasing band gaps, to optimize the efficiency of light absorption and radiant power conversion into H_2. This multijunction array will comprise one illuminated electrode of a photoelectrochemical cell; the second electrode will be metal. Anticipated problems with the illuminated electrode with respect to photocorrosion will be ameliorated through applications of thin protective layers and/or metallic islands deposited on the outer layer which contacts liquid water. The objective of these experiments will be to demonstrate the principle of voltage and conversion efficiency enhancement in a photoelectrolysis cell with a multiphoton-type electrode using well-defined semiconductor components.

Another configuration that will be studied and optimized will be a doubly-illuminated photoelectrolysis cell in which both photoanode and photocathode consist of n-type and p-type III-V semiconductors, respectively, and grown by MOCVD. Simultaneous, as well as successive illumination of the two electrodes will be investigated. The theoretical performance of these various multiphoton configurations will be calculated and compared to experimental results.

Keywords: Catalysis, Photoelectrolysis, Coatings and Films, Semiconductors

212. Novel Methods for Solar Hydrogen Production FY 1989 $350,000

DOE Contact: M. Gurevich, (202) 586-6104
SERI Contact: W. Hoagland, (303) 231-7383
Center for Electrochemical Systems and Hydrogen Research, Texas A&M University
Contact: John Appleby, (409) 845-8281

Research is being conducted in several areas of renewable hydrogen production. The purpose is (1) to develop practical photocell units that are capable of splitting water into hydrogen and oxygen with provision for separation of the two gases and storage of hydrogen, and to incorporate these cells into a membrane, (2) to investigate systems that incorporate active organic layers that contain photosensitive dyes for application in photoelectrochemical cells, and (3) to develop a theory for oxygen evolution electrocatalysis, to determine the relation to the efficiency of photoelectrochemical splitting of water. Efforts are directed toward the photoelectrochemical water splitting and the development of high efficiency, water splitting systems. Specific materials to be studied for catalyzation of photoelectrode surfaces are Pt, In, Ru and MnO_2. For the photoelectrode materials, amorphous silicon on n-GaAs is being considered.

Keywords: Catalysis, Coatings and Films, Semiconductors

OFFICE OF ENERGY RESEARCH

The Director of Energy Research is responsible for three major outlay programs: Basic Energy Sciences, High Energy and Nuclear Physics, and Magnetic Fusion Energy. The Director of Energy Research also advises the Secretary on DOE physical research programs, the Department's overall energy research and development activities, grants, and other forms of financial assistance. The Director also carries out additional duties assigned to the office related to basic and advanced research, and monitors the well-being and management of the multiprogram laboratories under the jurisdiction of the Department.

Four multiprogram and seven single-purpose laboratories are administratively assigned to the Office of Energy Research. The multiprogram facilities are Argonne National Laboratory, Oak Ridge National Laboratory, Brookhaven National Laboratory, and Lawrence Berkeley Laboratory. The single-purpose or specialized laboratories are the Bates Linear Accelerator Facility at the Massachusetts Institute of Technology, the Ames Laboratory at the Iowa State University, the Fermi National Accelerator Laboratory, the Notre Dame Radiation Laboratory, the Princeton University Plasma Physics Laboratory, the Michigan State University Plant Research Laboratory, and the Stanford Linear Accelerator Center. The multiprogram laboratories conduct significant research activities for other DOE programs (Conservation, Nuclear, etc.) and other Federal agencies, while the seven specialized laboratories are funded almost totally by the Office of Energy Research.

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
- Office of Health and Environmental Research: Division of Physical and Technologies Research
- Office of Fusion Energy
- Small Business Innovation Research Program

Office of Basic Energy Sciences

Division of Materials Sciences

This basic research program has several roles. One is to increase the understanding of materials properties, behavior, and phenomena in those classes of materials that either presently or in the future might be important to the mission of the Department of Energy. Another concerns the development of new forefront analytical instruments and facilities that are used to probe the structure and behavior of matter. Thus this program carries a major responsibility for many of the nation's premier research facilities including several neutron sources, a synchrotron radiation source, processing facilities, and frontier electron microscopes. Some of the materials research has a specific relationship to an identified energy technology (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, high temperature structural metals and ceramics); and some is important to fundamental understanding of new experimental and theoretical research tools.

This research is conducted at DOE laboratories, universities, and to a lesser extent at industrial laboratories by metallurgists, ceramists, solid state physicists, and materials chemists in about 100 different institutions.

There are three subprograms:

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

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

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

The operating funds for FY 1989 for the Division of Materials Sciences were $180,746,000. This was allocated to 434 projects. Many projects cross the traditional categories and, for example, involve property-structure relationships. Nevertheless, the approximate funding distribution for FY 1989 was:

	$ (Millions)
Materials Preparation, Synthesis, Deposition, Growth or Forming	20.2
Materials Structure and Composition	26.5
Materials Properties, Behavior, Characterization or Testing	78.0
Device or Component Fabrication, Behavior or Testing	--
Facilities	56.0

The DOE contact for this Division is Iran Thomas, (301) 353-3427. For specific detailed information, the reader is referred to DOE publication Materials Sciences Programs Fiscal Year 1989 (DOE/ER-0447P dated March 1990). This publication contains: summaries of all funded programs at DOE laboratories; summaries of all funded grant programs in universities and private sector organizations; summaries of all Small Business Innovation Research programs; major user facilities (descriptive information); other user facilities; cross-cutting indices: investigators, materials, techniques, phenomena, environment. Limited copies may be obtained by calling (301) 353-3427.

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) 353-5822.

The BES Geosciences Research Program supports research that is fundamental in nature and of long-term relevance to one or more energy technologies, national security, energy conservation, or the safety objectives of the Department of Energy. It is also concerned with the extraction and utilization of such resources in an environmentally acceptable way. The purpose of this program is to develop geoscience or geosciences-related information relevant to one or more of these Department of Energy objectives or to develop the broad, basic understanding of geoscientific 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 George A. Kolstad, (301) 353-5822.

Materials Properties, Behavior, Characterization or Testing

213. Bounds on Dynamic Plastic Deformation FY 1989
$129,000

DOE Contact: Oscar P. Manley, (301) 353-5822
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

214. Diffusion, Fluid Flow, and Sound Propagation in Disordered Media FY 1989
$70,380

DOE Contact: Oscar P. Manley, (301) 353-5822
Boston University Contact: Thomas Keyes, (617) 353-4730

The basic transport processes, of which those mentioned in the title are important examples, become extremely complicated in the presence of large amounts of disorder. For example, the effect of a low density of fixed scatterers upon diffusion is easy to calculate; at high density, diffusion may cease altogether and the problem becomes difficult. Lattice vibrations on an ordered lattice are described by perfect sound waves, but disorder—perhaps some broken bonds—can cause the vibrations to be "localized" with no ordinary long-wavelength sound at all (localization is thought to occur with an infinitesimal amount of disorder in two dimensions). Of course, large disorder is the rule in nature, as in the interior of a porous rock.

The aim of this project is to apply modern methods of nonequilibrium statistical mechanics to transport with large disorder. Those methods are the "Repeated Ring" kinetic equation, an extension of Boltzmann's equation to complicated systems, the Renormalization Group, and computer simulation. Transport coefficients and correlation functions are being calculated.

Keywords: Disordered Media, Statistical Mechanics

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

FY 1989
$183,000

DOE Contact: Oscar P. Manley, (301) 353-5822
Idaho National Engineering Laboratory Contact: J. R. Fincke, (208) 526-2031

Knowledge of in-flight particle temperature is fundamental to understanding particle/plasma interactions in the physical and/or chemical processing of fine powders. The measurement of in-flight particle temperature is based on a two wavelength pyrometry technique. In addition, simultaneous particle size is obtained by a light scattering technique. The requirement of coincidence between sizing and pyrometry signals insures that only particles for which temperature data are available will be sized. The technique has been demonstrated on laboratory scale plasma torches. The influence of particle size, injection rate, torch power, etc., are currently being examined in detail. In addition methods of simultaneously obtaining particle size, velocity and temperature are under development.

This project is one of six projects comprising a collaborative research program with the Massachusetts Institute of Technology.

Keywords: Plasma Processing, Particle/Plasma Interaction

216. Experimental Measurement of the Plasma/Particle Interaction FY 1989 $530,000

DOE Contact: Oscar P. Manley, (301) 353-5822
Idaho National Engineering Laboratory Contacts: C. B. Shaw, (208) 526-8818, S. C. Snyder, (208) 526-1507 and L. D. Reynolds, (208) 526-8335

The objective of this research is to quantitatively describe the heat mass, and momentum transfer associated with metallic or oxide particles immersed in thermal plasma environments. In order to characterize the interaction between plasma constituents and particles, new methods to determine plasma flow velocity and species compositions are being developed. Holographic interferometry is currently being considered for plasma flow velocity determination and planar laser induced fluorescence is being considered for compositional measurements adjacent to particle surfaces. Using these advanced techniques, temporal and spatially resolved distributions of the chemical and physical properties of the plasma/particle environment will be determined. Since this research is performed in collaboration with research at Massachusetts Institute of Technology, the resulting experimental data will be used to validate and correct theoretical models used for thermal plasma processing and for predictions relating to optimal torch and fixture design criteria. Experiments are currently being performed in two plasma torch designs, a constricted nozzle torch and an expanding nozzle torch. Input power dissipation levels ranging from 5 to 180 kW are being studied. These torch designs produce a representative plasma characteristic of those employed for industrial plasma processing.

Keywords: Particle/Plasma Interaction, Plasma Processing

217. Integrated Sensor/Model Development for Automated Welding FY 1989 $465,000

DOE Contact: Oscar P. Manley, (301) 353-5822
Idaho National Engineering Laboratory Contacts: H. B. Smartt, (208) 526-8333 and J. A. Johnson, (208) 526-9021

The objectives of this research are: (1) to develop models of the physical phenomena occurring in the gas metal arc welding process suitable for real-time process control, (2) to develop sensors and signal processing algorithms for arc welding processes including optical and ultrasonic techniques, and (3) to integrate the above models and sensing with advanced control methodologies. This project is part of a collaborative research program with the Massachusetts Institute of Technology.

A fundamental model of the gas metal arc welding process has been developed which considers wire melting and heat and mass transfer to the base metal. This model is being extended to account for droplet detachment modes and the dynamic aspects of heat and mass transfer through the arc.

Sensing of the weld pool solid/liquid interface location is being developed using noncontract transducers. Signal generation is by use of laser pulses directed on the weld pool. Signal analysis/pattern recognition techniques are being developed based on AI methods for automated measurements.

Independent control of heat and mass input to the weld has been demonstrated. Sensing algorithms to characterize droplet transfer mode by acoustic and electrical signals have been developed. Control of weld bead cooling rate during gas metal arc welding has been demonstrated where the cooling rate has been varied independently of the weld reinforcement. This has allowed near steady-state cooling rates to be achieved during weld start-up, an important factor in reducing weld defects.

Keywords: Welding, Ultrasonic Sensing, Optical Sensing

218. <u>Nondestructive Characterization of Fracture Dynamics and Crack Growth</u> <u>FY 1989</u>
$189,000

DOE Contact: Oscar P. Manley, (301) 353-5822
Idaho National Engineering Laboratory Contact: J. A. Johnson, (208) 526-9021

The purpose of this research is to develop instrumentation and models to measure and predict the emission and interaction of ultrasound from growing cracks in engineering materials, and to investigate methods of sensing the properties of growing cracks. A high speed digital acoustic emission (AE) data acquisition system is being developed and applied to fracture mechanics experiments that are part of the Elastic-Plastic Fracture Analysis program at INEL and the Modeling and Analysis of Surface Cracks program at the Massachusetts Institute of Technology. In addition, numerical methods are being used to model the interaction of acoustic emission stress waves with real crack geometries.

The AE detection system is being developed and is capable of detecting and digitizing AE signals with a larger bandwidth and with less dead time than in conventional systems. This will allow improved resolution in detecting the locations of the sources of emissions and in discriminating between types of sources. Automatic analysis methods are being developed for source location and source identification for each of the large number of acoustic emission events received in a typical fracture mechanics experiment. Other work includes transducer design, transducer calibration, generalized ray theory analysis (Green's functions), source location algorithms, and inverse source identification algorithms.

Models of the ultrasonic field/crack interaction are based on a numerical ray-tracing algorithm and on a numerical (finite difference) solution to the partial differential equations (PDE) describing the system. In the finite element model, a source of acoustic emission is modeled by changing boundary conditions and the ultrasonic fields that propagate from the source to a receiver are calculated. All mode conversions are automatically included in the numerical solution to the PDE with the boundary conditions of the system. These boundary conditions include the geometry of the macrocrack near the source of acoustic emission and thus calculate receiver signals which include effects that cannot be calculated using generalized ray theory.

Keywords: Nondestructive Evaluation, Fracture

219. High-Temperature Gas-Particle Reactions FY 1989
$130,000

DOE Contact: Oscar P. Manley, (301) 353-5822
MIT Contacts: J. F. Eliott, (617) 253-3305 and P. P. Bolsaitis, (617) 253-5069

The purpose of the research program is to examine the physicochemical behavior of individual inorganic particles in conditions simulating those to which particles are exposed during thermal plasma processing methods. The particle is suspended in a closed chamber by an electrostatic field, and it is heated by a pulsed laser beam. The composition of the gas in the reactor can be controlled, and the temperature of the particle can be measured with a time resolution as short as one or two milliseconds. Equipment is being installed for optical imaging of the particle during processing.

Study is in progress of melting and solidification of metal and oxide particles at high rates of heating and cooling. Measurements have been made of the evaporation of oxide particles while they are heated and cooled. Investigation of the ignition and combustion of metal particles is in progress also. Means have been developed for capturing individual particles and examining them by optical and electron microscopic methods.

This work is closely connected with the experimental program on plasma processing at the Idaho National Engineering Laboratory, and other plasma processing studies in the Department of Materials Science and Engineering at MIT.

Keywords: Plasma/Particle Interaction

220. Mathematical Modeling of Transport Phenomena in Plasma Systems FY 1989
$98,000

DOE Contact: Oscar P. Manley, (301) 353-5822
MIT Contact: J. Szekely, (617) 253-3305

The purpose of this investigation is to develop a comprehensive mathematical representation of the velocity field and of the temperature field in thermal plasma systems and to compare the theoretical predictions with experimental measurements.

The problem has been formulated through the statement of the axi-symmetric Navier-Stokes equations and the associated differential thermal energy and mass conservation relationships. The theoretical predictions for the gas temperature profiles were found to be in excellent agreement with the experimental measurements obtained by Dr. C. Shaw and Dr. J. Batdorf of the Idaho National Engineering Laboratory. The work is continuing with the objective of modeling gas mixing and representing the interaction between the plasma gas and solid particles.

Keywords: Plasma Systems, Transport Properties

221. Multivariable Control of the Gas-Metal Arc Welding Process — FY 1989 $161,000

DOE Contact: Oscar P. Manley, (301) 353-5822
MIT Contact: David E. Hardt, (617) 253-2429

The process of Gas-Metal Arc Welding (GMAW) involves many process control variables such as arc voltage, current, travel speed, wire feed rate, and voltage pulsing profile. These multiple inputs to the weld cause changes in multiple outputs such as weld width, depth, reinforcement height and thermal effects in the weldment. All existing work in closed-loop control of welding, however, has treated this highly coupled, multiple input-multiple output system as a single variable control problem, concentrating, for example, on controlling just the weld width or depth.

The objective of this work is to case the GMAW control problem in its most general sense and then examine the use of advanced multivariable control methods. We have so far progressed on two independent fronts: measurement and control of geometric properties of the weld and measurement and control of weldment properties via thermal history control.

For the latter we have analyzed the process to develop a 3 input-3 output process model. As for geometry control, we have concentrated on both bead contour measurement methods and on control models for the process.

Keywords: Welding, Control

222. Metal Transfer in Gas-Metal Arc Welding — FY 1989 $131,000

DOE Contact: Oscar P. Manley, (301) 353-5822
MIT Contact: T. W. Eagar, (617) 253-3229

The present research is part of a cooperative program among faculty at MIT and staff at Idaho National Engineering Laboratory to develop sensing and control methods which can be used to automate the gas-metal arc welding processes.

Current research emphasizes understanding of the forces controlling droplet detachment in gas-metal arc welding. Experimentally, a laser back lit viewing system has been developed which permits viewing of anode and cathode jet phenomena. Welds have been made with a variety of different metals (steel, aluminum and titanium) in different shielding gases (argon, helium, carbon dioxide). It is seen that the anode spot behavior changes dramatically with changes in both metal and gas composition.

This experimental information is being coupled with a model of the forces controlling metal transfer. These include gravitation, surface tension, aerodynamic drag, electromagnetic (Lorentz) force and plasma jet momentum. Initial studies show that globular transfer can be described quantitatively by previous theories which were presented originally in only a qualitative manner. Quantification of previous explanations of spray transfer depart markedly from the experimental observations. A new model of the globular to spray transition has been hypothesized and is currently being studied with a finite element model.

Keywords: Welding, Control

223. Modeling and Analysis of Surface Cracks — FY 1989 $199,000

DOE Contact: Oscar P. Manley, (301) 353-5822
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 determining parametric limits of applicability of the "dominant singularity" formalism at nonlinear fracture mechanics in these crack configurations as they are influenced (principally) by material strain hardening, load biaxiality, and crack geometry. When such single-parameter dominance is obtained, correlations of crack response with J-integral or related measures may be justified. The analysis requires detailed finite element computations which are too costly for routine applications, so further development of simplified analytical models such as the so-called "line-spring" model is underway. To date, detailed non-linear three-dimensional finite element studies of surface cracks under predominant tension show that the asymptotic HRR stress fields of power law hardening materials typically dominate for normal stress levels up to 75 percent of yield strength, with a rapid loss of dominance at higher load levels. Calculated crack front deformations are in good agreement with experimental measurements made at the Idaho National Engineering Laboratory. The line-spring has been generalized to include elastic/power law behavior, and resulting solutions are within a few percent of corresponding continuum solutions requiring more than an order of magnitude more computations.

Finally, detailed three-dimensional studies of through-cracks in "thin" sheets has accurately quantified the stress intensity variation through the thickness, as well as the boundary layer structure near the intersection of the crack front with the free surface.

Keywords: Fracture

224. Thermal Plasma Processing of Materials — FY 1989 $361,000

DOE Contact: Oscar P. Manley, (301) 353-5822
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The objective of this research project is a combined experimental and analytical study for thermal plasma processing of materials including the production of fine ceramic powders.

A new Triple Torch Plasma Reactor (TTPR) has been used for the synthesis of fine AlN powders. By controlling the aluminum nitrogen ratio a complete conversion can be achieved and with proper control of the quenching rate, single phase hexagonal AlN can be obtained. A computer simulation of this reaction has been performed in parallel with the experimental work.

Since the TTPR allows injection of powder into the hot core of converging plasma jets, plasma spraying of ceramic materials has been explored.

Zirconium hydroxide doped with yttrium hydroxide equivalent to 9 mole % yittria produced by a sol-gel reaction has been used for making coatings of zirconia on mild steel substrates.

An anode assembly for transferred arc operation has been designed and manufactured in order to study this mode of operation in the TTPR. A micron size powder feeding system is under investigation to improve particular feeding and resolve the problem encountered during the AlN synthesis.

Keywords: Plasma Processing, Plasma Diagnostics

225. Transport Properties of Disordered Porous Media from the Microstructure — FY 1989 $97,000

DOE Contact: Oscar P. Manley, (301) 353-5822
North Carolina State University Contact: S. Torquato, (919) 737-2365

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

The program has been broken down into four basic tasks: (1) the development of theoretical expressions for the bulk properties which depend upon the microstructure through various sets of statistical correlation functions, (2) the evaluation of these and other correlation functions that have arisen in the literature for nontrivial models of porous media, using results and methods of statistical mechanics, (3) the calculation of transport-property expressions which involve this statistical formulation, and (4) the comparison of theoretical results to experimental measurements of the conductivity and permeability of porous media. We are in the process of computing microstructure-sensitive property relations for models of porous media with heretofore unattained accuracy.

Keywords: Disordered Media

226. Inelastic Deformation and Damage at High Temperature — FY 1989 $129,400

DOE Contact: Oscar P. Manley, (301) 353-5822
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A combined theoretical and experimental investigation is performed to study the biaxial deformation and failure behavior of AISI Type 304 Stainless Steel 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 ratcheting 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.

The previously-developed viscoplasticity theory based on overstress (VBO) which uses neither a yield surface nor loading and unloading conditions will be augmented to include the effects of recovery and aging. This constitutive equation will be combined with an incremental damage accumulation law. It exists in uniaxial form and will be reviewed and extended to multiaxial, isotropic conditions. The theory will be checked against companion experiments.

For the experiments, an MTS servohydraulic axial/torsion test system is available together with an MTS Data/Control Processor. Induction heating (10 KHz frequency), MTS biaxial grips and an MTS biaxial extensometer will be used for the first time in this study of biaxial deformation and failure behavior. The biaxial test facility was checked out and is ready for testing.

Uniaxial and torsional ratcheting experiments showed considerable strain accumulation at room temperature and they demonstrate that ratcheting is due to viscous effects. Surprisingly, insignificant ratcheting and rate sensitivity were observed at 550, 600 and 650°C for uniaxial tests. This unexpected finding was attributed to strain aging in the stainless steel. Strain aging was further investigated by relaxation and strain-rate-jump tests at high temperature. A finite deformation theory of viscoplasticity based on overstress is being developed and is being implemented into a finite element computer program.

Keywords: Fracture, Damage

227. Energy Changes in Transforming Solids — FY 1989 — $170,000

DOE Contact: Oscar P. Manley, (301) 353-5822
Stanford University Contacts: George Herrmann, David M. Barnett, (415) 723-4143

A variety of processes occurring in stressed deformable solids, such as void formation, void growth, motion of dislocations and point defects, grain boundary sliding, etc., are accompanied by energy changes. It is these energy changes which give rise to the concept of generalized configurational (or material) forces and provide a most promising way to characterize state changes and the processes in question.

An anisotropic elastic boundary integral method has been developed and used to predict the existence of stable void lattices in irradiated FCC and BCC metals; numerical results are in close agreement with experimental observations quoted in the literature. An apparent paradox in the dislocation literature has been resolved. A new investigation of energy changes and forces associated with dislocations in anisotropic layered media is being undertaken, and the theory of interfacial waves in anisotropic elastic media is being extended to include piezoelectricity.

An integral equation method has been developed to study problems of interaction between holes and defects in elastostatics, including the calculation of energy release rates. An elementary theory of defective beams in bending and of bars in tension, compression, and torsion has been developed. Based on an extended circle theorem originally established in potential flow theory, the temperature distribution in an infinite region containing a circular cavity (defect) was determined in terms of the distribution existing in the same region without the cavity. The stress distribution induced by the presence of the defect was shown to be universal, i.e., it depends essentially only on the magnitude of the heat flux vector existing at the center of the defect before it was created.

Keywords: Stress Analysis, Materials Science

228. Nondestructive Testing FY 1989
$ 0

DOE Contact: Oscar P. Manley, (301) 353-5822
Stanford University: G. S. Kino, (415) 497-0205

The aim of this project is to arrive at techniques for contactless nondestructive testing and range sensing. Devices which can be rapidly scanned over a surface so as to detect flaws and measure their profiles are badly needed. The measurement of parameters such as surface roughness are also required. For this purpose, we are developing acoustic sensors operating in air and contactless photoacoustic techniques.

We have developed a new type of PZT ceramic acoustic transducer with a quarter wavelength matching layer of RTV rubber which operates in air in the frequency range of 18 MHz. The transducer itself has been used for range sensing and for photoacoustic measurements. As an example, it has enabled us to measure regions of high surface recombination rates on semiconductors by varying the number of injected carriers in a semiconductor, using a laser beam modulated at 2 MHz. We detect the rf term in the surface temperature due to recombination. Similar techniques have been used by us to measure film thicknesses and profiles.

We are now developing a new acoustic transducer operating in air which utilized a 1000 A thick pellicle of boron nitride as the detector of acoustic waves in the air. The deflection of the surface is measured by highly sensitive optical phase measurement of an optical beam reflected from the pellicle. The system is as sensitive as our previous acoustic transducer, but has the advantage that it can be operated over a bandwidth from a few Hz to several MHz.

Keywords: Nondestructive Evaluation, Acoustic Sensors

229. Effective Elastic Properties of Cracked Solids FY 1989
$57,000

DOE Contact: Oscar P. Manley, (301) 353-5822
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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 ansiotropic. 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

230. Laser Diagnostics of Plasma Assisted Chemical Vapor Deposition (PACVD) Processes FY 1989 $185,024

DOE Contact: Oscar P. Manley, (301) 353-5822
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The objectives of this research are to perform a comprehensive experimental investigation of the fundamental nonequilibrium reactive plasma assisted chemical vapor deposition (PACVD) process applicable to hard face coatings. Based on its superior erosion resistance, TiB_2 was selected as the initial coating for deposition onto a titanium alloy substrate (Ti-6Al-4V). In task I, novel non-intrusive laser diagnostic techniques (e.g., optical emission and absorption spectroscopy, Laser Induced Fluorescence Spectroscopy (LIFS), and Coherent Anti-Stokes Raman Spectroscopy (CARS)) are being used to determine, *in situ*, the reactive plasma composition, temperature, and species concentration and distribution in the gas phase. The second task includes use of Auger Electron Spectroscopy (AES), Ion Scattering Spectroscopy (ISS), Secondary Ion Mass Spectroscopy (SIMS) and other complementary techniques for detailed coating characterization. These are being combined with physical measurements of coating surface smoothness, density, hardness (state-of-the-art nanoindenter apparatus) and adherence (UTRC custom built pin-on-disc apparatus). These combined tasks will allow a correlation of the PACVD parameters with their required coating properties, thus providing a predictive capability that is severely lacking in the present science base of advanced protective coatings. Results to date include: (1) fabrication of a 5 kW rf PACVD reactor system integrated with a completely oil-free, high vacuum system (ultimate 10-8 torr); (2) exploratory spectral emission surveys for major molecular band and atomic line identification; (3) development of a collinear, scanned, narrowband CARS system; (4) implementation of an ultramicrohardness tester and adhesion test apparatus; (5) initial characterization of TiB_2 and diamond coatings; and (6) first time CARS measurement of several key species (e.g., B_2H_6).

Keywords: Coating, Plasma Diagnostics

231. Elastic-Plastic Fracture Analysis Emphasis on Surface Flaws — FY 1989 $454,000

DOE Contact: Oscar P. Manley, (301) 353-5822
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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. These results are used to make comparisons with data developed from specimens containing surface cracks.

These comparisons are presently underway for 6.4 and 12.7 mm thick surface-flawed specimens. 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

232. Continuous Damage Theory — FY 1989 $56,000

DOE Contact: Oscar P. Manley, (301) 353-5822
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The current state of development of the theory dealing with the brittle response of solids is characterized by a substantial arbitrariness reflected in a host of conflicting analytical models. The main objective of this research is to formulate a comprehensible continuum damage theory based on the improvements in the understanding of the underlying phenomena gained through experiments and application of micromechanics. Even though they are very useful micromechanical models typically require manipulations of very large databases causing significant computational complexities and presenting potent discouragement for their application in engineering practice.

The proposed model should retain the simplicity of a continuum theory without loosing the physical insights provided by the micromechanical studies. Once the theory has been checked on some benchmark problems (for which the pertinent micromechanical data are available) it will be possible to study more complicated problems.

The principal tasks of the initial phase of the project are: to select representative fluxes and affinities, to formulate a reasonable damage and failure surfaces and investigate the applicability of the normality property. Initial effort will be focused on the perfectly brittle response of solids such as concrete, rocks and ceramics.

Keywords: Metals: Ferrous, Fracture, Fatigue, Creep

233. <u>New Ultrasonic Imaging and Measurement Techniques for NDE</u> <u>FY 1989</u>
$258,000

DOE Contact: Oscar P. Manley, (301) 353-5822
Ames Laboratory, Iowa State University Contact: D. O. Thompson, (515) 294-5320

The objective of this project is to develop new knowledge and techniques for the nondestructive detection and characterization of flaws and nondestructive measurements of material properties that are of importance in obtaining reliability and integrity in materials and structures. In order to achieve this goal, use is made of new and unique multiviewing instrumentation that was previously developed in this work and which uses quantitative inverse elastic wave scattering theories in the interpretation of results. Three major thrusts are being pursued:

1. Nondestructive material characterization methods are being explored for high transition temperature superconducting ceramics using three types of probing fields: X-ray, eddy current, and ultrasound. Efforts are aimed at nondestructive measurements that can be used to monitor material processing techniques.

2. Novel techniques have been developed that allow the fabrication of ultrasonic transducers that have fundamentally important wave propagation properties of engineering significance. Two such transducers, a Gaussian beam transducer and a Bessel beam transducer, have been developed. The Gaussian beam is particularly desirable for inspection in the near field and the Bessel beam can potentially lead to diffraction-free elastic waves.

3. New techniques for ultrasonic computed tomographic imaging (reconstruction) are being explored that utilize elastic wave scattering models and the multiviewing instrumentation. This is an important innovation in that images so obtained are expected to be free of distortions due to effects of material anisotropy and complex surfaces encountered in some current imaging techniques.

Keywords: Nondestructive Evaluation, Ultrasonic, Fracture

234. Effects of Crack Geometry and Near-Crack Materials Behavior on Scattering of Ultrasonic Waves for QNDE Applications — FY 1989 $85,450

DOE Contact: Oscar P. Manley, (301) 353-5822
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A crack in a solid body can, in principle, be detected and characterized by its effect on an incident pulse of ultrasonic wave motion.

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. Several forward solutions to model problems have proven to be very helpful in the design of experimental configurations. They are also valuable in interpreting scattering data for the inverse problem.

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

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

Keywords: Nondestructive Evaluation, QNDE

235. Thermophysical Property Measurements in Fluid Mixtures FY 1989 $538,000

DOE Contact: Oscar P. Manley, (301) 353-5822
National Institute of Standards and Technology Contact: R. Kayser, (301) 975-2483 and J. M. H. Sengers, (301) 975-2463

The project aims at the development of accurate measurement capabilities for the thermophysical properties of complex, multiphase, fluid mixtures containing hydrocarbons. The research is being done jointly by two research groups within the Thermophysics Division of the NBS Center for Chemical Engineering. One group is located at the Gaithersburg, MD laboratories and the other at the Boulder, CO laboratories. The properties involved are PVT (pressure-volume-temperature), PVTx (pressure-volume-composition), phase equilibria (liquid-vapor and liquid-liquid equilibria), phase behavior in interfaces, and transport properties (viscosity, thermal conductivity, and diffusion coefficient). The apparatus will be designed for use in corrosive, highly corrosive, and sometimes toxic and flammable fluids with measurements extending to high temperatures (800K) and high pressure (30 MPa and, in some cases, 70 MPa). Also under study are methods for evaluating supercritical solvent mixtures and related fluid mixtures.

The most recently completed apparatus include a variable volume vapor-liquid equilibrium apparatus for moderate temperature ranges; a Langmuir film balance for use with aqueous, hydrocarbon, and biopolymer systems; a magnetic suspension densimeter for high temperatures and pressures; a torsional crystal viscometer for high temperatures and pressures; and a transient hot-wire apparatus for thermal conductivity measurements at high temperatures. The latter two apparatus are capable of reaching pressures near 70 MPa.

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

236. Flux Flow, Pinning, and Resistive Behavior in Superconducting Networks FY 1989 $63,594

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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.

This research will greatly enhance our fundamental understanding of pinning and flux flow resistance in superconducting materials. The results will have impact in understanding the magnetic properties of the new high T_c superconductors, and in the design of Josephson junction arrays for use as microwave detectors and generators.

Keywords: Flux Flow, Pinning, Vortex Motion, Superconductors

237. Thermodynamics of High Temperature Brines — FY 1989 $95,000

DOE Contact: George A. Kolstad, (301) 353-5822
Lawrence Berkeley Laboratory Contact: K. S. Pitzer, (415) 642-3472

This project covers theoretical and experimental studies concerning the thermodynamic properties of aqueous electrolytes at high temperatures. The components important in natural waters and brines are emphasized. The resulting data are important in understanding certain geothermal and other natural resources and in fission-product waste disposal. Moreover, this information has a wide range of applicability, since similar solutions arise in many industrial processes and in high-pressure steam power plants.

The experimental program involves measuring the heat capacities and heats of mixing or dilution of solutions exceeding 300°C and pressures to 1 kbar. The database for the principal components of natural waters has now become adequate for the prediction of mineral solubilities in brines up to about 300°C. Such calculations, based on the activity and osmotic coefficient equations of this project, were made for a number of systems containing $Na+$, $K+$, Mg^{2+}, Ca^{2+}, $Cl-$, $OH-$, SO_4^{2-}, and H_2O. Once the parameters are established for binary and common-ion ternary systems, no further parameters are needed for more complex brines, and calculations are truly predictive.

A theoretically based equation has been developed for the near-critical and supercritical properties of $NaCl-H_2O$. Parameters were fitted to the vapor-liquid coexistence surface for temperatures of 600°C and compositions from pure H_2O to that of the liquid on the three-phase line. Heat capacities and enthalpies were then predicted by this equation and agree satisfactory with the available experimental data.

Keywords: Electrolytes, Critical, Supercritical

238. Thermodynamic Properties of Silicate Materials

FY 1989
$70,000

DOE Contact: George A. Kolstad, (301) 353-5822
Lawrence Berkeley Laboratory Contact: D. A. Snyder, (415) 642-2577

This project measures high temperature thermodynamic properties of silicate liquids as a function of composition to enable the relevant quantities to be estimated for complex natural liquids. The iron redox state in silicate liquids has a dramatic effect on their volume, or their density. Measurements of the effect of temperature and oxygen fugacity on the ferric/ferrous iron ratio in natural liquids and liquids in the systems Na_2O-FeO-Fe_2O_3-SiO_2 and CaO-FeO-Fe_2O_3-SiO_2 have been used in conjunction with measurements of acoustic velocities to derive the compressibilities of liquids containing substantial amounts of ferric iron. With these data, values of the partial molar compressibilities of Fe_2O_3 and FeO in silicate liquids at 1 bar have been obtained.

As the iron redox state has a significant effect on the Fe/Mg distribution between crystals and silicate liquids, many of the trace metals, such as Ni and Co, will also have their distribution between liquid and crystals governed by the redox state, or the oxygen fugacity, of the magma. As magmas may encompass up to eight orders of magnitude of oxygen fugacity, experiments are underway to determine the effect of this range.

Keywords: Silicates, Thermodynamics

239. Studies of the Interactions Between Mineral Surfaces and Ions in Solution

FY 1989
$80,000

DOE Contact: George A. Kolstad, (301) 353-5822
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Studies have been conducted on the surface/solution interface reaction between galena (PbS) and copper(II) and chromium(VI) aqueous solutions using fluorescence techniques in conjunction with a synchrotron radiation source. The experiments, conducted at 25 °C and atmospheric pressure, were performed in order to gain a better understanding of the phenomenon of reductive chemisorption of a metal ion from solution. In this process, a metal ion in a higher oxidation state is removed from solution by a reducing substrate; the subsequent metal ion on the surface is then in a reduced (or lower) oxidation state.

Fluorescence microprobe data were taken in order to study the surface morphology of the adsorbed copper and chromium on the galena substrate. These data were compared to previously reported findings in which the surface morphology of the reacted galena was shown to be highly dependent on the chemical state of the initial, unreacted galena. With respect to the products formed upon reaction with the metal ions, the chemistry of the oxidized surface was markedly different from that of the unoxidized surface. The difference has been shown to be of both a chemical and morphological nature.

This work, a prelude to studying these same basic reaction systems at the Advanced Light Source (ALS) at Lawrence Berkeley Laboratory, has extremely widespread applications to energy conservation in a number of geochemically related processes. These studies, encompassing variable experimental chemical parameters such as pH, ion concentrations, temperature, and pressure, will lead to a better understanding of mechanisms and reaction products in several of these reaction systems. These same reactions will be studied by complementary surface approaches such as X-ray photoelectron, Auger, and scanning electron microscopy; in the cases of X-ray photoelectron and Auger spectroscopy, the preliminary research being done presently will be continued at the Advanced Light Source.

Keywords: Chemisorption, Fluorescence, Synchrotron Radiation

240. Thermodynamics, Kinetics, and Transport in Aqueous Electrolyte Solutions

FY 1989
$160,000

DOE Contact: George A. Kolstad, (301) 353-5822
Lawrence Livermore National Laboratory Contact: D. G. Miller, (415) 422-8074

Transport of dissolved chemical species is important in a wide variety of aqueous geochemical phenomena, including isolation of radioactive and chemical wastes, diagenesis and ore formation, and crystal growth and dissolution kinetics for certain types of minerals. The following types of transport experiments are being carried out in this context: 1) We have measured diffusion coefficients for aqueous solutions at 25°C using optical interferometry. Systems studied include most of the major and minor brine salts (except K_2SO_4 and alkali metal carbonates) and mixtures of NaCl with SrCl and with $MgCl_2$. 2) We have been measuring osmotic/activity coefficients for a variety of aqueous electrolytes and their mixtures up to saturation or supersaturation at 25°C including systems for which diffusion coefficients were measured. 3) Solubilities were measured for a number of these electrolytes using the isopiestic method. 4) We also measured densities of solutions used in the diffusion experiments.

This year we completed our extensive series of diffusion and density measurements for aqueous NaCl-$MgCl_2$ mixtures. This was done in collaboration with Dr. Luigi Paduano of the University of Naples, Italy, and with Professor John Albright and his students from Texas Christian University and is part of an international collaboration to thoroughly characterize this system. We will analyze data being measured at other laboratories (in the U.S.A., Australia, Canada, Germany, Argentina), which includes electrical conductances, viscosities, tracer diffusion coefficients, thermal diffusion coefficients, and transference numbers. Analysis of the seven compositions (out of 15) having complete sets of transport data has yielded preliminary values of the generalized transport coefficients 1_{ij} of irreversible thermodynamics. These are the quantities to be compared with statistical mechanical models of electrolyte mixtures. In addition, a preliminary comparison of these ternary 1_{ij} with a "mixture rule" that uses the binary 1_{ij} from NaCl-H_2O and MgCl-H_2O shows fairly good agreement. This implies reasonably good estimates of ternary properties from binary data.

Other studies include an analysis of the equal eigenvalue case in 3- and 4-components diffusion and derivation of relationships among mixture rules for electrical conductance. We have completed isopiestic measurements for aqueous $NaHSO_4$ and $NaHSO_4$-Na_2HSO_4. This system exhibits considerable deviations from ideal mixing rules due to HSO_4 formation. Previous activity data were restricted to lower molalities.

Keywords: Electrolytes, Diffusion

241. Thermodynamic Properties of Aqueous Solutions at High Temperatures and Pressures FY 1989 $125,000

DOE Contact: George A. Kolstad, (301) 353-5822
Los Alamos National Laboratory Contact: P. S. Z. Rogers, (505) 667-1765

Knowledge of the thermodynamic properties of electrolyte solutions at high temperatures is important in studies of geothermal systems, hydrothermal alteration processes, and element transport in deep brines such as those that have been encountered in the Continental Scientific Drilling Program (CSDP). Properties to at least 473 K for carbonates, hydroxy species, and organic complexes are especially needed to model cementation, mineral diagenesis, and element transport in sedimentary basin evolution. The purpose of this investigation is to determine the activity coefficients of geochemically important ionic species in aqueous solutions over a wide range of composition and temperature.

An automated flow calorimeter has been constructed to measure the heat capacities of concentrated, electrolyte solutions to 673 K and 40 MPa. Heat capacity data have been obtained for the systems NaCl-Na_2SO_4-H_2O, NaOH-H_2O, and Na_2CO_3-$NaHCO_3$-NaCl-H_2O to 39 MPa and 598 K.

Keywords: Electrolytes, Heat Capacity

242. Solubilities of Calcite and Dolomite in Hydrothermal Solutions FY 1989 $100,000

DOE Contact: George A. Kolstad, (301) 353-5822
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Equilibrium constants have been determined for the principal reactions that control the solubility of dolomite and calcite in hydrothermal solutions: $CaCo_3 + CO_2 + H_2O \rightarrow Ca^{2+} + 2HCO_3^-$ and $1/2CaMg(CO_3)_2 + CO_2O + H_2 \rightarrow 1/2Ca^{2+} + 1/2Mg^{2+} + 2HCO_3^-$ at temperatures of 50°, 100°, 150°, 200°, and 300°C and pressures of 300, 800, and 1300 bars. A co-solubility approach was selected, wherein equal molar proportions of calcite and dolomite were reacted with aqueous solutions with CO_2 concentrations varying from 0.04 to 2.3 m and ionic strengths less than 0.03. Run durations ranged from a few days to as much as 41 days. The equilibrium constants for both calcite and dolomite exhibit systematic retrograde behavior with non-zero heat capacities for the reactions. Reversals in the log K values were determined by ramping up and down pressure at a fixed temperature. Extrapolation of log K values for calcite to low pressure conditions agree with known calcite data. At 300 bars, log K values for calcite decrease from -4.86 at 100°C to -9.93 at 300°C, whereas log Ks for dolomite decrease from -5.20 to -10.44 over the same temperature interval. An increase in pressure results in an increase in the solubility, and this effect becomes more pronounced with increasing temperature. An increase of 1000 bars leads to an increase in solubility of calcite or dolomite by factors of 10 at 100°C and 100 at 300°C. This nonlinear behavior can best be normalized by a function that relates the log K values with the log density of water. Strict adherence of all the data to one simple function indicates that the data are precise to ±0.02 log K units for each solubility reaction. Data of this kind are essential for an understanding of the conditions that stabilize various carbonate phases (e.g., dolomite, siderite) and control permeability in diagenetic or geothermal systems via reactions such as the dolomitization of calcite ($2CaCO_3 + Mg^{2+} \rightarrow Ca^{2+} + CaMg(CO_3)_2$), which yields a 14.2 percent volume reduction.

Keywords: Carbonates, Solubility

243. Oxygen and Hydrogen Isotope Systematics of Brines FY 1989 $64,000

DOE Contact: George A. Kolstad, (301) 353-5822
Oak Ridge National Laboratory Contact: D. J. Wesolowski, (615) 574-6903

The activity coefficients of oxygen and hydrogen isotopes in natural brines differ substantially from unity as a function of salinity, composition, and temperature. The system $NaCl-H_2O$ has been studied at 100°C and seven salinities ranging from 0 to 5.5 molal NaCl. The D/H ratio of water vapor is 27 permil lower than that of coexisting pure liquid water at 100°C. As the salt content of the liquid phase increases, this different rises rapidly to a maximum of 38 to 40 permil at 0.5 molal NaCl and then decreases nearly linearly to approximately 20 permil at 5.5 molal. Presumably, the fractionation would become progressively smaller at higher salinities. These results are in excellent agreement with recent data reported in the Ph.D. thesis of K. Kazahaya at the Tokyo Institute of Technology. Preliminary results at 70°C indicate that the vapor-brine C/H fractionations differ significantly from our previous 100°C results for similar ionic strength solutions. At all NaCl molalities investigated at 70°C, the δD_{Vapor}-δD_{Brine} fractionations are less negative than the δD_{Vapor}-$\delta_{Pure\ H_2O}$ fractionation of -41 permil. For example, the δD_{Vapor}-δ_{Brine} values average approximately -30, -34, -36, -32, and -28 permil at 0.3, 0.5, 1, 3, and 4.9 m NaCl, respectively. These results are preliminary and require further confirmation with more experiments. At 100°C, the vapor-brine D/H fractionations are more negative (e.g., -35 to -39 permil at 1 m NaCl) than the vapor-pure water D/H fractionation (-27 permil) for NaCl molalities up to about 3.3. Above 3.3 m, the vapor-brine D/H values are less negative (e.g., -26 to -23 at 3.5 m NaCl) than the pure water system. The size and unexpected complexity of the salt effect at these conditions make it important to investigate this phenomenon in greater detail. Similar large effects are anticipated in systems with other important natural salts and mixtures thereof. These results suggest a small but fundamental change in the nature of bonding or the ratios of "free" versus "hydrated" water molecules in brines at temperature increases. The effects observed can lead to gross changes in the interpretation of isotopic data from natural systems. For instance, the kaolinite-pure water D/H fractionation changes by only 5 permil as temperature increases from 70 to 100°C. Our results indicate that if the water contains 1 molal dissolved NaCl, this change in the fractionation increases to 15 permil. Thus, the isotopic compositions of pore fluids in a subsiding sedimentary basin will experience major deviations from model prediction if the salinity effect is ignored or unquantified. This can results in erroneous interpretations of porosity-permeability evolution and fluid migration pathways in sedimentary basins and geothermal systems.

Keywords: Brines, Isotopic Composition

244. Sulfur Diffusion in Silicate Melts — FY 1989 $50,000

DOE Contact: George A. Kolstad, (301) 353-5822
Oak Ridge National Laboratory Contact: D. R. Cole, (615) 574-5473

Nearly 200 experiments have been conducted (900 to 1350°C, 1 atm, variable oxygen fugacity) to determine the sulfur diffusivities in three compositionally different silicate melts: low Fe^{2+}/Fe^{3+} basalt (McCoy Canyon), and Fe-deficient high-silica Na-Ca rich glass. Diffusion coefficients estimated from concentration-time plots for basalt and troctolite are remarkably similar despite their compositional differences. Values for log D (apparent diffusion coefficient, cm^2sec^{-1} range from about -6.7 and -7.3 at 1200°C to -6.3 and -6.6 at 1300°C for troctolite and basalt, respectively. In generally, reducing experimental conditions (QFM or below) resulted in slightly higher diffusion coefficients. This is true for both high- and low-silica melts. This redox trend may be due to the fact that all three starting compositions are more oxidized than the experimental conditions ultimately imposed on them via the CO_2/CO gas mixtures. The high-silica Na-Ca rich melts exhibit apparent diffusion coefficients approximately one order of magnitude less than the basalt (e.g., log D values of -8.7 at 1150 °C, -8.0 at 1250 °C, and -7.5 cm^2sec^{-1} at 1350 °C for fO_2 conditions defined by the NNO buffer). Diffusion coefficients calculated from electron microprobe profile data obtained on quenched high-silica glass spheres are in moderately good agreement with log D values estimated from the concentration versus time plots. The activation energies for diffusion vary between 40-50 and 55-65 kcal/mole for the low- and high-silica melts, respectively. These ranges are similar to those reported for sulfur diffusion in Ca-silicate and Ca-Al-silicate melts and those predicted by the Stokes-Einstein relation. A detailed examination of the sulfur K_α wavelength shifts by electron microprobe analysis of quenched glass indicates that the bulk of the sulfur occurs as sulfate rather than sulfide. The presence of sulfur as sulfate has been corroborated by using FTIR spectroscopy where we observed an absorption doublet as roughly 615 and 650 cm^{-1} in both high- and low-silica glasses. This doublet is not common in sulfur-deficient glasses and mimics doublets observed in many sulfate phases, particularly $CaSO_4$. Preliminary ESCA examination of our starting Na-Ca high-silica glass indicates that the sulfur appears to be bonded predominantly with Ca in the glass.

Keywords: Silicates, Sulfur, Diffusion

245. Diffusion/Dispersion Transport of Chemically Reacting Species — FY 1989, $121,000

DOE Contact: George A. Kolstad, (301) 353-5822
University of California, Berkeley Contact: H. C. Helgeson, (415) 642-1251

The project goal is the quantitative understanding of chemical mass transport attending fluid flow and water-rock interaction in geochemical processes. Recent research has focused on thermodynamic description of two geochemical systems: 1) concentrated aqueous electrolyte solutions at supercritical conditions and 2) the major organic compounds found in petroleum at temperature to 350 °C.

Analysis of literature conductance data for dilute NaCl, NaBr, NaI, HCl, and HBr solutions suggests that the activity coefficients of neutral ion pairs in hydrothermal solutions may vary significantly from unity. These conductance data were used to generate revised dissociation constants for neutral 1:1 complexes (K_1), limiting equivalent conductances, and Setchénow coefficients. The behavior of the computed Setchénow coefficients and of log K_1 suggests that neutral ion pairs may not be as abundant in concentrated supercritical electrolyte solutions as is commonly thought.

Molal stepwise dissociation constants for triple ions (K_2) of 14 alkali metal halides (e.g., Na_2Cl+) were computed for temperatures from 400° to 800 °C at pressures from 500 to 4000 bars with the aid of electrostatic theory. Species distributions calculated with these values, log K_1 values, and activity coefficients for relevant species taken from the literature indicate that triple ions predominate in low-pressure supercritical aqueous solutions at total concentrations ≥1.0 m. Supercritical aqueous solutions of the alkali metal halides thus are apparently dominated successively by single ions, neutral ion pairs, and triple ions with increasing solute concentration. As a consequence, polynuclear complexes, such as KNaCl+, $MgKCl_2^+$, $ZnNaCl_2^+$, $FeKCl_2^+$, etc., may have a significant effect on the solubilities of minerals in concentrated hydrothermal brines for many geochemical processes.

Preliminary calculations indicate that the thermodynamic properties of organic compounds at elevated temperatures can be used to characterize the interaction of petroleum with minerals and oil field brines. These properties have been computed for selected normal, branched and cyclic alkanes, alkenes, aromatics, naphalenes, alcohols, ketones, organic sulfides, and amino and carboxylic acids. The results have been used to predict the aqueous solubilities of organic species in petroleum at temperatures prevailing in hydrocarbon reservoirs. The importance of oxidation-reduction reactions among hydrocarbons and aqueous species in being assessed for processes responsible for the origin, transport, and deposition of oil and gas in hydrocarbon reservoirs.

Keywords: Electrolytes, Petroleum, Dissociation

246. Experimental Database and Predictive Theories for Thermodynamic Properties of Aqueous Solutions

FY 1989
$62,000

DOE Contact: George A. Kolstad, (301) 353-5822
University of Delaware Contact: R. H. Wood, (302) 451-2941

Measurements of the apparent molar heat capacity of aqueous solutions of H_2S, CO_2, and CH_4 are being made at twelve temperatures from 25° to 450°C and at pressure near 350 bar. Measurements of the apparent molar volume of aqueous solutions of H_2S, CO_2, and CH_4, are being made at the same twelve temperatures and at two different pressures. These measurements will accurately define the equilibrium properties of aqueous solutions of these gases at temperatures up to 450°C and pressures to 350 bar. These solutes are crucial reactants in a wide variety of geochemical processes and an accurate knowledge of their thermodynamic properties will permit a much better understanding of the driving forces for these processes. The measurements will double the amount of information available on volumes and heat capacities of aqueous nonelectrolytes at high temperatures. Theoretical models capable of representing these data and extrapolating them to higher temperatures and pressures are being investigated. Correlations and theoretical models that will allow the estimation of the properties of other nonelectrolytes of geochemical interest are also being investigated.

Keywords: Aqueous Solutions, Heat Capacity

247. Physical Characterization of Magma Samples FY 1989
$100,000

DOE Contact: George A. Kolstad, (301) 353-5822
University of Hawaii at Manoa Contact: M. H. Manghnani, (808) 948-7825

The main objectives of this project are: 1) to employ ultrasonic interferometry techniques to measure velocity and attenuation in natural and synthetic silicate melts; 2) to investigate interrelationships between the various physical, elastic and anelastic, and thermodynamic properties of silicate melts; and 3) to develop a Brillouin scattering technique for measuring the elastic and anelastic properties of melts in a wide range of temperature and pressure.

To accomplish these goals, laboratory studies are being conducted on natural rocks and synthetic silicate samples and their melts in three research areas: 1) characterization of physical, elastic and anelastic (V_p, V_s, Q^{-1}), and electrical properties of samples from Kilauea Iki lava lake and other related types of basalts; 2) development of Brillouin and Raman scattering measurements on synthetic and natural silicates and their melts, first as a function of temperature and then as a function of temperature and pressure, in an effort to understand the structure-property relationships in silicate melts; and 3) investigation of electrical conductivity of molten and partially molten rocks and silicates to understand the role of partial melting.

Ultrasonic measurements have been carried out on the melts of several types of natural rocks (basalts and komatiites) and on selected synthetic samples in the systems diopside ($CaMaSi_2O_6$)-anorthite ($CaAlSi_2O_8$) and albite ($NaAlSi_3O_8$)-anorthite ($CaAlSi_2O_8$) anorthite ($CaAlSi_2O_8$)-diopside ($CaMgSi_2O_6$) and to ~1600 C and in the frequency range 3-22 MHz. These measurements have enabled us to establish the velocity-density-composition (Birch's linear law) and attenuation-temperature-frequency systematics and to interpret the viscoelastic properties (viscosity, relaxation time, etc.) in terms of their composition and structure. We are now turning to employing the recently set up Brillouin scattering system and diamond anvil to study the compressibility of silicate melts at high pressures. The ultrasonic and Brillouin scattering results, to be extended to high pressures in the future, will provide important thermodynamic parameters (e.g., compressibility) for these melts at high pressure. The electrical conductivity measurements on the Kilauea Iki basalts have now been completed. In progress are the measurements on the nepheline-sodium disilicate ($NaAlSiO_4Na_2SiO_3$) system to ~1000° C to determine the effect of partial melting (solidus = 768° C) on the electrical properties.

Keywords: Silicates, Ultrasonics

248. Investigations of Ultrasonic Surface Wave Interaction with Porous Saturated Rocks

FY 1989
$55,000

DOE Contact: George A. Kolstad, (301) 353-5822
Ohio State University Contact: L. Adler, (614) 292-1974

This research work investigates the interaction of ultrasonic waves (including bulk waves, surface waves, and generalized Lamb waves) with fluid-saturated porous solids. The effort of the research should find applications in the geophysical evaluation of porous fluid bearing rocks where such parameters as porosity, tortuosity, permeability, surface flow impedance, saturation level or composition, and elastic properties of the skeleton frame and the saturated frame are of importance.

With the development of the theoretical treatment for reflection and transmission of fast, slow, and shear waves at a fluid/fluid-saturated porous medium interface, an alternate case concerning interactions of bulk waves with a plane interface separating two fluid-saturated porous media has been studied. The theoretical analysis includes developing property boundary equations and derivation of energy transmission and reflection coefficients for fast, slow, and shear waves through the interface. It has been shown that the surface flow impedance imposed previously for characterizing pore boundary conditions is a vector instead of a scalar quantity, and usually, only the normal component of the impedance vector plays a significant role in the analysis of reflection and transmission coefficients. Numerical calculations for energy transmission and reflection coefficients have been made for a case where the interface is formed by two porous media consisting of fused glass beads and fused lead beads with different porosities. The analysis is focused on the effect of pore interface conditions (determined by the value of the normal component of flow impedance vector). Predictions show in either fast or shear wave incidence the reflected and transmitted fast and shear waves behave with no evident difference at a sealed or an open pore interface, while the reflected or transmitted slow wave is affected strongly by the pore interface conditions. Numerical results show the amount of energy allocated from the fast or shear incident wave to the reflected and transmitted slow waves is negligible. For a normally incident slow wave with an open pore interface, about 88 percent energy is converted to the transmitted slow wave and 0.5 percent to the reflected slow wave while, with a sealed pore interface, a complete reflection occurs for the slow wave.

The investigation of generalized leaky Lamb wave interaction with a fluid-saturated porous plate has been conducted theoretically and experimentally. Using Biot's theory, numerical results for reflected and transmitted spectra through a thin porous plate immersed in a liquid has been obtained. Ultrasonic measurement of reflected signal spectra from porous plate at different angle has been performed to obtain phase velocity of various Lamb modes as function of product of frequency and thickness. Experimental results show that the measured lowest Lamb mode in a porous plate is attributed to the slow wave. At small incident angle, the horizontal axis of the asymptotic phase velocity of the measured lowest

Lamb mode is in coincidence with half of the slow wave velocity. The good agreement between experimental results and theoretical predictions shows that the Lamb wave technique provides a new approach for detecting slow wave in porous media.

Keywords: Ultrasonics, Lamb Waves

249. Zircons and Fluids: An Experimental Investigation with Applications for Radioactive Waste Storage — FY 1989 $60,000

DOE Contact: George A. Kolstad, (301) 353-5822
Virginia Polytechnic Institute and State University Contact: A. K. Sinha, (703) 231-5580

The purpose of this project is to study the relationship between hydrothermally induced mobility of uranium and lead isotopes and the chemical and mechanical properties of small populations of zircons ($ZrSiO_4$). The experiments utilized both natural and synthetic zircons as starting materials. During the first year of this project, techniques were refined for growing zircons in tungstate and molybdate fluxes. Variations in the size and morphology of the synthetic zircons are demonstrably related to both cooling rates and the addition of minor amounts of rare earths and other elements to the starting mixtures.

The hydrothermal stability of the U-Pb isotopic system of natural non-metamict zircons has been investigated at varying pressure and temperature conditions utilizing two fluid compositions, 2M NaCl and 2 percent HNO_3. Experiments were conducted at 4 and 6 kilobars, at 300° and 600°C, and for durations of 24, 200, and 720 hours. A large fraction (~30-40percent) of uranium (assumed to be bonded in the mineral structure) was removed from the zircon during the runs made with 2M NaCl, while the zircons treated with the HNO_3 solution lost less than 10 percent uranium at the same run conditions. Current research is investigating the relationship between crystallinity and chemistry of zircons, development of microfractures and the loss of uranium and lead from the experimental charge.

Preliminary SEM imaging of the run products indicates that microfractures are, to some extent, crystallographically controlled. Microprobe analyses suggest that trace constituents (other than uranium and lead), such as Hf, Y, and P, appear to be unaffected by the experimental solutions. Microfracture growth and nucleation mechanisms are being investigated using theoretical models. Models are being developed that relate the timing of microfracturing to changes in the surface/volume ratio and transport of uranium and lead out of zircons.

Keywords: Zircons, Uranium, Hydrothermally Induced Mobility

250. PVTX Properties of Fluid Systems: $NaCl-CaCl_2-H_2O$ FY 1989
$91,000

DOE Contact: George A. Kolstad, (301) 353-5822
Virginia Polytechnic Institute and State University Contact: R. J. Bodnar, (703) 961-7455

Most geologic processes in the Earth's crust take place in the presence of one or more fluid phases, and the compositions of these fluids vary from one environment to another. In order to derive thermodynamic properties of geologic fluids and fluid-melt systems and to interpret microthermometric data from fluid inclusions trapped in these environments, an experimental database on the PVTX properties of geologically important fluid systems must be established. Until recently, derivations of thermodynamic properties of geologic fluids and interpretations of fluid inclusion volumetric properties and phase equilibria have generally been based upon the PVTX properties of simple unary and binary subsets of the larger system $NaCl-KCl-CaCl_2-MgCl_2-H_2O-CO_2-CH_4$. These simple systems often do not adequately describe observed phase behavior in fluid inclusions, nor do they provide representative models for many of the more complex fluids found in nature.

This research program will determine accurately and completely the PVTX properties of geologically important fluid systems over the complete range of temperature, pressure, and composition conditions commonly encountered in the Earth's crust. These data have been and will continue to be gathered in a systematic manner, starting with relatively simple binary systems and progressing to more complex higher order systems. Studies of the $NaCl-H_2O$ and the $NaCl-KCl-H_2O$ system have been completed. Work on the $NaCl-H_2O-CO_2$ system is nearly completed. Study of phase equilibria and volumetric properties of the $NaCl-CaCl_2-H_2O$ system will be pursued next.

Information obtained in this study will add to knowledge of the physical and chemical properties of geologic fluids found at crustal P-T conditions. As such, the results will broaden our understanding of many important fluid-related geochemical processes of interest to geoscientists.

Keywords: Geological Fluids, Thermodynamic Properties

Materials Structure and Composition

251. Silicate Thermochemistry FY 1989
$30,000

DOE Contact: George A. Kolstad, (301) 353-5822
Princeton University Contact: A. Navrotsky, (609) 452-4674

A study was performed to examine the effects of the charge coupled substitution $Si^{4+} = T^{3+}\ Na^{1+}$ (T - Al, B, Fe, and Ga) on the overall stabilization of framework silicate glasses in the systems $xNaTO_2(1-x)SiO_2$. Enthalpies of solution in molten $2PbO \cdot B_2O_3$ at

973 K were determined for x ≥0.5. The heats of solution in each of these systems become increasingly endothermic with increasing x and exhibit a maximum near x - 0.5 reflecting an exothermic ΔH of mixing. In the glassy systems $M_{1/n}AlO_2$-SiO_2 (M - Li, NA, K, Rb, Cs, Mg, Ca, Sr, Ba, and Pb), the enthalpy of stabilization was found to scale inversely with the field strength (Z/R) of the non-framework cation, M. This implies that the stability of the aluminosilicate framework in these systems is controlled by the strength of the M-O bond and the concomitant weakening of the T-O-T angle. In the present study, ΔH_{stab} does not scale with the strength of the T-O bonds. Instead it appears that the stability of the aluminosilicate framework is controlled by the range of T-O-T bond angles permitted by the substitution of T^{3+} for Si^{4+}. The substitution of Al, Fe, Ga, and B for Si changes to varying degrees the range of bond angles that are energetically favorable. As this range decreases, the stability of the glass decreases.

A technique has been developed for solution calorimetry of oxides of highly charged cations in molten $2PbO \cdot B_2O_3$. It is used to obtain enthalpies of vitrification of crystalline $K_2(Ti, Zr)Si_4O_9$. Transposed-temperature-drop calorimetry experiments are being performed upon a glass that undergoes rapid glass-glass phase separation at 1173 K. These experiments indicate that it is possible to directly measure the enthalpies of unmixing of immiscible liquids and glasses. Thermodynamic mixing properties of glasses of the system K_2O-SiO_2-La_2O_3 are being measured.

Investigation continues of the structural and thermodynamic effects of aluminum substitution on tri-octahedral Fe-free micas. Nine synthetic samples along the join from $K_{0.94}(Mg_{2.93}Al_{0.04})$ - $(Al_{0.94}Si_{3.06})O_{10}(OH)_2$ to $K_{0.90}(Mg_{2.08}Al_{0.92})$ - $(Al_{1.83}Si_{2.17})O_{10}(OH)_2$ have been studied. Microprobe and thermogravimetric analyses of synthetic materials were completed. The five Si-rich samples had constant weight up to 1003 K, then they lost ~4.3wt% H_2O due to mica dehydroxylation. Weight loss occurred in two steps, probably due to a different in -OH sites and related to the Al content of the octahedral sheet. The Al-rich samples showed a gradual weight loss of up to 1.8 wt% in the 473-1003 K range that was temperature dependent and time independent. They lost 3.9-4.1 wt% H_2O in the 100-1423 K range due to mica dehydroxylation. Lattice parameter refinements have been completed. Calorimetric study to determine enthalpies of mixing is planned for later this spring. A series of amphiboles is also under study.

Keywords: Silicates, Glasses, Thermodynamics

Division of Advanced Energy Projects

Materials Preparation, Synthesis, Deposition, Growth or Forming

252. Gas Jet Deposition of Metallic, Semiconducting and Insulating Films FY 1989 $154,000

DOE Contact: Walter M. Polansky, (301) 353-5995
Schmitt Technology Associates Contact: Bret Halpern, (203) 432-4376

Gas Jet Deposition (GJD) is a new method for depositing thin films at high rate and controlled energy. The basic physics of GJD will be investigated in order to develop its technological capabilities. GJD deposits films by "seeding" atoms or molecules into a free jet expansion, e.g., of helium, and directing the jet at a substrate at relatively high pressure. GJD promises many advantages over established methods. Deposition rates of 10 microns per minute have been attained, and microns per second should be within range. The impact energy of depositing species can be gas dynamically controlled over a range of electron volts, so that film properties can be influenced during deposition. The substrate, which can be almost any material, can remain cool during deposition. Film composition and doping profile can be easily varied. Clusters can be deposited as well as atoms and molecules. GJD is flexible, and any metal, semiconductor, or insulator that can be seeded in the free jet can be deposited. The combination of these features in one method makes GJD singularly versatile. The goal of this project is to explore the feasibility of GJD as the basis of a usable technology. To do this, the fundamentals of GJD will be investigated. In particular, its high rate and impact energy control and the GJD apparatus will be refined. The properties of the films produced will be determined.

Keywords: Coatings and Films, Gas Jet Deposition

253. Growth of High T_c Superconducting Fibers Using a Miniaturized Laser-Heated Float Zone Process FY 1989 $477,000

DOE Contact: Walter M. Polansky, (301) 353-5995
Stanford University Contact: Robert S. Feigelson, (415) 723-4007

The primary objective of this project is to thoroughly explore the potential of the laser-heated pedestal (float zone) growth method for the preparation of flexible wires (fibers) of the new copper-oxide ceramic superconductors, in particular the Bi containing compounds which are capable of carrying high currents at temperatures above 77°K. This method, which involves drawing wires directly from a melt, has many advantages over other methods, most important of which is that it allows precise control of the growth process through the control of melt composition. Critical issues which will be considered in this superconducting fiber program include (1) determining the most suitable compositions to be grown, (2) the maximum allowable growth velocity which can be used to grow fibers with high T_c, and (3) the maximum length of fiber which can be produced. To address these issues, the program will involve an in-depth study of (1) the thermodynamic and kinetic factors which affect growth rate and the properties of the fibers produced, (2) the development of an advanced fiber growth system which permit better control of system parameters, and (3) the development of techniques to enhance fiber throughput via increased growth velocity, postgrowth heat treatments, and the possibility of growing many fibers simultaneously.

Keywords: Superconductivity, Laser-Heated Pedestal Growth

Materials Properties, Behavior, Characterization or Testing

254. Production of Fuels and Chemicals From Methane — FY 1989 $250,000

DOE Contact: Walter M. Polansky, (301) 353-5995
Argonne National Laboratory Contact: Victor A. Maroni, (312) 972-4547

In this project research is being carried out to develop novel bifunctional catalysts (BFCs) that can convert methane to fuels (e.g., liquefied petroleum gas or gasoline) and large volume industrial chemicals. The goal is to produce a catalyst that operates efficiently under moderate conditions of temperature ($<500°C$) and pressure (<10 atm), and for extended periods of time, without need for frequent regeneration or replacement. The BFC concept involves integrating into one material the properties of C-H bond activation and product-selective chemical synthesis. Several types of C-H bond activation catalysts that rely on unique oxidation state chemistries and coordination geometries are employed in combination with molecular sieve materials having well defined intracrystalline pores and channels that constrain the size and shape of the active catalytic species contained therein and the chemical species formed therein. This research is expected to culminate in a demonstration of the feasibility of efficient conversion of methane to a representative fuel and/or to one or more of the top 50 commodity chemicals.

Keywords: Catalysts, Molecular Sieves

Office of Health and Environmental Research

The Office of Health and Environmental Research supports a broad multidisciplinary program in basic and applied life sciences research for the purpose of achieving a comprehensive understanding of the health and environmental effects associated with energy technologies. Research is conducted to characterize and measure energy-related hazards, study transport and transformations in the environment, determine the biological and ecological response and define the potential impact on human health. In addition, new applications of nuclear science and energy technologies are developed for use in the diagnosis and treatment of human disease. Materials interests are primarily in development of sensors for radiation and chemical detection.

This Office sponsored no materials research in FY 1989.

Office of Fusion Energy*

The main goal of the magnetic fusion program is to establish the scientific and technological base required for an assessment of the feasibility of fusion energy. The strategy for providing this scientific and technological base is two-fold: (1) maintenance of a domestic R&D program that covers the necessary range of fusion science and technology adequately, and (2) use of international collaboration to advance the program in a timely way, especially through joint projects.

The work that must be accomplished to reach the program goal can be summarized by defining four key technical issues. The issues are associated with determining the properties of burning plasmas, improving magnetic confinement systems, formulating fusion materials and developing fusion nuclear technology. These issues have been agreed to by the Economic Summit Member's Fusion Working Group as the focus for planning future international research facilities. The U.S. program research on these issues constitutes the basis for participation in the world fusion program including participation in the four part ITER Design with the European community, Japan and the Soviet Union.

The third key issue is of specific relevance to this report. It addresses the identification and testing of materials for fusion systems. Not only is materials research vital to a successful experimental fusion program today but it is also the key to realizing the benefits of fusion. Materials play a central role in determining the environmental characteristics of a fusion reactor. Achievement of the program goal requires the development of new materials to enhance the economic and environmental potential of fusion. As part of the program's international strategy, this issue is being pursued through cooperative agreements which provide significant foreign contributions toward the operation of U.S. research facilities.

Small Business Innovation Research Program

The Small Business Innovation Research (SBIR) program was established in compliance with the Small Business Innovation Development Act of 1982, Public Law 97-219. 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

*No submission was received from the Office of Fusion Energy for FY 1989.

awards are limited to $50,000. Phase II is the principal research or research and development effort, and awards can be as high as $500,000 for work to be performed in periods of up to two years. Under Phase III, commercial applications of the research or research and development are to be pursued by small businesses with non-Federal capital or, alternatively, Phase III may involve follow-on non-SBIR Federal contracts for products or processes desired by the Government.

The materials-related projects, like all other projects in the DOE SBIR program, were selected using the specific evaluation criteria listed in the program solicitation. Conclusions were reached on the basis of detailed reports returned by reviewers drawn from DOE laboratories, universities, private industry, and government. In the case of Phase II, if several proposals were judged to be of approximately equal technical merit, preference was given to those proposals that had demonstrated third phase, non-Federal capital commitments.

The work supported in this program represents high-risk research, but the potential benefits are also high if the objectives are met. Brief descriptions of all DOE SBIR projects (not just those of interest in materials research) are given in the following publications: Abstracts of Phase I Awards, 1989 (DOE/ER-0417), Abstracts of Phase II Awards, 1989 (DOE/ER-0418), and Abstracts of Phase II Awards, 1988 (DOE/ER-0379). Copies of these publications may be obtained by calling Mrs. Gerry Washington on (301) 353-5867.

OFFICE OF NUCLEAR ENERGY

The Office of Nuclear Energy conducts research projects in the Office of Remedial Action and Waste Technology, the Office of Uranium Enrichment, 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 Remedial Action and Waste Technology

Division of Waste Treatment Projects

The mission of the Division of Waste Treatment Projects is to facilitate development of a reliable national system for managing low-level waste and to carry out a demonstration of immobilization of high-level radioactive waste in borosilicate glass at the West Valley Demonstration Project.

Materials Preparation, Synthesis, Deposition, Growth or Forming

255. Technical Support to West Valley Demonstration Project — FY 1989 $1,641,000

DOE Contact: T. W. McIntosh, (301) 353-3589
PNL Contact: W. A. Ross, (509) 376-3644

Pacific Northwest Laboratory (PNL) is providing technical assistance to the West Valley Demonstration Project by (a) characterizing high-level waste materials from West Valley storage tanks; (b) preparing Waste Qualification reports for the Department's high-level waste acceptance process; (c) developing an empirical model which relates the borosilicate glass composition to the chemical durability (including both the preparation and testing of materials and the statistical analysis of the results to allow modeling); (d) characterizing the individual process operations to show control of the process and the final waste form composition; (e) developing ion exchange media for plutonium removal from waste streams; and (f) providing remote technology systems support.

Keywords: Ion Exchange, Borosilicate Glass, Process Control, Radioactive Waste Host, Waste Qualification

Materials Properties, Behavior, Characterization or Testing

256. Materials Characterization Center Testing of West Valley Formulation Glass

FY 1989
$600,000

DOE Contact: H. F. Walter, (301) 353-5510
PNL Contact: G. B. Mellinger, (509) 376-9318

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 both nonradioactive glass containing surrogate elements for the radionuclides and radioactive glass doped with appropriate radionuclides. The MCC also initiated the fabrication of a glass containing actual West Valley high-level waste. The chemical durability of this glass will be determined in FY 1989.

Keywords: Radioactive Waste Host

257. Development of Test Methods and Testing of West Valley Reference Formulation Glass

FY 1989
$900,000

DOE Contact: E. A. Maestas, (716) 942-4314
CUA Contact: P. B. Macedo, (202) 635-5327

Vitreous State Laboratory, Catholic University of America (CUA) is (a) developing methods to test nonradioactive and radioactive borosilicate glass waste forms; (b) testing nonradioactive and uranium/thorium containing reference formulation glass waste forms for the West Valley Demonstration Project; (c) studying means to maximize the region of acceptable quality around the point of optimal durability for the borosilicate glass waste form; and (d) preparing Waste Qualification reports for the Department's high-level waste acceptance process.

Keywords: Radioactive Waste Host

258. Process and Product Quality Optimization for the West Valley Waste Form

FY 1989
$250,000

DOE Contact: E. A. Maestas, (716) 942-4314
AU Contact: L. D. Pye, (607) 871-2432

For the West Valley Demonstration Project, Alfred University (AU) is (a) studying properties and crystallization behavior of the West Valley glass composition, (b) developing methods for control of product quality during routine manufacture of the West Valley Demonstration Project waste form; and (c) preparing Waste Qualification reports for the Department's high-level waste acceptance process.

Keywords: Radioactive Waste Host

Office of Uranium Enrichment

The specific statutory authority which established the Department of Energy's role in the enrichment of uranium is the Atomic Energy Act of 1954, as amended. The goal of the Uranium Enrichment Program is to maintain this activity as a strong viable enterprise retaining a market share that preserves a long term competitive position. It is intended that these services be done for commercial and defense customers in an economical, reliable, safe, secure, and environmentally acceptable manner that will ensure a reasonable return on the Government's investment.

Revenues received by DOE for the enrichment of uranium are retained and used for the specific purposes of offsetting costs incurred by the Department in providing uranium enrichment service activities as authorized by Section 201 of Public Law 95-238, not withstanding the provisions of Section 3617 of the Revised Statutes (31 USC 484). The sum appropriated is reduced as uranium enrichment revenues are received during a fiscal year so as to result in no net fiscal year appropriations. Total obligations for all uranium enrichment activities in FY 1989 was approximately $1.3 billion.

Materials activities within the Office of Uranium Enrichment are varied and, for the most part, classified Restricted Data. The following summarizes these activities for the purpose of this report. The total outlay in FY 1989 was $21.6 million. The DOE contact is A. P. Litman, (301) 353-5777.

Gaseous Diffusion

Uranium as found in nature contains about 7/10ths of 1 percent uranium 235 which is fissionable. The remainder is essentially uranium 238 which is non-fissionable. The fissionable characteristics of uranium 235 make it desirable for use as nuclear fuel. To date, most nuclear reactors designed for producing electrical power require uranium 235 concentrations between 2 and 5 percent. Presently, uranium is enriched to the desired uranium 235 assay levels in gaseous diffusion plants. These plant operate on the principle that lighter weight gaseous isotopes have slightly higher average velocities and thus can be made to diffuse through a porous barrier more rapidly than heavier species. Two streams can be created, one enriched in the lighter isotope and one depleted. Because enrichment for a single cycle, or stage, is very small, a cascade of stages is required. For example, a plant constructed for producing 4 percent assay U-235 would contain about 1200 stages. Although many other methods for enrichment are still being investigated and another production technique is being used in parts of Europe, diffusion plants today still provide approximately 90 percent of the world's enrichment services. The United States gaseous diffusion 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.

Device or Component Fabrication, Behavior or Testing

259. Gaseous Diffusion: Barrier Quality

FY 1989
$2,587,000

Studies of the short- and long-term changes in the separative capability of the diffusion barrier. Methods to recover and maintain barrier quality and demonstration in the production facilities. This activity is a long-term undertaking and will be maintained at the appropriate levels of effort in the future.

Keywords: Nuclear Fuel Isotopic Separations, Gaseous Diffusion, Barrier, Uranium

260. Gaseous Diffusion: Materials and Chemistry Support

FY 1989
$3,473,000

Routine materials and chemistry support of the diffusion plants. Characterization of contaminant-process gas cascade reactions, physical/chemical properties of UF_6 substances, corrosion of materials, failure analyses, trapping technology, alternative materials replacement.

Keywords: Nuclear Fuel Isotopic Separations, Uranium, Gaseous Diffusion

Uranium-Atomic Vapor Laser Isotope Separation (U-AVLIS)

The U-AVLIS process is based on utilizing the differences in the electronic spectra of uranium isotopes to induce the selective absorption required for isotopic separation. The process utilizes the controlled vaporization of uranium atoms from metal feed followed by selective excitation and ionization of uranium 235 using tunable lasers in the visible regions of the spectrum. The resulting plasma of uranium enriched in uranium 235 ions can then be removed from the vapor using electromagnetic methods. Collection of the product is as a liquid metal that is allowed to solidify upon withdrawal.

In June 1985, DOE selected U-AVLIS for further development and possible future deployment into the uranium enrichment enterprise. The primary emphasis for U-AVLIS in FY 1989 was to continue activities that will enable a demonstration of U-AVLIS in full size equipment in 1992. This demonstration will provide a base of technical and economic information adequate to accomplish three goals: (1) support a detailed design for an

U-AVLIS production plant, (2) establish a high confidence plan for integration of U-AVLIS into the nuclear fuel cycle, and most important, (3) allow a U-AVLIS production plant deployment decision. Available resources in FY 1989 were focused on this goal and the activities included operation of large test beds and key subsystems. A separator facility continued operation in for FY 1989 to provide component development and design data for a full size separator. The U-AVLIS materials activities in FY 1989 were largely in support of the separator system and uranium processing activities. The latter technologies will have strong economic leverage for a U-AVLIS production plant and are receiving more attention this year. The overall goal of uranium processing is to develop and demonstrate low-cost paths for integrating the U-AVLIS metal feed and product into the existing uranium oxide/fluoride nuclear fuel cycle.

261. U-AVLIS: Separator Materials — FY 1989 $8,700,000

Selection and testing of alternative candidate structural and component materials and coatings for the U-AVLIS separator system. Fabrication of full size components and subsystems for U-AVLIS verification tests.

Keywords: Enrichment, Uranium, Laser Isotope Separation, Uranium-Atomic Vapor Laser Isotope Separation (U-AVLIS)

262. U-AVLIS: Uranium Processing — FY 1989 $6,900,000

Bench-scale experiments and design studies on three alternatives for preparation of U-AVLIS feed from precursor oxide. Design of a demonstration system for U-AVLIS metal product conversion to precursor oxide for light water power reactor fuel. Environmental, safety and health compliance activities. Interaction with fuel fabricators to assure integration into the nuclear fuel cycle.

Keywords: Enrichment, Uranium, Laser Isotope Separation, Uranium-Atomic Vapor Laser Isotope Separation (U-AVLIS)

Office of Civilian Reactor Development

Office of Advanced Reactor Programs

Division of High Temperature Gas-Cooled Reactors

The objective of this division is to develop the base technology, systems concepts, and reactor designs which will permit the Government, in cooperation with utilities and private industry, to commercialize the High Temperature Gas-Cooled Reactor (HTGR). The materials interests of this division include those required for the development of coated particles fuels, graphite moderator and reflector blocks, graphite core support blocks and posts, and heat exchanger tubing and tube sheets. The DOE contact for these projects is J. E. Fox, (301) 353-3985.

Materials Preparation, Synthesis, Deposition, Growth or Forming

263. Fuel Process Development — FY 1989 $775,000

DOE Contact: J. E. Fox, (301) 353-3985
GA Technologies Contact: R. F. Turner, (619) 455-2306

This work includes establishing, characterizing, and qualifying fabrication processes and equipment for the preparation of microsphere fuel particles of uranium-oxycarbide (UCO) coated with layers of pyrolytic carbon (2) and silicon carbide (1). Major processing operations include solution mixing, kernel forming, drying, calcining, and sintering. Coatings are applied in a fluidized-bed furnace at temperatures up to 1600°C. The objective is to develop kernel fabrication and coating specifications, which yield very low fractions of defective particles. This work also includes development of the process for fabricating the fuel compacts (short rods).

Keywords: Fuel, Ceramics, Sintering, Coatings, Chemical Vapor Deposition

Materials Properties, Behavior, Characterization or Testing

264. Fuel Materials Development — FY 1989 $515,000

DOE Contact: J. E. Fox, (301) 353-3985
GA Technologies Contact: R. F. Turner, (619) 455-2306

This work includes development of the technology base required to design, qualify, and license the fuel systems for near-term steam cycle and advanced process heat HTGRs. These efforts are focused on the low enriched uranium-oxycarbide/thorium-oxide fuel system. Major elements of the work include the preparation and evaluation of irradiation specimens, development and verification of fuel performance models, and preparation and updating of fuel specifications and a design data manual.

Keywords: Fuel, Ceramics, Coatings, Microstructure, Radiation Effects, Diffusion, High Temperature Service

265. Fuel Development and Testing

FY 1989
$2,500,000

DOE Contact: J. E. Fox, (301) 353-3985
ORNL Contact: M. J. Kania, (615) 576-4856

This work supports development of the technology base required to design, qualify, and license the fuels systems for near-term steam cycle and advanced process heat HTGRs. These efforts are focused on the low-enriched uranium-oxycarbide/thorium-oxide fuel system. Major elements of the work include services associated with the design, assembly, and irradiation of fuel capsules, and post-irradiation examination work in support of qualification and licensing of the reference fuel system. This work also includes support of International Cooperatives with West Germany and Japan, and a fuel test program in the French CEA COMEDIE Test Facility.

Keywords: Fuel, Ceramics, Coatings, Microstructure, Radiation Effects, Diffusion, High Temperature Service

266. Graphite Development

FY 1989
$65,000

DOE Contact: J. E. Fox, (301) 353-3985
GA Technologies Contact: R. Vollman, (619) 455-3310

This work supports the evaluation and qualification of graphite materials for applications in HTGRs. Major goals of this work are to develop high strength graphites with sufficient stability under irradiation to be qualified for core components, and with sufficient oxidation resistance to be qualified for core support components. The major element of this work is the development of graphite materials test specifications and failure criteria required for reliable design analyses.

Keywords: Graphite, Ceramics, Irradiation Effects, Strength, Corrosion, High Temperature Service

267. Graphite Development and Testing

FY 1989
$460,000

DOE Contact: J. E. Fox, (301) 353-3985
ORNL Contact: T. D. Burchell, (615) 576-8595

This work includes the selection, characterization, and qualification of graphite materials for applications in HTGRs. These efforts are focused on the development of fundamental understanding of the behavior of graphite under representative HTGR environmental and loading conditions. Major goals of this work are to develop high strength graphites with sufficient stability under irradiation to be qualified for core components, and with sufficient oxidation resistance to be qualified for core support components. The major elements of this work include characterization of the mechanical, physical, and chemical properties of candidate graphites and determinations of the effects of irradiation on mechanical and physical properties.

Keywords: Graphite, Ceramics, Irradiation Effects, Strength, Corrosion, High Temperature Service

268. Metals Technology Development — FY 1989 $30,000

DOE Contact: J. E. Fox, (301) 353-3985
GA Technologies Contact: R. F. Turner, (619) 455-2306

This work includes activities to characterize and qualify the metallic materials selected for applications in the HTGR system. Tasks involve work to establish the database required for design validations and code qualifications. Principal alloys include SA508 and 533 steels, 2¼ Cr-1 Mo steel, and Alloy 800H.

Keywords: Alloys, Strength, Corrosion, Joining, Microstructure, High Temperature Service

269. Structural Materials Development — FY 1989 $800,000

DOE Contact: J. E. Fox, (301) 353-3985
ORNL Contact: P. L. Rittenhouse, (615) 574-5103

This work includes testing activities to characterize and qualify the metallic materials selected for application in HTGR components and structures. The emphasis of the work is to provide design data or components which operate in the primary coolant circuit, where the service temperatures are the highest and the materials may be adversely affected by trace amounts of impurities in the helium coolant. The primary testing activities include evaluations of the effects of extended high temperature exposures in simulated helium and air environments on mechanical properties and the effects of irradiation on the nil-ductility transition temperature.

Keywords: Alloys, Strength, Corrosion, Joining, Microstructure, High Temperature Service

270. Advanced Gas Reactor Materials Development — FY 1989 $170,000

DOE Contact: J. E. Fox, (301) 353-3985
ORNL Contact: O. F. Kimball, (615) 574-8258

This work includes testing and evaluation of the high temperature alloys required for applications in advanced HTGRs that will operate at temperatures about 750°C. The primary activity is operation of a testing laboratory specifically designed for extended high temperature exposures of mechanical property specimens and corrosion samples in simulated helium reactor environments. Major work elements include mechanical property and corrosion testing of commercial available and developmental candidate alloys and the generation of a database for development of high temperature design criteria and code qualification rules.

Keywords: High Temperature Alloys, Mechanical Properties, Corrosion

Office of Technology Support Programs (LMRs)

The applied research and development technology activities, conducted at several national laboratories, industrial organizations, universities, and through bilateral and trilateral technology programs and exchanges with foreign nations, relate to current and advanced reactor systems. The scope of these activities include the following areas: fuel cycles; design and performance of high quality core components for fuels, blanket, and control systems; development of the structural materials used in these components and systems; development and demonstration of equipment, processes, and procedures for fabricating, processing, handling, and producing mixed oxide bearing fuels, binary and ternary metal fuels, materials, and components; sodium technology; standards and quality assurance; assuring a reliable high quality economical fuel supply for LMRs; destructive and nondestructive testing, examination, and evaluation of core components and the facilities and capabilities for conducting such examinations; responsibility for engineering and supporting facilities; associated safety, safeguards, and nonproliferation; maintaining competent capabilities in the several contractor organizations that conduct the pertinent R&D activities and programs. These activities are responsive to the administration's policies and goals and, to the DOE programs that support them.

In-reactor and out-of-reactor property evaluations are being conducted on core materials, clad/ducts, fuels and absorber materials. Through irradiation testing in FFTF and EBR-II, the Technology Support Programs are developing, qualifying, and verifying the use of reference, improved and advanced mixed oxide and metal fuels and boron carbide absorbers, including full-size driver and blanket fuels, and absorber element pins and assemblies—same for carbide fuels. Fabrication development, evaluation, qualification, and verification (raw material processing, melting, hot working, cold working, and finishing) are conducted on reference, improved, and advanced alloys including in-reactor qualification of pins, ducts, and assemblies. Improved and advanced materials are being tested for use in future cores. The testing for these programs is primarily conducted at government laboratories: Argonne National Laboratory at Chicago, Illinois and Idaho Falls, Idaho; Oak Ridge National Laboratory at Oak Ridge, Tennessee; and Westinghouse Hanford Company at Richland, Washington.

Fuels and Core Materials

Materials Properties, Behavior, Characterization or Testing

271. Fuel Performance Demonstration

FY 1989
$7,600,000

DOE Contact: Andrew Van Echo, (301) 353-3930/FTS 233-3930
ANL Contact: Leon C. Walters, (208) 526-7384/FTS 583-7384

Establish U-Pu-Zr fuel fabrication process, irradiation performance characteristics and high burn-up capability. EBR-II lead test achieved 17.1 and 18.4 a/o burn-up and were removed for PIE. Program plans to complete initial off-normal testing in EBR-II, including RBCB and fabrication variable tests.

Keywords: Breeder Reactor, Actinides, Fuel

272. Pyroprocess Development

FY 1989
$5,000,000

DOE Contact: Eli I. Goodman, (301) 353-2966/FTS 233-2966
ANL Contact: James E. Battles, (312) 972-4538/FTS 972-4538

Establish technical feasibility of the proposed pyroprocesses including electrorefining, chemical reduction, and waste treatment processes. Program will select optimum cathode configuration for electrorefining process, conduct engineering scale (10 kg) demonstration of electrorefining with uranium, and run laboratory-scale demonstration of waste treatment processes.

Keywords: Waste Treatment, Electrorefining, Pyroprocesses

273. Fuel Safety Experiments and Analysis

FY 1989
$4,000,000

DOE Contact: Philip B. Hemmig, (301) 353-3579/FTS 233-3579
ANL Contact: John Marchaterre, (312) 972-4561/FTS 972-4561

Conduct analyses and experiments required for the demonstration of the safety performance of metallic fuel in fast reactor systems. Include transient fuel behavior, validated models and codes which describe fuel behavior, and safety mechanisms which contribute to inherent safety. Program will initiate analysis of TREAT test M7 with irradiated U-Pu-Zr fuels, and continue preparations for two PRF/TREAT tests.

Keywords: Reactor Safety, Actinides, Fuel

274. Core Design Studies FY 1989
$4,300,000

DOE Contact: Philip B. Hemmig, (301) 353-3579/FTS 233-3579
ANL Contact: D. C. Wade, (312) 972-4858/FTS 972-4858

Provide direct support in developing optimized metallic core designs for ALMR and establish a validated design and safety analysis methodology suitable for initiation of detailed design and for licensing interactions. Conduct studies of fuel management strategies for the closed fuel cycle including physics and economic impacts of self-sufficient uranium start-up versus maximized breeding ratio start-up of sequential plan modules. Evaluate impact of actinide self-consumption in the metal fuel cycle.

Keywords: Actinides, Reactor Design, Breeding Ratio, Metal Core

275. Fuel Cycle Studies FY 1989
$5,300,000

DOE Contact: Eli I. Goodman, (301) 353-2966/FTS 233-2966
ANL Contact: M. J. Lineberry, (312) 972-7434/FTS 972-7434

Initiate planning for fuel cycle demonstration, including in-cell equipment system development. This activity provides semi-prototypic testing of pyroprocess and fabrication equipment systems prior to design of in-cell models. Quantify the ultimate fuel cycle economics through development of commercial fuel cycle facility design and cost estimates. Program will initiate equipment development activities for remotized in-cell application, including reusable mold concept for injection-casting furnace, semi-automated pin processor, engineering-scale pyroprocessing equipment, etc. Refine and update commercial-scale fuel cycle facility design and cost estimates, including sensitivities to throughput requirements and develop initial set of prototype equipment systems.

Keywords: Fuel, In-Cell, Remotized, Injection-Casting

276. LMR Technology R&D FY 1989
$2,100,000

DOE Contacts: Philip Hemmig, (301) 353-3579/FTS 233-3579 and C. Chester Bigelow (Seismic), (301) 353-4299/FTS 233-4299
ANL Contact: D. C. Wade, (312) 972-4858/FTS 972-4858

Continue seismic analyses and test support for the ALMR design. Provide test and analyses support for the ALMR mechanical components. Continue inherent safety controllability testing and analyses to demonstrate the passive safety aspects of the IFR concept and how they could be applied in the ALMR design.

Keywords: Seismic Tolerance, Enhanced Reactor Safety, Inherent Safety Features, Fuel

Structural Materials and Design Methodology

Materials Properties, Behavior, Characterization and Testing

277. Structural Design/Life Assurance Technology — FY 1989 $ 0 (Funded by JAPC)

DOE Contact: Andrew Van Echo, (301) 353-3930/FTS 233-3930
ORNL Contact: Jim Corum, (615) 574-0718/FTS 624-0718

Program was to develop the structural design methods and criteria for use of modified 9 Cr-1 Mo steel in liquid metal reactor environment; however, it has been closed out in FY 1989. The program is now supported under a DOE/Japanese exchange agreement, funded jointly by DOE and Japanese Atomic Power Company (JAPC).

Keywords: Fatigue, Failure Testing, Joining and Welding, Creep

278. Modified 9 Cr-1 Mo Steel Design Properties — FY 1989 $ 0 (Funded by JAPC)

DOE Contact: Andrew Van Echo, (301) 353-3930/FTS 233-3930
ORNL Contact: Phil Rittenhouse, (615) 574-5103/FTS 624-5103

The program had been conducting long-term thermal aging effects on mechanical properties, long-term creep-rupture tests on base and weldment materials, creep-fatigue tests in air and high vacuum environments and creep-crack propagation tests on modified 9 Cr-1 Mo steel. The program is now supported under a DOE/Japanese exchange agreement, funded jointly by DOE and Japanese Atomic Power Company (JAPC).

Keywords: Creep, Fatigue, Tensile Testing, Toughness

279. Nondestructive Testing Technology for Heat Exchangers — FY 1989 $ 0

DOE Contact: Andrew Van Echo, (301) 353-3930/FTS 233-3930
ORNL Contact: Donald D. McGuire, (615) 574-4835/FTS 624-4835

The program had been conducting nondestructive eddy-current and ultrasonic probes development for operation at 400°F in sodium; however, the program has been phased out in FY 1989.

Keywords: Nondestructive Testing, Eddy Currents, Ultrasonic

280. Nuclear Systems Materials Handbook — FY 1989: $ 0

DOE Contact: C. Chester Bigelow, (301) 353-4299/FTS 233-4299
ORNL Contact: Martin F. Marchbanks, (615) 574-1091/FTS 624-1091

Program was developing mechanical property correlations for input into the Nuclear Systems Materials Handbook. It was closed out in FY 1989.

Keywords: Mechanical Properties, Creep, Fatigue

281. MOTA Fabrication and Operation — FY 1989: $1,100,000

DOE Contact: Andrew Van Echo, (301) 353-3930/FTS 233-3930
WHC Contact: Ray J. Puigh, (509) 376-3766/FTS 444-3766

Conduct activities to provide a known and controlled environment for materials irradiation tests in FFTF. Principal tests include HT9 irradiation supporting Series III fuel design, international tests, FFTF structural materials surveillance, and non-LMR tests. Fabricate and assemble MOTA irradiation vehicle for insertion into FFTF. Upon discharge of MOTA from FFTF, examine specimens and reconstitute all samples into a new MOTA vehicle during the reactor outage. Monitor and document the operations of MOTA. Issue MOTA 1F operations report and complete fabrication and assembly of MOTA 1H test train to be loaded into FFTF cycle 12A.

Keywords: Irradiation, Environmental Testing

282. Absorber Development — FY 1989: $700,000

DOE Contact: C. Chester Bigelow, (301) 353-4299/FTS 233-4299, Andrew Van Echo, (301) 353-3930/FTS 233-3930
WHC Contact: Alan E. Waltar, (509) 376-5514/FTS 444-5514

Conduct activities to support Series III control rod design and monitor ongoing FFTF absorber tests. This includes completing irradiation of HEHB and ADVAB-1B experiments and providing analytical support to extend FFTF absorber lifetime to 900 Effective Full Power Days (EEPD). Provide report on absorber performance to date in FFTF.

Keywords: Control Rods, Nuclear Absorbers

283. FFTF Metal Fuel Testing FY 1989
$1,100,000

DOE Contact: Andrew Van Echo, (301) 353-3930/FTS 233-3930
WHC Contact: Alan E. Waltar, (509) 376-5514/FTS 444-5514

Continue activities for FFTF metal fuel irradiations and transient testing in TREAT. Fabricate full HT9 clad FFTF binary metal fuel driver test assemblies at nominal fuel conditions (MFF-4, -5, and -6) and at 2-sigma hot channel conditions (MFF-3).

Keywords: Fuel, Non-ferrous Metals

284. Core Demonstration Experiment (CDE) FY 1989
$1,600,000

DOE Contact: Jacob Glatter, (301) 353-3921/FTS 233-3921
WHC Contact: Alan E. Waltar, (509) 376-5514/FTS 444-5514

Continue Core Demonstration Experiment (CDE) irradiation in FFTF supporting the extension of fuel lifetime to 1,200 EFPD. Complete PIE report on TREAT tests. Draft Cycle 10 CDE report, evaluate data for justifying continued irradiation of CDE beyond goal exposure (1200 EFPD) based on steady-state and transient data. Complete FCTT testing on high-exposure HT9 clad ACO-1R pins from MFF-1A. Evaluate high exposure HT9 data to determine toughness.

Keywords: Fuel, Non-ferrous Metals

285. International Collaboration FY 1989
$750,000

DOE Contact: Jacob Glatter, (301) 353-3921/FTS 233-3921
WHC Contact: Alan E. Waltar, (509) 376-5514/FTS 444-5514

Complete fabrication of the DSF-1 fuel test with cladding types agreed to with DOE and PNC. Monitor irradiation performance in FFTF of PNC fuel (MFA-1 and -2) and blanket (MBA-1) assemblies. Characterize production lots of MA957 cladding. Reconstitute MOTA NAM-1 test specimens. Ship C-1 pins to PNC.

Keywords: Dispersion Strengthened Ferritic (DSF), Fuel, Cladding

Office of Space and Defense Power Systems

The Office of Space and Defense Power Systems is responsible for the development, system safety and production of radioisotope 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

286. Development of Improved Thermoelectric Materials for Space Nuclear Power Systems

FY 1989
$30,000

DOE Contact: W. Barnett, (303) 353-3097
General Electric Co., Space Systems Division Contact: P. D. Gorsuch, (215) 354-5047

The prime objective of this program is to optimize the thermoelectric performance of silicon-germanium type materials by a systematic study of compositional (i.e., alloy and dopant additions) and processing (i.e., powder preparation techniques, including rapid solidification, powder particle size, hot pressing variables, etc.) parameters. Property characterization included the following: electrical resistivity, Seebeck voltage, thermal conductivity, Hall effect and density measurements. Structural characterization shall employ the following evaluation techniques: optical microscopy, X-ray diffraction, SEM, STEM, EDAX, ESCA and EXAFS. The goal is an average figure of merit, Z, of $1 \times 10^{-3} \cdot C^{-1}$ over the temperature range of 300-1000°C.

During FY 1989, studies were focused on the role of gallium phosphide additions to N-type 80Si-20Ge type alloys. Optimization of preparation parameters and resulting structure has led to the identification of a family of N-type composition which offer the potential of a 40 percent or more improvement in figure of merit. A final report will be issued in the first quarter of 1989.

Improved thermoelectric materials are required to enhance the performance of advanced radioisotope thermoelectric generators, the primary space power system employed in NASA spacecraft for deep space exploration.

Keywords: Consolidation of Powder, Powder Synthesis, Semiconductors, Thermoelectrics

287. Development of an Improved Process for the Manufacture of DOP-26 Iridium Alloy Blanks

FY 1989
$600,000

DOE Contact: W. Barnett, (303) 353-3097
RNL Contact: 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 such as Voyager and

Galileo. This program is aimed at the development of an improved process route for the production of DOP-26 iridium alloy sheet, namely a consumable arc cast/extrusion/"warm" rolling route. Thermomechanical process parameters shall be optimized with respect to uniformity of product grain morphology, high strain rate, high temperature ductility and formability. The product must meet or exceed existing DOP-26 iridium alloy specifications.

It is anticipated that the consumable arc cast/extrusion route process will replace the currently employed arc drop cast ingot/warm roll sheet process and shall yield a significant improvement in process yields and product quality. A prime goal for the new process is a 50 percent reduction in reject rate (i.e., from 30-15 percent or below) due to ultrasonic indications (i.e., laminar type defects).

During FY 1989 extrusion billet surface quality problems were solved by scale-up to a 2½" diameter x 10 kg. arc cast ingot size coupled with minor surface conditioning. Extrusion problems were solved by adopting a slight increase in extrusion temperature plus the adoption of a glass lubrication practice. Beds were received on a state-of-the-art consumable arc melting furnace. Optimization of rolling processes was continued.

Keywords: Consumable Arc Melt, Extrusion, Noble Metal

288. Carbon Bonded Carbon Fiber Insulation Manufacturing Process Development and Product Characterization — FY 1989 $650,000

DOE Contact: W. Barnett, (303) 353-3097
ORNL Contact: R. L. Beatty, (615) 574-4536

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) which will power the spacecraft for the NASA Galileo and NASA/ESA Ulysses missions. This CBCF process development program is intended to accommodate a replacement carbon fiber (present specified fiber is no longer available), improve process controls, and optimize process parameters. The product shall meet prior flight quality CBCF specification. Product characterization shall include chemical purity, density, compressive strength, and thermal conductivity.

During FY 1989, process and product qualification activities and procedure preparation or updating were 90 percent complete. A minor problem, the occasional occurrence of small low binder content fiber clusters exceeding X-ray density limits, appears to have been solved by a combination of wet melling and ultrasonic slurry agitation. Training of two machinists was initiated. Adaptation of a computer-aided image analyzer to X-ray (film) inspection will be initiated in FY 1990.

Keywords: Insulators/Thermal, High Temperature Service, Fibers

Device or Component Fabrication, Behavior or Testing

289. Nondestructive Testing Methods Development and Application to Thermoelectric Materials and Devices

FY 1989
$150,000

DOE Contact: W. Barnett, (303) 353-3097
ORNL Contact: B. E. Foster, (615) 574-4837

Continued support program aimed at the development and application of state-of-the-art nondestructive examination (NDE) techniques for Si-Ge thermoelectric materials, multicouples and multicouple subassemblies. Particular attention was directed toward the evaluation of glass bonds and hot shoe bonds, and the post-test diagnostic evaluation of multicouples.

Keywords: NDE, Semiconductor Devices, Thermoelectrics

Materials Properties, Behavior, Characterization or Testing

290. Characterization of State-of-the-Art Improved Silicon-Germanium Thermoelectric Device/Materials and Silicon-Germanium Materials Development

FY 1989
$400,000

DOE Contact: W. Barnett, (303) 353-3097
Iowa State University Contact: B. Beaudry, (515) 294-1366

This program is concerned with the evaluation and characterization of state-of-the-art Si-Ge/GaP and other "improved" silicon-germanium type thermoelectric materials. Also the compatibility of materials employed in the manufacture of the multicouple (i.e., glass bonded closs packed arrays of silicon-germanium couples) device was studied. Long-term stability of thermal and electrical properties of thermoelectric materials and devices was also studied.

In addition, exploratory studies of the potential of mechanical alloying for producing unique high performance Silicon-Germanium type thermoelectric materials were initiated. Processing techniques were developed in FY 1989.

Keywords: Semiconductor, Thermoelectrics, Powder Processing, Mechanical Alloying

Office of Naval Reactors

The Materials Research and Development Program is in the Reactor Materials Division under the Deputy Assistant Secretary for Naval Reactors. The 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 in the high power density and long life 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 $77 million in FY 1989 including approximately $42 million as the cost for irradiation testing in the Advanced Test Reactor. The Naval Reactors contact is Robert H. Steele, (703) 557-5565.

OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT

Office of Systems Integration and Regulations*

Office of Civilian Radioactive Waste Management/Yucca Mountain Project (OCRWM/YMP)

The primary goal of the OCRWM/YMP materials program is the development of tuff specific waste packages that meet the NRC's performance requirements. This work includes the definition of physical and chemical conditions of the site, evaluation of the package materials, waste package design and performance assessment, prototype waste package fabrication, and performance testing. (As a result of the Nuclear Waste Policy Act Amendments, the Salt Repository Project and the Basalt Waste Isolation Project were terminated effective March 1989.)

Materials Properties, Behavior, Characterization or Testing

291. Waste Package Environment — FY 1989 $1,699,000

DOE Contact: C. P. Gertz, (702) 794-7920
LLNL Contact: David Short, (415) 422-1287

Characterize the time-dependent behavior of the hydrogeologic environment in which the waste packages will reside in order to establish the envelope of conditions that define package design parameters, materials testing conditions, and boundary conditions for performance analysis.

Keywords: Near Field Environment

*No submission was received from this office for FY 1989.

292. Waste Form Testing FY 1989
$2,342,000

DOE Contact: C. P. Gertz, (702) 794-7920
LLNL Contact: David Short, (415) 422-1287

Characterize the behavior of and determine the radionuclide release rates for the various waste forms in the geological tuff environment and as modified by corrosion products in the Metal Barrier Testing. This includes work on both borosilicate glass and spent fuel.

Keywords: Radioactive Waste Host, Materials Degradation

293. Metal Barrier Testing FY 1989
$2,264,000

DOE Contact: C. P. Gertz, (702) 794-7920
LLNL Contact: David Short, (415) 422-1287

Characterize the behavior of and determine the degradation modes and rates for candidate metallic barrier materials in the environment. This information is needed to establish the data base to support license applications predictions of containment of radioactivity for times required by NRC 10 CFR 60. Characterize the properties and behavior of other engineered barrier waste package components that may be present in a repository.

Keywords: Materials Degradation, Radioactive Waste Host

294. Other Engineered Barrier Waste Package Components FY 1989
$4,000

DOE Contact: C. P. Gertz, (702) 794-7920
LLNL Contact: David Short, (415) 422-1287

Characterize the properties and behavior of other engineered barrier waste package components that may be present in a repository. This information is needed to establish the predicted performance of other materials, such as packing materials, that may be present to assist waste forms and metal barriers in meeting NRC 10 CFR 60 performance requirements.

Keywords: Near Field Environment

295. Integrated Testing

FY 1989
$1,435,000

DOE Contact: C. P. Gertz, (702) 794-7920
LLNL Contact: David Short, (415) 422-1287

Characterize the integrated behavior of the waste form, barrier materials, and surrounding environment. Determine thermodynamic properties of Actinide and fission products.

Keywords: Actinide Chemistry, Waste Package Testing, Thermodynamic Data Base

296. Waste Package: Performance Assessment

FY 1989
$686,000

DOE Contact: C. P. Gertz, (702) 794-7920
LLNL Contact: David Short, (415) 422-1287

Provide a quantitative prediction of long-term waste package performance. This information, including uncertainties, is needed to provide feedback to design optimization studies, to demonstrate compliance with NRC performance objectives for the Waste Package Subsystem, and to provide a source term for the Engineered Barrier System and the Total System performance assessments required by NRC 10 CFR 60 and EPA 40 CFR 191.

Keywords: Waste Package Performance, Uncertainty Analysis

297. Research on Geochemical Modeling of Radionuclide Interaction with a Fractured Rock Matrix

FY 1989
$1,376,000

DOE Contact: C. P. Gertz, (702) 794-7920
LLNL Contact: David Short, (415) 422-1287

Further develop the geochemical modeling code EQ3/6 for use in long-term predictions of radionuclide release from a nuclear waste repository.

Keywords: Goechemical Modeling, Computer Modeling, Rock-Water-Waste Interaction

Device or Component Fabrication, Behavior or Testing

298. Waste Package: Design, Fabrication and Prototype Testing — FY 1989 $1,748,000

DOE Contact: C. P. Gertz, (702) 794-7920
LLNL Contact: David Short, (415) 422-1287

Develop, analyze, fabricate, and test waste package designs that incorporate qualified materials which are fully compatible with the repository design. This work supports license application by demonstrating conformance with requirements for safe handling, emplacement, possible retrieval, and credible accident conditions per NRC 10 CFR 60 and EPA 40 CFR 191 in a cost-effective manner.

Keywords: Radioactive Waste Package Development

299. Waste Package Environment Field Tests — FY 1989 $1,584,000

DOE Contact: C. P. Gertz, (702) 794-7920
LLNL Contact: David Short, (415) 422-1287

Develop a detailed engineering test plan for the waste package environment in situ testing program and evaluate, design, fabricate, and test thermomechanical and hydrologic instrumentation for waste package in situ test measurements.

Keywords: Radioactive Waste Packaging Tests, Instrumentation and Technique Development, Field Testing

Sandia National Laboratories: Brittle Fracture Technology Program

The objective of this program is to qualify alternate materials (other than stainless steel) for use in nuclear spent fuel cask construction. Candidate materials include nodular cast iron and ferritic steel. The main technical issue which must be addressed is the application of fracture mechanics to cask analysis and design. Materials, such as nodular cast iron, exhibit a ductile/brittle failure mode transition. Hence, a cask constructed out of this material may be susceptible to brittle fracture under certain environmental and loading conditions. The application of fracture mechanics can provide the cask analyst/designer the ability to guarantee ductile cask material response to design loadings.

Materials Structure and Composition

300. Microstructure Investigations of Nodular Cast Iron — FY 1989 $15,000

DOE Contact: F. Falci, (301) 353-3595
SNL Contact: K. B. Sorenson, (505) 845-8431

Standard metallography techniques are being used to quantify graphite nodule size and spacing in sample test specimens used for obtaining fracture toughness values. A strong correlation is evident between nodule size and spacing and fracture toughness. Similar studies were done to establish the effect of nodule size and spacing on tensile properties (tensile strength and ductility).

Keywords: Fracture Toughness, Nodular Cast Iron

301. Composition Investigation of Nodular Cast Iron — FY 1989 $10,000

DOE Contact: F. Falci, (301) 353-3595
SNL Contact: K. B. Sorenson, (505) 845-8431

The investigation concluded that compositional features controlled the tensile behaviors of nodular cast iron, particularly nickel and silicon. Compositional features had no apparent effect on fracture toughness.

The conclusion drawn from the above two studies was that fracture is a phenomena controlled by microstructural features, whereas tensile properties (ductility) are controlled by compositional features. There is no apparent mechanistic link between fracture toughness and ductility.

Keywords: Microstructure, Nodular Cast Iron

Materials Properties, Behavior, Characterization, or Testing

302. Generate Material Property Database for Nodular Cast Iron — FY 1989 $50,000

DOE Contact: F. Falci, (301) 353-3595
SNL Contact: K. B. Sorenson, (505) 845-8431

Existing material property data for nodular cast iron are being assimilated into a common format. Data sources include technical reports and industry (foundries and cask vendors). In addition, testing is being performed to fill in gaps of the existing database. Significant lack of data includes fracture toughness values as a function of strain rate and temperature. The main focus of the testing program is to generate fracture toughness values for nodular cast iron.

Keywords: Database, Fracture Toughness, Nodular Cast Iron

303. Mosaik Brittle Fracture Test Program — FY 1989 $75,000

DOE Contact: F. Falci, (301) 353-3595
SNL Contact: K. B. Sorenson, (505) 845-8431

A drop test program is being developed whereby a ductile cast iron cask (mosaik) will be dropped in order to demonstrate a proof of principle for the fracture mechanics design approach.

Keywords: Fracture Toughness, Ductile Cast Iron

304. Investigate Thickness Effects on Impact and Toughness Properties of Ferritic Steel — FY 1989 $80,000

DOE Contact: F. Falci, (301) 353-3595
SNL Contact: K. B. Sorenson, (505) 845-8431

Materials testing is being done to measure nilductility (NDT) transition temperature, Charpy and fracture toughness properties as a function of section thickness. These measurements will be compared directly with the values established by the NRC to qualify certain grades of ferritic steel for transport cask construction.

Keywords: Ferritic Steel, Fracture Toughness

305. Investigate the Feasibility of Using Depleted Uranium as a Structural Component in Cask Construction — FY 1989 — $25,000

Doe Contact: F. Falci, (301) 353-3595
SNL Contact: K. B. Sorenson, (505) 845-8431

A brief literature search was conducted to determine the feasibility of using depleted uranium (DU) as a structural component in cask body construction. Sandia has performed a study (1982) to identify material properties pertinent to structural considerations. The material may be suitable for this application. It exhibits a relatively strong toughness and high tensile strength. A 2 percent Mo alloy exhibits better mechanical properties than unalloyed DU. An extensive testing program would be required to qualify this material for cask construction. Fracture toughness values as a function of strain rate and temperature need to be generated.

Keywords: Radioactive Waste Casks, Uranium

306. Use State-of-the-Art Data Acquisition Ductile Cast Iron Drop Test — FY 1989 — $100,000

DOE Contact: F. Falci, (301) 353-3595
SNL Contact: K. B. Sorenson, (505) 845-8431

The Mosaik Instrumentation Data Acquisition System (MIDAS) will be used to support data acquisition needs for drop tests being conducted in Albuquerque, New Mexico, and West Germany under DOE sponsorship.

Keywords: MIDAS, Data Acquisition

OFFICE OF DEFENSE PROGRAMS

Assistant Secretary for Defense Programs

The Assistant Secretary for Defense Programs directs the Nation's nuclear weapons research, development, testing, production, and surveillance programs. In addition, the Assistant Secretary coordinates a safeguards and security program to provide accountability and physical protection of special nuclear materials, including research and development for improvements, testing, evaluation, and implementation of safeguards systems. Additional responsibilities include management of the inertial fusion development and nuclear materials production programs, classification and declassification of sensitive weapons information, and analysis and coordination of international activities related to nuclear technology and materials.

Materials activities in Defense Programs are concentrated in the Office of Weapons Research, Development, and Testing and in the Office of Nuclear Materials Production. Within the Office of Weapons Research, Development, and Testing, materials activities are supported by the Inertial Fusion Division and by the Weapons Research Division.

Office of Defense Waste and Transportation Management

Waste Research and Development Division*

The objective of the Defense High-Level Waste (HLW) Technology Program is to develop the technology for ending interim storage and achieving permanent disposal of all U.S. defense HLW. Defense HLW generated by atomic energy defense activities is stored on an interim basis at three U.S. Department of Energy (DOE) operating locations: the Savannah River Site in South Carolina, the Hanford Site in Washington, and the Idaho National Engineering Laboratory in Idaho. HLW will be immobilized for disposal in a geologic repository. Other waste will be stabilized in-place if, after completion of the National Environmental Policy Act (NEPA) process, it is determined, on a site-specific basis, that this option is safe, cost effective and environmentally sound. The orderly transition from interim storage to permanent disposal at the three DOE sites will proceed sequentially in order to permit technical developments at the first site to be utilized at the other sites and thereby achieve a more efficient use of resources. The immediate program focus is on implementing the waste disposal strategy selected in compliance with the NEPA process at

*In November 1989, this program was transferred from Defense Programs to the new Office of Environmental Restoration and Waste Management and placed under the Office of Waste Operations.

Savannah River and Hanford, while continuing progress toward development of final waste disposal strategy at Idaho.

At Savannah River HLW will be retrieved from underground storage tanks, immobilized as borosilicate glass, stored on-site for an interim period, and eventually shipped to a geologic repository. A Defense Waste Processing Facility (DWPF) to immobilize Savannah River waste is under construction.

At Hanford a final Environmental Impact Statement (EIS) was prepared to support selection of a disposal strategy for Hanford high-level, transuranic and tank wastes. The Preferred Alternative recommended proceeding with disposal of double-shell tank waste, retrievably-stored transuranic waste and encapsulated cesium and strontium. Further development and evaluation is required for the remaining three types of wastes: single-shell tank waste, TRU-contaminated soil site, and pre-1970 buried suspect TRU-contaminated solid waste. A Record of Decision was signed April 18, 1989, selecting the Preferred Alternative.

At Idaho several alternative waste management strategies have been identified and their relative rankings evaluated. One of these strategies will eventually be selected in compliance with the NEPA process for disposal of Idaho HLW.

Materials Properties, Behavior, Characterization or Testing

307. Waste Form Qualification — FY 1989 $6,000

DOE Contacts: Ken Chacey, (301) 427-1621, and Marv Furman, (509) 376-7062
Westinghouse Hanford Company Contact: Steve Schaus, (509) 376-8365

These studies provide the fundamental data for immobilizing defense waste (e.g., borosilicate glass, crystalline ceramics). The related compliance activities for acceptance at a geologic repository and site specific testing (e.g., MCC-1) are included in this work. Additionally, data are generated which are used for start-up of the Defense Waste Processing Facility and related process control tests. The documentation supporting waste form qualification is used to support waste compliance disposal requirements and demonstrates the suitability of the defense waste form in a geologic repository.

Keywords: Waste, Waste Form, Borosilicate Glass, Waste Acceptance Specifications (OGR/B-8)

308. Immobilization/Volume Reduction/In-place Stabilization FY 1989
$6,746

DOE Contacts: Ken Chacey, (301) 427-1621, and Marv Furman, (509) 376-7062
Westinghouse Hanford Company Contact: Steve Schaus, (509) 376-8365

These studies provide the process flowsheets for treatment of HLW streams at Richland and Idaho. The focus of the work is on reduction of immobilized waste volumes. These studies include waste characterization, retrieval technology, and waste processing requirements. Additionally, technology for in-place stabilization is investigated, where appropriate, to ensure all disposal strategies are included in evaluating the disposal requirements for defense waste at Richland and Idaho.

Keywords: High-Level Waste, Volume Reduction, In-Place Stabilization

Office of Weapons Research, Development, and Testing

Weapons Research Division

Sandia National Laboratories - Albuquerque

Solid State Sciences Directorate, 1100

Ion Solid Interactions and Surface Sciences Research Department, 1110

The mission of Department 1110 is to provide Sandia National Laboratories with a comprehensive research program and technology base in the surface and interface science ion implantation, ion-solid microanalysis/channeling thin film kinetics and epitaxy, and defects and hydrogen in solids. The research is designed to enhance fundamental understanding of the physical and chemical processes necessary to control the near-surface and interfacial regions of solids as well as to develop new techniques for the controlled synthesis, modification and analysis of these near-surface and interfacial regions. A major aspect of the work is thus to develop an underlying understanding and control of defects, thin film kinetics, epitaxy, hydrogen-materials interactions alloying processes, and the formation of metastable and amorphous phases. In addition, the mission of the department is to relate this knowledge to laboratory problems and needs in the development of advanced weapons and energy systems.

Materials Properties, Behavior, Characterization or Testing

309. Ion Implantation Studies for Friction, Wear and Microhardness

FY 1989
$300,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
SNL (Contract No. DE-AC04-76DP00789) Contacts D. M. Follstaedt, (505) 844-2102, S. M. Myers, (505) 844-6076 and L. E. Pope, (505) 844-5041

Ion implantation is used to modify the surface and near-surface regions of metals, and these implantation-modified materials are evaluated for their improved friction and wear characteristics. Of particular interest is the implantation of Ti + C into bearing steels to concentrations sufficient to form amorphous layers in the near-surface region. These amorphous layers have been found to yield significantly improved friction and wear behavior for steels, independent of the structure and composition of the starting material. Extensions of these studies to vacuum applications are under investigation. A second area is the formation of ultrahard and stable Al alloys by oxygen implantation.

Keywords: Ion Implantation, Friction, Wear, Amorphous Metals

310. Silicon-Based Radiation Hardened Microelectronics

FY 1989
$670,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
SNL (Contract No. DE-AC04-76DP00789) Contacts: H. J. Stein, (505) 844-6279, B. L. Doyle, (505) 844-2609 and J. A. Knapp, (505) 844-2305

Optical, electrical and compositional measurements, in conjunction with electron paramagnetic resonance, Rutherford backscattering/channeling, and related techniques are used to determine the fundamental defect structures and materials properties required for radiation-hardened Si-based microelectronics. Recent studies have concentrated on amorphous silicon nitride, which is the charge storage medium for radiation-hard nonvolatile semiconductor memories; defects in SiO_2 and at the Si-SiO_2 interface, which markedly affect the radiation tolerance of MOS devices, and the formation of buried dielectric layers which may be essential for next generation radiation hard microelectronics. Relationships between the materials composition, chemical bonding, and defect configurations and the electrical performance are evaluated to permit long-term prediction of the performance of devices in a radiation environment and to develop new structures with particular properties.

Keywords: Microelectronics, Radiation Hardened, Silicon Nitride, Silicon, Silicon Dioxide, Defects

311. Surface Science FY 1989
$400,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
SNL Contact: T. A. Michalski, (505) 844-5829

Scanning tunneling microscopy, field ion microscopy, Auger electron spectroscopy, synchrotron and lab-based UV photoemission spectroscopy, and thermal desorption are being used to understand at an atomic level the early stages of epitaxy, oxidation and corrosion of metals and semiconductors, the nature of the adhesion of polymers to metals and how to improve it, and the formation of interface states and fine structures. Novel chemical vapor deposition techniques are being developed to explore formation of more uniform and reliable high temperature coatings.

Keywords: Surface Physics, Scanning Tunneling Microscopy, Field Ion Microscopy, Auger Electron Microscopy, UV Photoemission Spectroscopy, Oxidation, Corrosion, Adhesion

Laser and Chemical Physics Research Department, 1120

Materials processing science studies emphasizing chemical vapor deposition and plasma- and photo-enhanced chemical vapor deposition and etching are carried out. Emphasis is on microelectronic and optoelectronic materials and processing methods. Examples of ongoing studies include:

Materials Properties, Behavior, Characterization or Testing

312. Plasma Etching FY 1989
$500,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
SNL Contacts: K. E. Greenberg, (505) 844-1243 and P. J. Hargis, (505) 844-2821

Optical diagnostics are emphasized in fundamental studies of plasmas of the type widely used in the manufacture of large-scale and very-large-scale integrated electronic circuits to etch small features in semiconductors, dielectrics and conductors. Emphasis is placed on gaining improved understanding of the underlying physics and chemistry of technologically-important processes occurring both in the volume and on the surface. The goal of this study is the development of new process methods and methodologies that give improved pattern-transfer fidelity and less damage to the underlying material. A secondary goal is the development of process monitors that may lead to improved process reliability.

Keywords: Plasma Etching, Microelectronics

313. Plasma-Enhanced Chemical Vapor Deposition FY 1989
$100,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
SNL Contacts: K. E. Greenberg, (505) 844-1243 and P. J. Hargis, (505) 844-2821

Optical diagnostics are emphasized in fundamental studies of plasma-enhanced chemical vapor deposition, PECVD, of thin-film materials of the type that are used in the manufacture of microelectronic devices. Plasma-enhanced CVD offers advantages in comparison to thermal CVD in that high-quality materials can be deposited at lower temperatures. Lower-temperature processing offers latitude in device fabrication, especially as to how a particular fabrication step may affect the properties of materials that were defined in previous process steps. The goal of these studies is to develop processes that give higher quality materials having good adhesion to the underlying structure. A secondary goal is to develop *in situ* monitors for process control.

Keywords: Plasma Deposition, Microelectronics, Chemical Vapor Deposition

314. Laser-Controlled Etching and Deposition of Materials FY 1989
$250,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
SNL Contact: A. Wayne Johnson, (505) 844-8782

We are studying the underlying science and the technological limits of laser-controlled deposition and etching of conductors and insulators on microelectronic circuits. This technology is expected to find important applications for the correction of design errors in prototype circuits and for customization of large-scale integrated circuits.

Keywords: Laser Etching, Laser-Induced Chemistry, Microelectronics

315. Surface Chemistry of Organometallics for Compound Semiconductor Epitaxy

FY 1989
$300,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
SNL Contact: J. R. Creighton, (505) 844-3955

The motivation for this study stems from the extensive use of organometallic compounds ($Ga(CH_3)_3$, $Al(CH_3)_3$, etc.) as sources of elemental constituents for the growth of compound semiconductors by such techniques as metallorganic chemical-vapor deposition (MOCVC) chemical-beam epitaxy (CBE), and atomic layer epitaxy (ALE). Technology is leading science in these important compound semiconductor growth processes, and our lack of a detailed understanding of the underlying physics and chemistry, especially surface chemistry, is hindering advances necessary to produce future generations of optoelectronic materials and devices. Breakthroughs in understanding the underlying surface chemistry require a break from conventional methods of trial and error system optimization. Here we probe the primary chemical surface reactions to gain a scientific understanding of these technologically important systems. With the emergence of new understanding, higher quality materials should follow.

Keywords: Surface, Deposition, Epitaxial Growth, Chemical Vapor Deposition

316. Metallorganic Chemical Vapor Deposition

FY 1989
$520,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
SNL Contacts: K. P. Killeen, (505) 844-5164 and M. E. Coltrin, (505) 844-7843

The deposition of thin films of III-V compound semiconductor materials to produce scientifically tailored semiconductor structures is often done by thermal chemical vapor deposition using Group III organometallic compounds ($Ga(CH_3)_3$, $Al(CH_3)_3$, etc., and Group V hydrides (AsH_3, PH_3, etc.) or alkyls ($As(CH_3)_3$, $P(C_2H_5)_3$, etc.). The control of these technologically important processes to give quality material is an art with little scientific foundation. In this program we are applying comprehensive theoretical modelling of the fluid dynamics and both the volume and the surface chemistry, as well as an extensive array of *in situ* measurement tools to gain new insight into the underlying physics and chemistry of the process. The goal of this work is the development of processes and process-control procedures that yield higher quality materials and more abrupt heterointerfaces. Another objective of the work is to identify chemical precursors that are less toxic and otherwise more safe to handle.

Keywords: Chemical Vapor Deposition, Process Modelling, Thin Films

Compound Semiconductor and Device Research Department, 1140

Study and application of semiconductor strained-layer superlattices and heterojunction materials to explore solutions to new and existing semiconductor materials problems by coordination of semiconductor physics (theory and experiment) and materials science. This program investigates fundamental material properties including band structure, electronic transport, crystal stability, and linear and nonlinear optical properties. It also includes investigation of thin film high temperature superconductors for hybrid compound semiconductor/superconductor applications. The materials under study have a wide range of applications for high speed and microwave technology, optical detectors, lasers, and optical modulation and switching.

Materials Preparation, Synthesis, Deposition, Growth or Forming

317. Materials Growth by Molecular Beam Epitaxy (MBE) — FY 1989 $500,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
Sandia Contacts: L. R. Dawson, (505) 846-3451, T. M. Brennan, (505) 844-3233 and J. F. Klem, (505) 844-9102

Growth of AlGaAs/GaAs, InAsSb/InAl, InGaAs/GaAs and AlInAs/GaInAs strained layer superlattice (SLS) and strained quantum well (SQW) structures for electronic and optoelectronic applications. These structures are either uniformly doped for application in a typical electronic device or modulation doped for novel device structures, including high speed electronic devices, light emitting diodes and detectors.

Keywords: Semiconductor Device Fabrication, Strained Layer Superlattices, Strained Quantum Well

318. Materials Growth by MOCVD FY 1989
$400,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
Sandia Contact: R. M. Biefield, (505) 844-1556

Growth of GaP/GaAsP and InAsSb/InSb SLS's for high temperature radiation-hard electronic devices and for long wavelength IR detectors, respectively. Another major effort centers on the AlGaAs/GaAs and InGaAs/GaAs systems for detailed studies of the electrical and optical properties. This work has led to a variety of devices, including bistable optical switches, photon-hard photodetectors and high speed p-channel modulation doped FET's.

Keywords: Semiconductor Devices, Fabrication, Strained-Layer Superlattices, Radiation Hardened Semiconductors

319. Strained Layer Superlattices for IR Detectors FY 1989
$300,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
Sandia Contacts: S. R. Kurtz, (505) 844-5436 and L. R. Dawson, (505) 846-3451

Strained layer superlattices based on the InAsSb/InSb and InAsSb/InSb/AlSb systems are being investigated for use as attractive alternatives to the unstable HgCdTe alloys for IR detector applications in the 8-12 μm range. These IR materials are being grown by both MBE and MOCVD techniques and evaluated by electrical and optical techniques. Photovoltaic detectors with $D^* > 1 \times 10^{10}$ cm $\sqrt{HZ}/W$ at 10 μm and 77K and photoconductive detection to 15 μm have been demonstrated.

Keywords: Strained-Layer Superlattices, Infrared Detectors

320. Novel Processing Technology for Semiconductor Technologies FY 1989
$500,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
Sandia Contact: D. S. Ginley, (505) 844-8863.

This program involves studies of new technologies for formation of diffusion barriers for improved epitaxial growth, novel metallurgies for Shottky barrier and Ohmic contact formation, passivation layer development, and development of new metallurgical techniques for deposition of reactive alloys, and deposition and patterning of high temperature superconductors to interconnects on semiconductor devices.

Keywords: Semiconductor Devices

321. Thin Film Superconductors FY 1989
$300,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
Sandia Contact: D. S. Ginley, (505) 844-8863

Thin films of the high temperature superconductors in the Y-Ba-Cu-O and Tl-Ca-Ba-Cu-O systems are being prepared by MBE, E-beam evaporation and sputtering. Oriented and random films with T_cs to 112K are being produced. Strongly-linked polycrystalline films with critical currents approaching 1,000,000 A/cm^2 or 77K have been demonstrated. Patterning and contacting technology for the films for device applications is also being developed.

Keywords: Thin Films, High Temperature Superconductors, Coatings and Films

Condensed Matter Research Department, 1150

The mission of Department 1150 is to provide fundamental understanding and strong technology bases in novel materials and structures, surface physics and shock wave physics and chemistry. Both experimental and theoretical research are performed. Current areas of emphasis include high T_c superconductors, shock-induced solid state chemistry, disordered materials, high temperature semiconducting borides defects in semiconductors, surface desorption and ferroelectrics.

Materials Properties, Behavior, Characterization or Testing

322. Superconductivity FY 1989
$650,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
Sandia Contact: B. Morosin, (505) 844-8169

Transport, magnetic and structural measurements to access the fundamental factors which limit the performance of ceramic superconductors. Development of theoretical models of high temperature superconductivity. Development of new processing technologies for ceramic superconductors, in particular high pressure, high temperature oxygen treatments.

Keywords: Superconductivity, Ceramics

323. Shock Physics and Chemistry — FY 1989 $500,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
Sandia Contact: R. A. Graham, (505) 844-1931

Both organic and inorganic solids are being investigated to determine the influence of molecular structure on shock-induced bond scission, and the influence of line and point defects on the observed enhanced, shock-induced solid state reactivity. Shock-induced, highly exothermic chemical reactions are being investigated for potential applications. The influence of shock modification on the properties and synthesis of high T_c superconductors is being explored. Shock-activated thermal batteries are being studied to determine the mechanisms and materials parameters which influence electrical output. The work also provides insights about the nature of the shock process itself. A revolutionary time-resolved dynamic stress gauge using the piezoelectric polymer PVF_2 is being developed for laboratory, field testing and component diagnostics application. The mechanism for the operation of the gauge is being investigated.

Keywords: Organic Solids, Inorganic Solids, Molecular Structure, Shock, Chemical Reactions

324. Semiconductors — FY 1989 $600,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
Sandia Contacts: D. Emin, (505) 844-3431 and H. P. Hjalmarson, (505) 846-0355

Theoretical and experimental studies of electronic properties of boron carbide at high temperatures. Radiation-induced defects and their deep electronic levels in silicon and compound semiconductors and the role of these defects in device degradation. Physics of light-hole devices based on strained layer superlattices.

Keywords: Semiconductors, Boron Carbides, Defects, Deep Levels

325. Surface Science — FY 1989 $650,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
Sandia Contact: D. R. Jennison, (505) 844-5909

Detection and analysis of neutral atoms and molecules desorbed from surfaces. Theory of electronically stimulated desorption. Theory of surface electronic structure. Hydrogen in metals.

Keywords: Surface, Desorption, Predictive Modeling

326. Disordered Materials FY 1989
$600,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
Sandia Contact: G. A. Samara, (505) 844-6653

Application of polymeric synthesis routes to ceramic materials. Gas phase materials processing. Gelation in foam precursors and sol-gel glasses. Fundamentals of film formation. The physics and formation of microemulsions.

Keywords: Glass-Ceramics, Sol Gel Process, Thin Films, Microemulsions

Optoelectronics and Microsensor Research Department, 1160

The mission of Department 1160 is to provide Sandia National Laboratories with a comprehensive science and technology base in photonics and microsensor research. A fundamental understanding of the interaction of materials with both electromagnetic and mechanical forms of energy as well as their chemical environment are used to facilitate the design of new photonic and sensor devices. Activities include research into advanced materials and devices for: optical sources, modulators and detectors; information processing; and chemical sensing.

Materials Properties, Behavior, Characterization or Testing

327. New Concepts in Microsensors FY 1989
$750,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
SNL Contacts: R. C. Hughes, (505) 844-8172, A. J. Ricco, (505) 844-4907 and M. A. Butler, (505) 844-6897

New concepts in microsensors are being developed for a variety of stimuli, including radiation, magnetic fields, chemical species, and liquid-surface interactions using principles of semiconductor device operation and fabrication, surface acoustic wave propation, and optical properties of solids. Microsensors based on the properties of semiconductor surfaces include a radiation-sensing field-effect transistor (RADFET), which operates by the trapping of radiation-produced holes in the silicon dioxide gate dielectric of the FET, and chemical sensors which operate by inducing charged layers at the metal-silicon dioxide interface in response to the chemical species. Acoustic wave devices have been developed which offer new capabilities for detection and solid-liquid interface phenomena like viscosity, freezing, and low level chemical detection. Optically-based corrosion and energy impulse detectors based on the properties of new materials, like coated optical fibers, are being developed for high speed impulse detection and remote corrosive species detection. A miniature optical fiber micromirror chemical detector has been developed which can distinguish between water and common organic solvents which might be present in a contaminated toxic waste site.

Keywords: Microsensors, Microcircuitry

Organic and Electronic Materials Department, 1810

Department 1810 provides support to Sandia projects through selection, development, and characterization of organic and electronic materials and associated manufacturing processes. Responsibilities span exploratory development through design, production, and stockpile life. The Department provides the Laboratories with knowledge and engineering data on properties and reliability of organic and electronic materials pertinent to our unique applications and conducts in-depth studies in order to understand and improve these properties. Department 1810 investigates unique and innovative approaches to applying organic materials to problems of interest at Sandia.

Chemistry of Organic Materials Division, 1811

Division 1811 supports the Laboratories in the area of chemistry of organic materials. It is responsible for selecting, formulating, and characterizing polymer films and coatings, adhesives, and resins for casting and molding as well as developing or synthesizing new organic materials for unique and innovative applications. This division coordinates aging and compatibility studies throughout the Laboratories. To accomplish these goals, the Division carries out in-depth chemical investigations to characterize the reaction chemistry of these materials which influence their formulation, processing, or aging.

Materials Preparation, Synthesis, Deposition, Growth or Forming

328. Sulfonated Aromatic Polysulfones — FY 1989 $100,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
SNL Contacts: R. L. Clough, (505) 844-3492, C. Arnold, Jr., (505) 844-8728 and R. A. Assink, (505) 844-6372

Sulfonated alpha-methyl polystyrenes are being synthesized and evaluated as chemically-stable, thin-film, cation-permeable membranes which have a large cost advantage compared with fluorinated materials. Aging and resistivity tests are continuing. Sulfonation of other high-stability polymers including polyphenylene, as well as preparation of commercial microporous membrane materials with the new cation-permeable polymers is underway. This latter work is aimed at enhancing the efficiency of commercial membrane systems.

Keywords: Polymers, Coatings and Films, Batteries

329. Carbon Foams — FY 1989 — $150,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
SNL Contacts: R. L. Clough, (505) 844-3492 and A. P. Sylvester, (505) 844-8151

We are developing a new type of microporous carbon foam, based upon high-temperature carbonization of solvent-cast, phase-separated polyacrylonitrile (PAN) polymer foams. These materials have a variety of DOE-related applications including use as target pellets for pulse-power fusion experiments, and for porous battery electrodes.

Keywords: Carbon Foam

Materials Properties, Behavior, Characterization or Testing

330. Radiation Hardened Dielectrics — FY 1989 — $100,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
SNL Contacts: R. L. Clough, (505) 844-3492 and C. Arnold, Jr., (505) 844-8728

Polymer dielectrics are being developed that display a minimum radiation-induced conductivity (RIC). These materials will be used in capacitors and cables exposed to high dose rate radiation so that little charge is lost due to RIC in this environment. Mylar doped with an electron acceptor complex (TNF) has been shown to be a very effective rad-hard material. Studies on the aging behavior of this material are underway. A large production run on the material has been completed, and another is planned. Capacitors made from this material have been fabricated and successfully tested. A parametric study on processing conditions has been carried out, and this will lead to a formal production specification.

Keywords: Radiation Effects, Polymers, Weapons

331. Organic Nonlinear Optical Materials FY 1989
$125,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
SNL Contacts: R. L. Clough, (505) 844-3492, P. A. Cahill, (505) 844-5754, G. E. Pike, (505) 844-7562, and M. B. Sinclair, (505) 844-5506

Both second and third order organic nonlinear optical materials (dyes and polymers) are being synthesized for applications including electro-optic and photonic switching, frequency summation (through an anomalous-dispersion phase-matching process), and spatial light modulation. Some of the new materials exhibit nonlinearities an order of magnitude larger than other organic materials. Recently-initiated research on the fabrication of devices based on these materials is aimed at integrated optical devices on semiconductor substrates.

Keywords: Nonlinear, Optics, Optical, Organic, Waveguides

Physical Chemistry and Mechanical Properties of Polymers Division, 1812

Division 1812 develops new organic materials, structurally and chemically characterizes organic materials, and studies their mechanical properties. It is responsible for characterizing the molecular, electronic, and microphase structure of organic materials and their chemical reactivity toward the use environment as well as formulation of organic composites and adhesives.

Materials Preparation, Synthesis, Deposition, Growth or Forming

332. Chemistry of Plasma Etching and Deposition Processes FY 1989
$130,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
SNL Contacts: C. L. Renschler, (505) 844-0324 and R. J. Buss, (505) 844-7494

The chemistry of glow discharge plasmas, used in a wide range of materials processing applications, is being studied with molecular beam and laser techniques. In microelectronic fabrication, the feature morphology is directly related to the detailed etch mechanism of the plasma for different materials. The interactions of plasma-generated radicals with electronic materials are being investigated to identify the significant chemistry leading to etch selectivity. Also being studied are plasma cleaning and chemical modification processes with are used extensively in weapons-component manufacture. The complex plasma chemistry determines the conditions under which the required cleaning as opposed to undesirable deposition will occur. Molecular beam and laser probing techniques are being used to identify the reactive species and their chemistry and thereby optimize the plasma processing and develop new applications. The same methods are being used to determine the important depositing species in the plasmas used to produce solar cell materials and thin carbon/hydrogen ("diamond-like") films.

Keywords: Plasma Etching, Plasma Deposition

Materials Structure and Composition

333. Materials Structure, Dynamics, and Property Studies by Multinuclear Pulsed NMR Spectroscopy — FY 1989 $75,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
SNL Contacts: C. L. Renschler, (505) 844-0324 and R. A. Assink, (505) 844-6392

Multinuclear nuclear magnetic resonance spectroscopy of liquid and solid samples is being applied to several materials related problems. The ^{13}C and ^{1}H spectroscopy of liquids was used to determine the molecular weight and stereochemistry of precursors used in the preparation of encapsulants and foams. The chemical structures of newly synthesized explosives were also analyzed. Both liquid and solid state spectroscopy are being applied to the study of degradation pathways and products in organic materials. Imaging techniques have been used to characterize liquid foams and will be adapted to solid foams.

Keywords: Polymers, Organics, Coatings, Coatings and Films

334. Mechanistic and Kinetic Studies of Polymer Aging — FY 1989 $250,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
SNL Contacts: C. L. Renschler, (505) 844-0324, K. T. Gillen, (505) 844-7494 and R. L. Clough, (505) 844-3492

Polymer aging under a variety of environmental stresses (e.g., thermal, radiation), is critically important in a wide range of applications. The understanding of dose rate effects is particularly important to the formulation of a predictive capability for radiation aging situations. We have developed several experimental techniques, including density and modulus profiling, to monitor the depth-dependent aging of thin polymer samples. The data obtained from these experiments have then been used to validate kinetic theory which we developed to predict oxidative aging effects in a quantitative way.

Keywords: Polymer Aging, Profiling, Kinetics

335. Theory of Polymer Dynamics FY 1989
$100,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
SNL Contacts: J. M. Zeigler, (505) 844-0324

A number of constructs, most notably reputation and modified reputation theories (e.g., tube renewal, constraint release) have been developed in an attempt to explain the dynamics of polymer liquids (blends, melts). These theories generally begin with assumptions which are plausible, but somewhat arbitrary. More troublesome is the fact that predictions arising from these theories are often not borne out by experiment. We are developing a model of the dynamics of polymer, liquids based on microscopic statistical mechanics. This model calculates structure-property relationships from first principles with no adjustable parameters and no a priori assumptions about liquid structure or mode of motion. We anticipate eventual extension of the theory to glasses.

Keywords: Polymer Liquids, Dynamics

Physical Properties of Polymers Division, 1813

Division 1813 provides support to Sandia projects through selection, development, and processing of foams, elastomers, encapsulants, and molding compounds. It is responsible for characterizing the physical properties and aging behavior of these materials. This Division also carries out in-depth physical property studies when necessary in order to understand or improve these properties.

Materials Preparation, Synthesis, Deposition, Growth or Forming

336. Microporous Foam Development FY 1989
$157,500

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
SNL Contacts: J. G. Curro, (505) 844-3963, J. H. Aubert, (505) 844-3305 and P. B. Rand, (505) 844-7953

We are developing new polymer and carbon foams which have both low density and very small cell sizes (0.1 to 10 microns). The process utilizes thermally induced phase separation followed by solvent removal steps such as extraction or freeze-drying. It has been applied to many polymers such as polystyrene, polyethylene, and polyacrylonitrile (PAN). PAN foams have many potential applications.

Keywords: Foams, Microcellular, Phase Separation, Carbon

337. Development of Removable Encapsulants FY 1989
$157,500

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
SNL Contacts: J. G. Curro, (505) 844-3963, D. B. Adolf, (505) 844-4773 and P. B. Rand, (505) 844-7953

In order to allow the "rework" of expensive electronic components, a removable encapsulant is being developed. This new concept for a removable encapsulant involves coating glass microballoons with a thin layer of a thermoplastic polymer. A blowing agent, such as pentane or a chlorofluorocarbon, is then absorbed into the polymer coating. The coated beads, with the blowing agent, are a free flowing powder which can be poured into an electronic assembly. After filling, the component is heated to a temperature above the glass transition temperature of the polymer. As the polymer softens and foams, the microspheres are fused together to form a syntactic foam. The resultant syntactic foam has good compressive strength, high modulus, and a low coefficient of thermal expansion thus making an excellent encapsulant. Removal of the encapsulant for rework is easily achieved by solvent treatment. Processes are currently being developed to encapsulate large complex electronic assemblies with this material.

Keywords: Polymers, Foam, Encapsulants

Materials Properties, Behavior, Characterization or Testing

338. Mechanical Properties of Encapsulants FY 1989
$21,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
SNL Contact: J. G. Curro, (505) 844-3963 and D. B. Adolf, (505) 844-4773

Accurate thermophysical properties are essential as input to computer codes designed to calculate stress levels in electronic components. To date, we have measured those linear elastic properties (coefficient of thermal expansion, bulk modulus, and shear modulus) as functions of temperature that lead to stresses upon thermal cycling for common polymeric encapsulants used at Sandia. Future studies will focus on the ultimate properties of these materials for use in determining failure criteria in the computer codes.

Keywords: Polymeric Encapsulants, Organic, Tests, Bulk Modulus

339. Deformation of Kevlar Fabrics FY 1989
$73,500

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
SNL Contacts: J. G. Curro, (505) 844-3963 and W. E. Warren, (505) 844-4445

The effects of weave geometry and the size, spacing and elastic properties of individual Kevlar yarns on the effective elastic response of woven Kevlar fabrics are being investigated both experimentally and theoretically. The results are important for understanding the effects of fabric structure on mechanical response. They will improve our ability to design high performance fabrics such as those required for new parachute applications.

Keywords: Fibers, Polymers, Fracture, Creep, Parachutes

340. Moisture Permeation in Encapsulants, Adhesives and Seals FY 1989
$50,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
SNL Contacts: J. G. Curro, (505) 844-3963 and P. F. Green, (505) 844-2466

Polymeric materials are used as encapsulants, seals and adhesives in hundreds of weapon components. The long term reliability of weapon components depend on knowledge of the moisture permeation characteristics of these polymeric materials. Data concerning water permeation in such materials is unavailable in most cases. This program is being initiated to study the moisture permeation characteristics of some of the more commonly used polymeric encapsulating, sealant and adhesive materials.

Keywords: Polymers, Encapsulants, Adhesives, Seals, Moisture, Permeation

Electronic Property Materials Division, 1815

Division 1815 provides support to Sandia programs through selection, development, and characterization of electronic materials. Responsibilities span exploratory development through design, production, and stockpiling. The Division also performs in-depth studies in order to understand material properties and associated electronic phenomena. Areas of activity include electronic materials, dielectrics, and optical materials.

Materials Properties, Behavior, Characterization or Testing

341. Nonlinear Optical Materials — FY 1989 — $100,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
SNL Contacts: G. E. Pike, (505) 844-7562 and M. L. Sinclair, (505) 844-5506

Measurements of the second and third order hyperpolarizabilities of organic molecules and polymers are being made. New techniques using attenuated total reflection by either waveguide coupling or surface plasmon creation are being developed to make these measurements.

Keywords: Nonlinear Optical, Organic

342. Hydrogen Effects in Silicon — FY 1989 — $100,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
SNL Contacts: G. E. Pike, (505) 855-7562 and R. A. Anderson, (505) 844-7676

Measurements have been made of hydrogen diffusion through metal contacts into boron doped silicon. The hydrogen is found to bond to the boron and phosphorous as a complex and passivate them as dopants. This strongly affects the formation of Schottky barriers in this type of silicon, and is sometimes an accidental side effect of low temperature processing in a hydrogen ambient.

Keywords: Silicon, Boron Doping, Hydrogen Complexes, Phosphorous Doping

343. Rapid Thermal Processing of Gate Oxides — FY 1989 — $100,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
SNL Contacts: G. E. Pike, (505) 844-7562 and W. K. Schubert, (505) 846-6548

High quality thin SiO_2 layers are required for new generations of microelectronics. Silicon has been oxidized to a thickness of 20 nm and characterized for various electrical properties. The effect of X-rays in producing radiation defects is tested using capacitance-voltage techniques. The dielectric breakdown strength is tested using Fowler-Nordheim current measurements.

Keywords: Rapid Thermal Oxidation, Silicon, Radiation Hardness

Materials Characterization Department, 1820

Department 1820 performs chemical, and physical analyses of materials in support of weapons and energy programs throughout the Laboratories. The department also has the responsibility for the development of advanced analytical techniques to meet existing or anticipated needs. Consulting and process reviews are other important functions of the department.

Analytical Chemistry Division, 1821

The Analytical Chemistry Division, 1821, is responsible for performing chemical analyses in support of weapon and energy programs at Sandia. The division is equipped to analyze a variety of samples such as gases, polymers, liquids, solutions, solids, organics, inorganics, glasses, alloys, ceramics, and geological materials. Analyses are performed by a variety of techniques using absorption and emission spectroscopy, gas chromatography, gas chromatography/mass spectrometry, ion chromatography, neutron activation analysis, electrochemistry, combustion, and classical methods of chemical analysis.

Instrumentation and Facilities

344. Development of Automated Methods for Chemical Analysis — FY 1989 $250,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
SNL Contact: S. H. Weissman, (505) 846-0820/FTS 846-0820

New automated methods for chemical analysis of materials are being developed to meet new or anticipated needs and to improve accuracy, precision and efficiency of analyses. A new gas chromatography system has recently been installed and will be used for quantitative Fourier transform mass spectrometer support of a variety of applied and basic research programs, such as development of materials for energy resource with an ion trap detector photovoltaic materials, geo energy process research, and development of materials to be used for fusion energy. A computerized data base is being developed to better manage data and use chemical standard reference materials in a variety of analytical procedures. New atomic spectroscopic and ion chromatographic procedures are being developed to analyze aerosols generated in simulated nuclear reactor accidents and in analysis of glass and electrolytes being developed for use in new batteries.

Keywords: Instrumentation and/or Technique Development, Atomic Spectroscopy, Ion Chromatography, Mass Spectrometry, Analytical Chemistry

Electron Optics and X-ray Analysis Division, 1822

The Electron Optics and X-ray Analysis Division 1822 characterizes the microstructures of engineering materials and develops a basis for understanding processing microstructure property relationships in a wide range of materials including metals, ceramics, and semiconductor materials. The analytical techniques used include light microscopy, scanning electron microscopy, electron probe microanalysis, analytical electron microscopy, and X-ray diffraction. Methods are also developed for extending microstructural characterization capabilities, and for applying image analysis techniques to the characterization for microstructural features.

Materials Preparation, Synthesis, Deposition, Growth or Forming

345. Thermomechanical Treatment of U Alloys — FY 1989 $40,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
SNL Contact: K. H. Eckelmeyer, (505) 844-7775/FTS 234-7775

Strengthening mechanisms were investigated in U-Ti alloys with the goals of simplifying processing procedures and increasing strength-ductility combinations. Past work has shown that remarkable improvements can be obtained by employing thermomechanical processing rather than aging as a strengthening approach. More recently it has been shown that thermomechanical processing results in substantial tensile-compressive anisotropy. Current work is concentrating on applying these principles to realistic engineering geometries and processing conditions.

Keywords: Uranium Alloys, Strengthening Mechanisms, Thermomechanical Processing

Instrumentation and Facilities

346. Advanced Methods for Electron Optical, X-ray, and Image Analysis — FY 1989 $200,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
SNL Contact: W. F. Chambers, (505) 844-6163/FTS 234-6163

Advanced methods of automated electron and X-ray instrumental analysis are being developed to improve resolution, accuracy, and efficiency and to allow us to undertake and solve more difficult problems. The microstructural image analysis system includes image analyzers connected to a copy stand, a light microscope, scanning an electron microprobe, and an analytical electron microscope as well as a central file server and image storage facility. The emphasis during the past year has been on the development of improved methods for incorporating chemical information into particle characterization and sorting routines. Current projects include the development of quantitative imaging techniques for the electron microprobe and of particulate screening techniques for analytical electron microscope.

Keywords: Automation, Electron Optics, Transmission Electron Microscopy, Instrumentation and Technique Development

Surface Chemistry and Analyses Division, 1823

The Surface Chemistry and Analyses Division 1823 provides analytical surface and optical analyses of materials in support of Sandia programs throughout the Laboratories. In addition, staff members in the division engage in advanced materials research and in research funded by specific weapons or energy programs which can be uniquely investigated using their expertise. Specific techniques employed within the division include Auger spectroscopy, x-ray photoelectron spectroscopy, low energy ion scattering and secondary ion mass spectroscopies, energetic ion analysis methods, fluorescence and Raman spectroscopies, dispersive and Fourier transform infrared spectroscopies.

Instrumentation and Facilities

347. Advanced Methods for Surface and Optical Analysis — FY 1989 $500,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
SNL Contact: J. A. Borders, (505) 844-8855/FTS 234-8855

State-of-the-art facilities, methods and data analysis techniques for surface and optical materials characterization are being developed. An ion microscope is being added, primarily to support semiconductor materials development and processing. Chemometric statistical data correlation methods have been developed for infrared spectroscopy and are now being extended to Auger electron spectroscopy, ion mobility spectrometry and Raman spectroscopy. These materials can enable the prediction of physical properties from spectroscopic data.

Keywords: Ion Microscope, Chemometric Data Correlation Methods, Infrared Spectroscopy, Auger Electron Spectroscopy, Ion Mobility Spectrometry, Raman Spectroscopy

Metallurgy Department, 1830

Department 1830 selects, develops, and characterizes the non-electronic behavior of all metals and processes that may be needed to meet systems and components requirements. Responsibilities span exploratory development through design, production, and stockpile life. If either current or anticipated demands cannot be met by commercially-available metals and processes, Department 1830 is responsible for the necessary development. Understanding mechanisms of alloy bulk and surface behavior provides the basis for alloy and process development and increases the confidence of predictions of behavior. Surface treatment and coating processes receive special emphasis because of the close coupling of the surface and "bulk" behavior.

Physical Metallurgy Division, 1831

The Physical Metallurgy Division selects, develops and characterizes the physical behavior of all metals that may be needed to meet systems and components requirements. This includes the selection and development of alloys to insure a sufficiently long service life while maintaining fabricability. Responsibilities span exploratory development through design, production and stockpile life. If commercial technology does not meet engineering requirements, Division 1831, working with the other divisions in Department 1830, will develop the required technology. Understanding the relationship between alloy processing, alloy microstructure and alloy behavior is the basis for alloy selection and development and provides the input required to predict, via thermodynamic and kinetic modeling, the physical behavior of the alloy through its service life. The objective of Division 1831 is, therefore, to use this understanding to extend the capabilities of the design engineers and to increase confidence in alloy performance.

Materials Properties, Behavior, Characterization or Testing

348. Analytical Electron Microscopy of Engineering Materials — FY 1989 $50,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
SNL Contacts: A. D. Romig, (505) 844-8358, M. J. Carr, (505) 846-1405 and T. J. Headley (505) 844-4787

The capability to establish chemical concentrations at high spatial resolutions quantitatively has progressed very significantly in recent years. Through proper experimental techniques and the appropriate mathematical manipulation (with Monte Carlo simulations of electron trajectories in solids) of the experimental data, the capability to measure segregation to grain boundaries, stacking faults and dislocations quantitatively has been developed. These techniques are being applies to a variety of materials including Fe-Ni based and Ni-based superalloys, intermetallic compound alloys, IC metallizations and Si used for microelectronic applications.

Keywords: Electron Microscopy, Microstructure

349. Segregation Behavior During Solidification of Alloys — FY 1989 — $100,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
SNL Contacts: C. V. Robino, (505) 844-6557, A. D. Romig, (505) 844-8358 and M. J. Cieslak, (505) 846-7500

Alloying element segregation is an important consequence in the solidification of welds in many engineering materials. Under certain conditions, selected elements may form minor low melting point constituents which remain the last liquid to solidify. Under the stresses generated during cooling, the material may crack (called hot-cracking) in the region containing these low melting point constituents. To understand this behavior, the distribution of elements following solidification must be known quantitatively. The current program is solving the solidification problem more rigorously than has been done in the past. Diffusion in the solid, solidification in multicomponent system and for non-planar front solidification are being treated.

Keywords: Solidification, Alloys, Diffusion

350. Solid State Reactions Between Metal Substrates and Solders — FY 1989 — $150,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
SNL Contacts: A. D. Romig, (505) 844-8358, J. J. Stephens, (505) 846-9962, M. M. Karnowsky, (505) 844-4134 and G. C. Nelson, (505) 844-5200

Reactions between fusible alloy solders, based on Pb, Sn, In, etc., and metallic substrates such as Au and Cu can occur at room temperature. The most common manifestation of these reactions is the formation of intermetallic compounds. These compounds alter the mechanical and electrical performance of the solder joint, often degrading performance and reliability. In an integrated experimental and diffusion modeling program, a variety of important systems are being examined. The experimental efforts are aimed at determining the stability of the intermediate phases as a function of temperature and at determining the rates at which they form. Both bulk alloy and thin film substrates are under study. The modeling efforts are directed at determining reaction constants and activation energies and at using the results to model joint behavior through a variety of potential thermal cycles. Systems currently under study include Au/Pb-In, Au-Pd/Pb-In, Cu/Pb-Sn, Cu/Pb-In, and Pd/Pb-In.

Keywords: Solder, Intermetallic Compounds

351. Fluxless Soldering FY 1989
$75,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
SNL Contacts: F. M. Hosking, (505) 844-4925, C. V. Robino, (505) 844-6557, and D. R. Frear, (505) 846-4713

Fluxes promote wetting when soldering, but present potential long term reliability problems with respect to the potential for corrosion if their residues are not removed. Reducing gasses, such as molecular hydrogen or formic acid, are sometimes used to circumvent fluxing. Thermodynamic modeling suggests that atomic and/or ionic hydrogen should be more effective. In this study, the feasibility of using nonmolecular hydrogen and other atmospheres to reduce surface oxides and enhance wetting is being examined. The goal of this work is to find a reactive gas and specific processing conditions which produce solder joints which are comparable to those produced using rosin based fluxes, but are not environmentally hazardous either alone or with subsequent cleaning operations.

Keywords: Solder, Flux, Modeling

352. Stress Voiding of Aluminum Interconnect Lines FY 1989
$100,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
SNL Contacts: A. D. Romig, (505) 844-8358, F. G. Yost, (505) 846-5446 and J. A. Van Den Avyle, (505) 844-1016

Current generation and near-future generation integrated circuits use aluminum interconnect lines. With times, stress driven diffusion can cause the lines to open and the circuit to fail. During manufacturing, large tensile stress and stress gradients are generated in the Al. These stresses are generated by a thermal expansion mismatch between the Al line and the glass passivation layer which is deposited by CVD at 450°C. The stress gradients generate a chemical potential gradient which drives mass transport causing the lines to void. A diffusion model has been developed which predicts the rate of void formation as a function of stress. Current efforts are addressing the measurement of the stress as a guide to assessing product reliability and the development of a suitable accelerated aging test.

Keywords: Integrated Circuits, Interconnections

353. Grain Boundary Segregation in Al-Cu Metallization Interconnect Lines

FY 1989
$50,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
SNL Contacts: A. D. Romig, (505) 844-8358, D. R. Frear, (505) 846-4713 and C. R. Hills, (505) 844-4787

Cu is added to Al interconnect lines to improve the resistance to failure by electromigration. The need to develop electromigration resistant metallizations is becoming more critical as current densities increase concomitant with decreases in line dimensions. Despite the evidence that Cu improves resistance to electromigration voiding, the mechanism by which this benefit is obtained is unknown, although one current popular theory suggests that the grain boundaries are coated with a few monolayers of Cu. Current efforts are directed at understanding the microstructural role of Cu. The program is multifaceted in that the problem is being addressed experimentally (analytical electron microscopy, high resolution electron microscopy) and by thermodynamic and kinetic modeling. Initial results have shown that the grain boundaries are free of Cu, except for the formation of $CuAl_2$ precipitates. Work is progress is studying the time-temperature dependent evolution of these microstructures in detail, especially with respect to the distribution of C.

Keywords: Electromigration, Grain Boundary

Mechanical Metallurgy Division, 1832

The mission of the Mechanical Metallurgy Division 1832 is to provide the characterization and understanding of the mechanical and corrosion properties of metals and alloys. This includes the selection of alloys and the conduct of research in alloy design and thermomechanical effects on material behavior. Sophisticated mechanical and corrosion testing capabilities are part of this division, and extensive use is made of the analytical capabilities at Sandia.

Materials Properties, Behavior, Characterization or Testing

354. Micromechanical Testing — FY 1989 $100,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
SNL Contacts: W. B. Jones, (505) 845-8301 and R. J. Boucier, (505) 844-6638

The structural response of very fine scale features is of growing concern in microelectronics. The mechanical response of thin layers of aluminum on silicon, of glass on silicon, of tungsten on silicon, and many others must be measured in order to proceed with future design refinements. We are developing techniques for conducting tensile and creep tests on structures which have dimensions in the range of a few micrometers. Constitutive models will be developed which describe the time independent inelastic and the time dependent creep and relaxation response of these very fine structures.

Keywords: Mechanical Properties, Micromechanical Testing

355. Toughness of Ductile Alloys — FY 1989 $330,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
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The elastic-plastic fracture toughness (J_{Ic}) has the potential to allow a fracture-related material property to be used in the design of structures using ductile alloys. For this to come about, valid testing procedures need to be developed and candidate materials need to be studied. Single-specimen J-testing procedures are being studied and the fracture behavior of ductile cast irons is being examined. The goal of the current work is to have the fracture behavior of this alloy well enough characterized and understood that nuclear material shipping casks can be designed with it using a fracture toughness methodology.

Keywords: Metals: Ferrous, Fracture, Predictive Behavior Modeling

356. Low Melting Point Alloy Studies FY 1989
$200,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
SNL Contacts: W. B. Jones, (505) 845-8301 and D. R. Frear, (505) 846-4713

Solder alloys operate in service conditions at temperatures ranging from 0.5 to 0.8 of their absolute melting points. Failure of solder joints under conditions of cooldown from processing temperatures or thermal fatigue is an important concern in the reliability of electronic components. Our studies include the examination of various alloys under conditions of isothermal mechanical fatigue and thermomechanical fatigue. We have found that microstructural instability plays a large role in strain localization during thermomechanical fatigue. Mechanisms for this behavior are being developed with the goal of developing fatigue design methodologies which could be used in solder joint design.

Keywords: Solder Alloys, Thermomechanical Fatigue

Process Metallurgy Division, 1833

The Process Metallurgy Division supports the Laboratories by selecting, characterizing, and developing metallurgical processes needed in the manufacture of components and systems. The objective is to provide process definition and control by understanding the mechanisms which operate. Attention is devoted toward structure-property modifications that occur during manufacturing processes. Principal processes currently under study include laser welding, arc welding (GTA and plasma), brazing, soldering, vacuum induction melting, vacuum arc remelting, and investment casting.

Materials Preparation, Synthesis, Deposition, Growth or Forming

357. Vacuum Arc Remelting FY 1989
$300,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
SNL Contact: F. J. Zanner, (505) 844-7073

Arc plasmas during vacuum arc remelting are being studied with the goal of reducing inhomogeneities and defects in structural alloys and uranium alloys. Improvements in the control of melting and solidification are being incorporated into production processes to increase production yields and improve the ingot quality. This work involves experimental verification of models. Currently the heat energy balance in the plasma arc is being evaluated on the basis of boundary temperatures. Spectrographic studies to characterize the plasma are determining the importance of alloy chemicals.

Keywords: Metals: Ferrous and Non-Ferrous, Conventional Solidification

Device or Component Fabrication, Behavior or Testing

358. Electronbeam Melting FY 1989 $200,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
SNL Contact: F. J. Zanner, (505) 844-7073

A program to study the control of melting and solidification during electron beam melting has been initiated. A research electron beam system that includes two differentially pumped 30 kV electron guns has been completed. A special capability of the system is the rapid raster of both beams so as to affect spatial and temporal control of the heat flux. Raster rates are orders of magnitude faster than diffusion rates within the melt pool, which permits control of melting and solidification. Studies are directed toward the recycling of uranium alloy scrap.

Keywords: Electronbeam Melting, Electron Guns

359. Electroslag Remelting FY 1989 $300,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
SNL Contact: M. C. Maquire, (505) 844-4925

A study directed at the control of the electroslag remelting process has been initiated. An experimental electroslag melting system has been established that is capable of producing 1000 pound steel ingots. This process is used to refine the ingot microstructure and eliminate impurities via electrochemical reactions with the slag. Impedance measurements of the melting current have been made on both the experimental system as well as industrial systems. The goal is to develop a control methodology that will result in uniform optimum properties throughout the length of the ingot.

Keywords: Electrical Melting, Microstructure

360. Welding of Nickel-Based Alloys FY 1989 $250,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
SNL Contacts: M. J. Cieslak, (505) 846-7500 and G. A. Knorovsky, (505) 844-1109

The combination of advanced design requirements and recent progress in glass-to-metal sealing technology has stimulated a program to obtain higher-strength hermetic seals than is afforded by conventional austenitic stainless steel-borosilicate glasses. Both solid-solution strengthened and precipitation strengthened nickel-based alloys are being considered as replacements for stainless steel. Studies have been initiated to identify the constituents responsible for hot-cracking in these classes of alloys. Initial results indicate that solidification in these alloys generally terminates with the formation of one or more topologically close-packed phases. Fundamental alloy studies remain to be completed for both Inconel 625 and Inconel 718 to determine the roles of minor alloying components. Commercialization of modified Inconel 625 chemistries is in progress.

Keywords: Metals: Non-Ferrous, Joining and Welding, Conventional Solidification

361. Plasma Arc Welding — FY 1989 $100,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
SNL Contacts: P. W. Fuerschbach, (505) 846-2464 and J. L. Jellison, (505) 844-6397

Few fusion welding processes are suitable for joining aluminum alloys in the vicinity of heat-sensitive components. Initial experiments suggest that plasma-arc welding can markedly reduce heat input compared to conventional gas tungsten arc welding. A variable-polarity plasma-arc welding power supply has been developed. Studies evaluating cathodic cleaning, welding efficiency, and arc stability as a function of the current-voltage characteristics are in progress.

Keywords: Metals: Non-Ferrous, Joining and Welding, Conventional Solidification

362. Laser Welding — FY 1989 $50,000

DOE Contact: A. E. Evans, (301) 353-3098 /FTS 233-3098
SNL Contact: J. L. Jellison, (505) 844-6397

Pulsed Nd:YAG laser welding is a complex process both in terms of the number of control parameters and materials-process interactions. To improve the understanding of the process with the ultimate goal of developing weld schedules on the basis of process modeling, process characterization studies are being conducted. These include calorimetry experiments, plume characterization studies, and experimental validation of heat-transfer codes. Current studies are directed towards determining the roles of surface-driven convection and refraction of the beam by the plume.

Keywords: Lasers, Joining and Welding, Process Modeling

363. Development of Materials for Magnetic Fusion Reactors — FY 1989 $200,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
SNL Contact: M. F. Smith, (505) 846-4270

Materials used in magnetically confined fusion energy devices experience severe environments. Two materials have been developed for these applications. A low-pressure chamber plasma spray process has been successfully developed to deposit ceramic/metal (SiC/Al) coatings. The ceramic/metal coatings may be used for low atomic number, low activation armor coating for first wall surfaces or for a graded thermal expansion transition coating to accommodate large thermal expansion differences. Tests to evaluate these materials are continuing.

Keywords: Magnetic Fusion, Coatings and Films, Ceramics, Plasma Synthesis

Surface and Interface Technology Division, 1834

The Surface Metallurgy Division 1834 is concerned with the influence of surface and near-surface regions on the engineering application of materials. Basic and applied research is conducted to understand and control deposition processes for reproducible surface modification and to correlate surface properties (composition, structure, and stress) with friction, wear, and electrical contact resistance. Controlled deposition of amorphous materials by sputtering, reactive ion beam deposition of compound films, low-pressure plasma spraying, and surface modification by ion implantation are techniques used to tailor surface properties. This division also supports design and component groups in areas where surface properties are critical.

Materials Preparation, Synthesis, Deposition, Growth or Forming

364. Development of Hard, Wear-Resistant Coatings for Mechanical Applications

FY 1989
$80,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
SNL Contact: J. K. G. Panitz, (505) 844-8604

Currently, we are beginning a study of the friction and wear properties of carbon coatings which are sputter deposited (1) with and without a dopant, (2) in varying mixtures of hydrogen and methane, (3) with and without atomic hydrogen provided by an incandescent tungsten filament supplementing and atomic hydrogen present in the glow discharge, (4) at different substrate temperatures, and (5) with different levels of ion bombardment during deposition. Here the objective will be to deposit hard diamond-like or diamond coatings with low coefficients of friction without the high levels of residual stress and poor adhesion that are typically characteristic of the diamond coatings currently produced by chemical vapor deposition. A hybrid TVD/CVD apparatus for depositing these coatings has been constructed.

Keywords: Carbon Coatings, Erosion/Wear/Tribology

Materials Properties, Behavior, Characterization or Testing

365. Modification of Mechanical Properties by Ion Implantation FY 1989 $40,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
SNL Contacts: L. E. Pope, (505) 844-5041; D. M. Follstaedt, (505) 844-2102; S. T. Picraux, (505) 844-7681 and J. A. Knapp, (505) 844-2305

Stainless steel parts which undergo relative motion can have large coefficients of friction and can experience severe wear, specifically galling. The dual implantation of titanium and carbon into stainless steels produces an amorphous film on the surface which decreases both the friction coefficient and the wear rate; the implantation process is effective for stainless steels and permits self-mating wear couples, 304 rubbing on 304 stainless steel, for example. Though amorphous films can be produced with titanium or carbon alone, superior performance occurs if both titanium and carbon are incorporated. Oxygen is needed in the ambient for best performance.

Keywords: Ion Implantation, Coatings and Films, Erosion/Wear/Tribology, Structure, Surface

366. Corrosion Predictions FY 1989 $100,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
SNL Contact: N. F. Sorenson, (505) 846-6024

Acoustic plate mode sensors are being developed to allow for the measurement of small amounts of metallic corrosion. These data will be used to generate determine rate coefficients for corrosion reaction in non-accelerated experiments, allowing for realistic corrosion lifetime predictions.

Keywords: Corrosion, Prediction, Sensors

367. Solvent Substitutive Program FY 1989 $50,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
SNL Contact: M. C. Oborny, (505) 844-1038

A program to evaluate alternative solvents to halogenerated solvents for use in cleaning and coating processes has begun. Long term materials compatibility issues are being addressed.

Keywords: Solvents, Halogenerated

Device or Component Fabrication, Behavior or Testing

368. Process Control Ultrasonic Cleaning of Delicate Parts

FY 1989
$70,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
SNL Contact: M. C. Oborny, (505) 844-1038

Ultrasonic cavitation has long been used to improve the effectiveness of solvent cleaning. It is especially effective in the cleaning of small parts with complex geometries. However, ultrasonic cleaning can cause surface damage and fatigue failures in some materials and parts. A new generation of ultrasonic cleaner claims to avoid these problems by operating in a swept frequency mode and also controlling the energy injection rate into the cleaning solution by the control of five physical parameters associated with the ultrasonic bath. This process control ultrasonic system has been purchased and is now undergoing characterization studies. Future studies will focus on the use of this system for the cleaning of delicate parts such as ceramics and ferrites. Correlations will be made between cleaning effectiveness, material damage and the ultrasonic bath process parameters.

Keywords: Ceramics, Erosion/Wear/Tribology, Fracture, Weapons

369. Plasma Oxidation and Reduction Studies

FY 1989
$80,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
SNL Contact: E. P. Lopez, (505) 846-8979

Plasma treatments employing both oxidizing and reducing atmospheres are being studied using a Branson Barrel Etcher. The removal of organic contamination using an oxygen plasma is a well known phenomenon. However, surface oxidation is of concern since it could create wetting problems in subsequent soldering operations. Preliminary results indicate that a reducing atmosphere will restore an oxidized surface. Future studies will include temperature profiling of the plasma barrel etcher utilizing a Luxtron Temperature Probe.

Keywords: Surface, Joining and Welding, Plasma Synthesis, Metals

Instrumentation and Facilities

370. Ion Beam Reactive Deposition System FY 1989 $50,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
SNL Contact: D. E. Peebles, (505) 844-1647

The properties of deposited films may vary with stoichiometry, substrate temperature, system pressure and ionization state and acceleration. A system has been in use to study these effects on film deposition by controlled use of atom/molecule/ion beams. The system has now been modified to allow studies of films deposited at much higher current densities and substrate temperatures, and to study the deposition of multi-element films. These films (TiN and TiAlN at the present) are being evaluated for tribological performance.

Keywords: Coatings and Films, Erosion/Wear/Tribology, Surface

371. Deposition and Evaluation of Titanium Nitride Films FY 1989 $50,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
SNL Contacts: D. E. Peebles, (505) 844-1647 and L. E. Pope, (505) 844-5041

Titanium nitride films have proven useful as tribological coatings for increased hardness and wear resistance in a variety of applications. However, films properties, structure, and wear behavior have been shown to be highly dependent on substrate properties and deposition parameters. Films have been deposited by controlled low temperature reactive evaporation in an ultrahigh vacuum system. Effects of parameters such as substrate material, deposition temperature, deposition pressure, ionization, contamination, stoichiometry and film thickness have been evaluated in terms of film microstructure, adhesion and wear behavior. In addition, commercially prepared films on identical substrates have been evaluated in parallel. Future work will involve continued investigation of deposition parameter effects and the extension to titanium aluminum nitride films.

Keywords: Titanium Nitride, Coatings and Films, Erosion/Wear/Tribology, Structure, Surface

372. *In Situ* Friction, Wear, and Electrical Contact Resistance Systems FY 1989 $40,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
SNL Contacts: L. E. Pope, (505) 844-5041 and D. E. Peebles, (505) 844-1647

Friction, wear, and electrical contact resistance can depend critically on the surface composition of the outer 2.5 nm of material. A device has been assembled to complete oscillatory or unidirectional sliding friction experiments in a scanning Auger analytical system while monitoring the coefficient of friction and the electrical contact resistance. Auger surface analysis is completed *in situ*. A gas handling/introduction capability has been added for atmosphere control; the dynamic gas partial pressure can be controlled from 10^{-10} to 10^{-5} torr or at static pressures up to one atmosphere. Segregation of sulfur to wear track surfaces due to sliding alone has been measured for a gold alloy, which increased the electrical contact resistance.

Keywords: Surface, Erosion/Wear/Tribology, Structure

Chemistry and Ceramics Department, 1840

Department 1840 supports Sandia weapons and energy programs by selecting, developing, and characterizing ceramics, glasses and glass-ceramics. A variety of approaches are used, including gas-phase synthesis and reactions, solution preparation, as well as more traditional ceramic processing. The department promotes advanced weapons and energy concepts by providing new materials and developing new prototype components.

Interfacial Chemistry and Coating Research Division, 1841

Division 1841 is responsible for developing an understanding of the materials and processes involved in the formation of coatings and thin film structures. This work may be applicable to processes in use at Sandia, such as CVD tungsten films, as well as to new types of coatings, such as electroporetic formation of dielectric films. The division develops CVD and aerosol techniques for preparing ceramic powders. There is a major effort in understanding the interaction of hydrogen with metals.

Electronic Ceramic Division, 1842

Division 1842 develops and determines the properties of new ceramics for electronic and optical applications in Sandia systems. Examples are PZT for nonvolatile, radiation hard semiconductor memories, high-field ZnO varistors, $KNbO_3$ for optical switches, and cuprate high temperature superconductors.

Ceramics Development Division, 1845

Division 1845 is responsible for supporting laboratory programs involving glass- or ceramic-to-metal seals and other uses of glass or ceramics in moderate temperature environments. Expertise in the division includes the following areas: fracture surface analysis of brittle materials; seal design and fabrication processes; and glass and ceramic properties, i.e., strength, electrical conductivity. The division also maintains an active materials development program to formulate new glass or glass ceramics to meet particular requirements, e.g., corrosion resistance or high thermal expansion.

Inorganic Materials Chemistry Division, 1846

Division 1846 develops new processes for making ceramic powders and films using solution chemistry techniques. Understanding the structure and chemistry of sol-gel bulk and film materials is a significant part of this activity. The division also develops understanding of small particle-metal interactions that has led to new catalyst materials.

Materials Preparation, Synthesis, Deposition, Growth or Forming

373. Electrolytic and Electrophoretic Methods for Materials Processing — FY 1989 $150,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
SNL Contact: Sylvia Tsao, (505) 846-6753

Electrophoresis as a technique has been used for some time to apply organic and ceramic coatings to large, irregularly-shaped objects. Our research has been directed towards the application of electrophoretically-deposited organic and organic/ceramic composite coatings as insulators and IEMP hardeners for electronic component packages. Present systems under study are acrylic/fluorocarbon copolymers and acrylic/titanium dioxide composites. Future work will include the development of insulator/conductor composites.

Keywords: Coatings and Films, Polymeric Insulators/Dielectrics, Ceramic Insulators/Dielectrics, Electrophoretic Deposition

374. Aerosol Production of Fine Ceramic Powders — FY 1989 $200,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
SNL Contact: Sylvia Tsao, (505) 846-6753

We have recently begun developing a "generic" method to coat powders. The objective is to coat some powder, A, with B, such that subsequent processing may be assessed for its compatibility with B. The nature of A then becomes irrelevant and may be changed at will with no effect on the process. We use an aerosol method since particle agglomeration is minimized. The powder ($<1\mu m$ in diameter) is entrained in a carrier gas and the coating material condensed on it and reacted further if necessary. We are currently characterizing the instrumentation (atomizer, condensation nuclei counter) we will use to atomize and measure the aerosol.

Keywords: Aerosols, Ceramic Powder, Coatings

375. Chemically Prepared Ceramic Films for Opto-Electronic Applications

FY 1989
$1,200,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
SNL Contact: B. C. Bunker, (505) 844-8940

We have fabricated and characterized the first ferroelectric, chemically-prepared thin films of PZT doped with niobium. The ideal ferroelectric thin film for nonvolatile semiconductor memory devices has the following properties: (1) high remanent polarization, (2) low coercive field, (3) minimal aging and (4) minimal fatigue. Possible improvements in the aging characteristics of ferroelectric films may be achieved by donor doping. Specifically, doping with the aliovalent niobium ion in bulk PZT has significantly decreased ferroelectric aging by suppressing the number of oxygen vacancy-acceptor defect dipoles. The final issue of fatigue, the decrease in remanent polarization with repeated cycling, may be addressed by fabricating ferroelectric thin films with preferred orientation. For example, rhombohedral ferroelectric thin films with a preferred (111) orientation would have very few 71° and 109° domains. Thus, the ferroelastic contribution to ferroelectric fatigue would be eliminated. We have surveyed existing ferroelectric materials and determined that the best material for semiconductor memory applications would be a PZT material in the vicinity of the morphotropic phase boundary that is donor doped.

We have developed and characterized the first ferroelectric $KNbO_3$ thin films. Although previous investigators have attempted to make $KNbO_3$ thin films by liquid phase epitaxy and various vapor phase techniques, our chemically-prepared films are the only $KNbO_3$ films reported to be ferroelectric. The geometry used for electrical testing consists of a sapphire or fused silica substrate onto which a 0.2 μm thick layer of platinum is vapor deposited. Our best films are produced using multiple dip coating with 700°C heat treatments between each coating step and a final firing temperature of 800°C. Five coatings result in a 0.4 μm thick film of polycrystalline $KNbO_3$ on the platinum after the 800°C heat treatment. An array of platinum top electrode dots, which are 0.5-1.0 mm in diameter and 0.2 μm thick, is deposited onto the potassium niobate. For a 1 kHz, sinusoidal applied field of 300 kV/cm, we measured the following ferroelectric properties: (1) a spontaneous polarization of 8.4 $\mu C/cm^2$, (2) a remanent polarization of 4.1 $\mu C/cm^2$, and (3) a coercive field of 55 kV/cm. For films heated at 700°C and 800°C, we measured dielectric constants of 300 with dissipation factors of 0.05, in reasonable agreement with bulk, polycrystalline $KNbO_3$ dielectric properties.

Keywords: Ceramic Coatings, Chemical Synthesis, Ceramics

376. Development of New Glasses and Glass-Ceramics FY 1989
$500,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
SNL Contact: J. W. Rogers, Jr., (505) 844-1141

A family of glass ceramics is being developed to match the thermal expansion of a number of metal systems. We have developed a group of lithium silicate glass ceramics that are being used to make hermetic seals to a variety of stainless and superalloys for actuator headers and other electronic components. A family of phosphate-based glasses is being used to form seals to Al, Cu, and stainless steels. Previously we developed a new glass that is very corrosion resistant to Li ambient temperature battery environments. This glass is presently used in batteries (active and reserve) and has an expected life of five years. We have developed a more advanced sealing glass with a 10-year life and have begun using it to replace the earlier, shorter-lived version. Transformation-toughened glass ceramics based on the precipitation of metastable ZrO_2 in a glass matrix have been developed. The objective of this program is to develop tougher glass ceramics for electrical insulator applications.

Keywords: Ceramics, Glasses, Electrical Insulators, Corrosion

377. Preparation of Ceramic Powders by Chemical Techniques FY 1989
$1,500,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
SNL Contact: D. H. Doughty, (505) 844-1933

High-purity, homogeneous ceramic powders are being prepared by sol-gel chemistry techniques. Materials prepared include ZrO_2, PZT, ZnO, Al_2O_3, and titanate catalyst supports. The first three materials are utilized in ceramic electronic components at Sandia. Alumina is being toughened by coprecipitation with ZrO_2. The catalysts are used in our coal liquefaction program currently, and may find more general application. Novel glasses are also being prepared by sol-gel techniques. Our studies include basic research on precursors as well as applied development. Experimental techniques include small angle X-ray scattering, nuclear magnetic resonance, and several spectroscopic techniques to characterize precursor solutions and products. Glasses have been successfully evaluated on solar thermal receiver tubes and on photovoltaic cells. Dielectric barriers for a number of weapon applications have also been developed and are being evaluated.

Keywords: Ceramics, Glasses, Chemistry, Surface Characterization and Treatment

Materials Structure and Composition

378. Structure of Novel Glasses

FY 1989
$250,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
SNL Contact: J. W. Rogers, Jr., (505) 844-1141

The goal of this program is to develop a general understanding of the relationships between the structure and properties of a glass in order to design compositions for specific applications. To that end, we characterize the effects of composition on the structures of simple glasses, using a number of spectroscopic techniques including X-ray photoelectron spectroscopy (XPS), Raman spectroscopy, and magic angle spinning nuclear magnetic resonance (MAS NMR) spectroscopy.

Fluorophosphate glasses are candidate materials for high expansion sealing applications. We have examined a series of sodium phosphate glasses with increasing F-substitution for oxygen. This substitution alters the glass structure by systematically reducing the bridging-to-nonbridging oxygen ratio, as determined from the O1s spectra collected by XPS. The development of peaks associated with P-F vibrations in the Raman spectra are consistent with this structural depolymerization. The reduction in the average phosphate chain length with F-incorporation explains the substantial decrease in glass transition temperature for high-F glasses.

We have also examined several series of sodium aluminophosphate glasses. MAS NMR analyses reveal that the average Al-coordination number (CN) is dependent on glass composition. Octahedral aluminophosphate groups are preferred in acidic compositions, whereas tetrahedral species are favored in basic compositions. The transition from Al(6) to Al(4) with changing composition has a dramatic effect on glass properties, primarily because fewer nonbridging oxygen are consumed to make the tetrahedral sites. Al-coordination can also be tailored by changing the field strength of the modifying cation; increasing the field strength decreases the average Al-CN.

Keywords: Ceramics, Glasses, Electric Insulators

379. Structure of Sol-Gel Films

FY 1989
$150,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
SNL Contacts: D. H. Doughty, (505) 844-1933

Control of the microstructures of sol-gel-derived thin films (e.g., pore volume, surface area, pore size, refractive index) is important for such applications as protective and planarization layers, dielectric passivation layers, and sensor surfaces. This collaborative program explores the fundamentals of sol-gel film deposition using such techniques as imaging and conventional ellipsometry, FTIR microscopy, and gas sorption on SAW substrates.

Ellipsometric imaging of mixed water-alcohol solvents shows that water may be concentrated at the drying line. Therefore film deposition from coating sols containing water in excess of the azeotropic composition may occur primarily within water rather than alcohol. Based on surface area analyses of bulk gels, we found that replacement of alcohol with water causes a dramatic compaction of the structure in the final stage of drying. No doubt a similar effect occurs in thin films, which may explain the observation that film refractive indices increases with the H_2O/M ratio of the precursor sol.

Thicker entrained films obtained for high substrate withdrawal speeds take longer to dry than thin films, because evaporation can occur only from the film/vapor surface. For aggregating systems, longer drying times allow increased aggregation prior to final drying causing the film porosity to increase (refractive index decreases with substrate speed). For non-aggregating systems composed of repulsive monosized particles, slower drying provides additional time for the particles to arrange (perhaps order) on the substrate surface causing the refractive index to increase with U. The deposition of ordered arrangements of monosized particles is an attractive method for obtaining large pore sizes with narrow pore size distributions.

Keywords: Ceramic Coatings, Glasses, Sol-Gel, Films

Materials Properties, Behavior, Characterization or Testing

380. Molecular Beam Studies of Hydrogen in Metals — FY 1989 $400,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
SNL Contact: Sylvia Tsao, (505) 846-6753

In an effort to elucidate the dynamics of chemical reactions occurring on metal surfaces, we have undertaken a quantum-resolved study of HCl formed during the reactive collision of a beam of gaseous H-atoms with a chlorinated Au(111) surface. This is the first surface chemical reaction to be studied in a quantum specific manner. The nascent rotational and vibrational distributions of the HCl product are determined using resonantly enhanced multiphoton ionization laser spectroscopy. The thermochemistry for this reaction indicates that product formation proceeding through chemisorbed H-atoms is near thermoneutral, while direct reaction of a gas phase H-atom with Au(111):Cl is highly exothermic (~50kcal/mole). The H-atom reaction probability and the angular distributions of the reactively scattered HCl are determined in a quantum specific manner as a function of surface temperature.

The HCl produced in v=O is rotationally equilibrated with the surface (170K <T_s <800K) while the HCl produced in v=1 has a rotational temperature of 300K independent of surface temperature. The J integrated flux of v=O HCl produced in the reaction is independent of surface temperature while the flux of v=1 HCl increases with surface temperature in an Arrhennius fashion with an activation energy of ~500 cm^{-1}. This activation energy is ~5X smaller than the vibrational splitting (2900 cm^{-1}) in HCl. These findings clearly indicate that the v=O and v=1 channels arise from dynamically distinct channels. We tentatively ascribe the v=O channel to reaction occurring between chemisorbed H and Cl atoms and the v=1 channel to the direct reaction of a gas phase H-atom with a vibrationally excited Cl atom chemisorbed to Au(111). The Au(111):Cl bond vibrational frequency is ~550 cm^{-1}. Current efforts are aimed at the reactions of H atoms with Pd(111):Cl and Pd(111):D forming HCl and HD respectively.

Keywords: Hydrogen Effects, Surface Characterization and Treatment, Surface Modification

381. Electronic Ceramics — FY 1989 $600,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
SNL Contact: B. C. Bunker, (505) 844-8940

Studies of electronic ceramics include: (1) development of high field ZnO-based varistors and understanding microstructure-property relationships; (2) development of ZnO and dielectric granules for lightning arrestor connectors; (3) studying the electrical transport properties of boron carbides for thermoelectric generator and neutron detector applications; (4) study of the electrical properties of PZT films for nonvolatile semiconductor memories; and (5) relating processing, microstructure and Jc in $YBa_2Cu_3O_{7-x}$.

Keywords: Ceramics, Ceramic Coatings, Electronic Structure

382. Ceramic Fracture — FY 1989 $300,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
SNL Contact: J. W. Rogers, Jr., (505) 844-1141

The fracture properties of ceramics often limit their application in weapon and energy systems. Our program includes basic research to better understand fracture processes and to develop tougher ceramics based on this understanding. The effects of microstructure in glass ceramics, phase separation in glasses, and of the environment are presently being studied. Basic studies on the effect of environment in crack propagation of glasses have led to an atomistic model which explains the chemical interaction between a wide range of environments and strained silicate bonds in glasses. A program to develop tough ceramic composites and glass ceramics is also underway.

Keywords: Ceramics, Glasses, Fracture, Strength, Corrosion

383. Superplastic Ceramics — FY 1989 $100,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
SNL Contact: J. W. Rogers, Jr., (505) 844-1141

Superplastic ceramics are ultra-fine-grained ceramics with an intrinsic capability to deform extensively at moderate temperatures. This presents the possibility that they can be near-net-formed into complex shapes without the time, expense, and deleterious flaws generated by machining. In addition, these ceramics possess significant other advantages over their larger-grained commercial counterparts; lower sintering temperatures, enhanced diffusional bonding to other materials, and superior toughness.

The thrust of the current program is to manufacture and test ceramics with nanometer-scale grain sizes. From superplasticity theory, such ceramics would be capable of being deformed, like metals, into complex shapes in a matter of minutes. To date, we have achieved the first step of that goal, the production of ultrafine fine starting powder in bulk quantities. Our ZrO_2 -3mol% Y_2O_3 powders are only 10-12 nm in size and can easily be produced in multi-gram quantities. The only other U.S. attempt to develop nanometer-scale powders has resulted in only milligrams of material per batch. The current technique uses conventional chemical precipitation from chloride salts, but with significant attention to detail concerning pH, rate of solute addition, and post-precipitation rinsing. Agglomerates are produced, but they are weak and can easily be broken up into individual nanocrystals by ball milling or ultrasonic dispersion.

Keywords: Toughened Ceramics, Ceramic Powder, Superplastic Forming, Zirconia

384. Reactivity and Bonding of Glasses and Ceramics to Metals — FY 1989 $400,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
SNL Contact: J. W. Rogers, Jr., (505) 844-1141

We study reactions between metals and glasses or ceramics using sessile drop experiments and detailed analyses of reaction zones by SEM, TEM, Electron microprobe, AES and XPS techniques. Systems under development include glass-ceramic to 304 stainless steel, glass to aluminum, and Ti-containing alloys on alumina, mullite, and zirconia toughened mullite. The objective of these studies is to develop sealing techniques that give strong, hermetic bonds with minimum mechanical stress.

Keywords: Glasses, Ceramics, Surface Microstructure, Metal-Ceramic, Surface Phases, Surface Characterization and Treatment

Device or Component Fabrication, Behavior or Testing

385. Sensor Development FY 1989
$200,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
SNL Contact: Sylvia Tsao, (505) 846-6753

We are jointly investigating the use of integrated anodic oxide moisture sensors in IC packages as a means of identifying defective hermetic seals. Thin aluminum oxide dielectric films, when grown in acidic electrolytes such as sulfur acid, develop a crystalline morphology characterized by pore structures exhibiting significant moisture adsorption. Water has a dielectric constant of about 80, and therefore produces large increases in electrical capacitance when adsorbed in the oxide. When this structure is incorporated as the dielectric in a capacitor, a large capacitance response to humidity is observed. We speculate that the pores derive from the voids which results from oxide crystallization that takes place during growth. It is also known that the films contain (SO_4=) and (OH-) anions, which may additionally contribute to hygroscopic activity observed in these small (<1 micrometer) pores.

Keywords: Moisture Sensors, Oxides, Dielectric Films

386. SAW Development FY 1989
$200,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
SNL Contact: D. H. Doughty, (505) 844-1933

The detection of organic species in water is important in the analysis of waste water as well as in the monitoring of drinking water. Since some polymers absorb organic species much readily than they absorb water, they should be useful for detecting the presence of organic contaminants in an aqueous system. The sensitivity of acoustic plate mode (APM) devices, which can be effectively operated in contact with liquids, to mass changes in a polymer film contacting the device can be used as the sensing mechanism.

A preliminary investigation into this type of sensor was performed using a polystyrene coated APM device. A characterization of device response as a function of the concentration of both methylene chloride (CH_2Cl_2) and carbon tetrachloride (CCl_4) was obtained. The organic species caused a detectable response: frequency shifts of 25 and 615 ppm for CH_2Cl_2 (16 percent of saturation) and CCl_4 (23 percent of saturation), respectively. The response for CH_2Cl_2 was relatively linear with concentration up to over 60 percent of saturation. Larger responses should be observed for polymers with large absorption capabilities as well as for thicker polymers. Even though polymers are not highly selective, they do exhibit selectivity for types of organics and, therefore, an array of sensors of this type should be useful for obtaining information about the concentration of various types of organic species in water.

Keywords: Organic Detection, Acoustic Plate Mode, Organic Sensors

Sandia National Laboratories - Livermore

Materials Preparation, Synthesis, Deposition, Growth or Forming

387. Powder Metallurgy | FY 1989 | $200,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
SNL Contacts: M. I. Baskes, (415) 294-3226; J. E. Smugeresky, (415) 294-2910

In addition to extensive powder handling and characterization capabilities including automated image analysis, facilities exist to produce rapidly solidified structures by inert atomization, melt spinning, and spark erosion. Emphasis is being placed on the effect of processing parameters on material characteristics.

Metallurgical studies are being conducted on a variety of alloy systems. The relationship between strength, toughness, microstructure, and fracture modes of blended elemental PM titanium alloys is being studied to optimize HIP cycles and heat treatments for improved properties of near-net-shape processed components. The relationships between starting powder size and sintering parameters on the microstructure, permeation and filtration characteristics of porous stainless steel compacts is being established. The dynamic compaction of Al-Si alloys has produced fully dense compacts, retained metastable microstructures of the original powder, and has provided further insight into the mechanisms at inter-particle bonding. The effect of particle size distribution and morphology on the quality of compacts is also being established. The new rapid solidification processing facilities will also be utilized to produce powders for metal matrix composites.

Keywords: Alloys, Rapid Solidification, Metals, Shock Wave Compaction

388. Advanced Electrodeposition Studies FY 1989 $100,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
SNL Contacts: R. E. Stoltz, (415) 294-2162, H. R. Johnson, (415) 294-2822, W. D. Bonivert, (415) 294-2987

Engineering applications, electroanalytical development, and fundamental studies are being pursued in the areas of electrodeposition and electroforming. Electrodeposition of a variety of metals is being studied with a focus on the relationship between critical process variables and the mechanical properties of the deposit. The role surface active agents play in this process is being studied using an in situ real-time monitor for organic additives developed at SNLL. Process variables to produce a crack-free deposit for a NaS battery case are being defined and techniques are being evaluated to measure and control residual stresses during the electroplating process.

Keywords: Metals, Electrodeposition, Electroforming, Mechanical Properties, Chromium

389. Metal Forming FY 1989 $200,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
SNL Contacts: J. Lipkin, (415) 294-2417, T. C. Lowe, (415) 294-3187 and D. A. Hughes, (415) 294-2686

Fundamental understanding of inelastic deformation is being developed through crystal plasticity modeling and experimentation. Recent studies in this area relate to the properties of metals which have been altered by deformation-induced anisotropy. In particularly, we have examined elastic response and reversibility of microstructure evolution following unloading and reverse loading of highly deformed cylinders. This effort is a departure from previous work which has considered only monotonic loading histories. It is clear, however, that more general, non-monotonic and non-proportional loading paths are common in metal forming operations. Numerical and experimental results for more general loading histories have thus been useful in resolving key issues related to the design of constitutive relations for such processes. Further progress in this area includes the development of a new apparatus for measuring anisotropic material response during torsion of short gage length, thin walled tubes. The results of these torsion experiments have enabled us to obtain a complete set of constitutive model constants for an engineering material, 304L stainless steel. Companion finite element analyses of metal forming operations, including a 304L stainless steel closed-die extrusion process, are in progress. Additional, physically-based, insight for designing constitutive relations is emerging from studies of the evolution of dislocation substructures in large-strain torsion experiments. Recent results provide new evidence that these structures evolve in a stable manner without localized shearing. This observation is in sharp contrast to previous investigations which have emphasized instabilities in the formation of dislocation microstructures.

Keywords: Metals: Ferrous and Non-Ferrous, Fracture, Near-Net-Shape Forming

390. Advanced Organic Materials — FY 1989 $200,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
SNL Contacts: D. L. Lindner, (415) 294-3306 and W. R. Even, (415) 294-3217

Recent developments in our understanding of the relationship between microstructure and macroscopic properties in preparation of low density polymer foam materials has led to the ability to produce foams with unique physical properties in collaboration with personnel at Sandia National Laboratories, Albuquerque. Engineering applications and basic studies designed to optimize properties are being pursued. We have begun determining the relationship between these unique microstructures and physical and mechanized properties of the foams. We have been successful in producing a continuum in morphologies ranging from very open cell-low density, to nearly closed cell-higher density polymeric foams. We have developed several different methods to produce such materials in a variety of modifications. These materials are ideal candidates for catalyst support structures or low-pressure-drop, high-efficiency filters. By incorporating molecular sieves into the structure, foams that adsorb and retain various gases and liquids under specific temperature and pressure conditions can be produced.

Keywords: Polymers, Catalysis, Molding, Microstructure

391. Particulate Technology — FY 1989 $50,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
SNL Contacts: D. L. Lindner, (415) 294-3306 and W. R. Even, (415) 294-3217

We are using controlled precipitation and subsequent pyrolysis of various actinide compounds to prepare actinide oxide particles of very small size and of specific morphology. We have used this method to prepare uranium and thorium oxides as platelates, as needles, and as "starbursts." We have examined and optimized the conditions required to produce these powders, we have characterized the resulting materials, and we have investigated their hydrodynamic properties.

Keywords: Actinides, Refractory Oxides, Powder Synthesis

392. Tritium Getter Technology FY 1989
$50,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
SNL Contacts: D. L. Lindner, (415) 294-3306 and T. Shepodd, (514) 294-2791

We are investigating the use of solid alkynes and alkenes as organic tritium getters. Currently we use several alkynes as hydrogen getters in controlled environments (ie., in the absence of oxygen and water). We have demonstrated that the use of these materials can be extended to applications in which a limited amount of oxygen and/or water is present as well as investigating their use to getter tritium without producing HTO or gaseous tritided species as hazardous by-products. Work with 1,4-bis (phenylethynyl) benzene has shown that when mixed with appropriate catalysis, it can quickly getter tritium (as it does hydrogen). Aging studies of the tritiated getter demonstrate that no gaseous tritided species are evolved over extended periods of time. We are now modifying these getter systems to provide materials that will provide enhanced stability and functionality in the radiolytic environment.

Keywords: Hydrogen Getters, Tritium

393. Molded Desiccant Foam FY 1989
$100,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
SNL Contacts: D. L. Lindner, (415) 294-3306 and C. B. Frost, (415) 294-2048

We have developed a zeolite-loaded polyurethane foam that we are using in applications in which we require both structural support and desiccation. The urethane foam is loaded with a zeolite powder during formulation and casting, and then activated *in situ*. We can produce parts from this material at quite high densities (up to 1.4 g/cc) and up to 50 weight percent zeolite. The material can be formulated and processed with conventional polyurethane foam processing equipment. Our work with this material has shown that parts can be conveniently cast directly with it or, alternatively, blanks can be machined to final dimension. We have also examined the electrical properties of these foams as a function of water content and have found that conductivity is not significantly affected as the material takes up water. We are now examining the possibility that it can be used as a desiccating electrical potting material.

Keywords: Encapsulants, Organic Foams, Desiccants

394. Plasma Processing FY 1989
$200,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
SNL Contact: W. L. Hsu, (415) 294-2379

Plasma processes are used to develop new and advanced material coatings. In particular, hard amorphous carbon films and diamond films have been deposited for applications as tritium permeation barriers, corrosion barriers, and sealants against moisture absorption. Film growth is achieved by using a plasma discharge to break down and enhance the reactivity of the fill gas, which is typically a mixture of hydrogen and methane. The research program emphasizes three areas of investigation: gas phase chemistry induced by the plasma, nucleation kinetics, and characterization of film properties. In situ diagnostics, such as mass spectroscopy with energy filter, optical emission spectroscopy, and Langmuir probes, are developed for studying the plasma-gas phase reactions. Laser Raman spectroscopy has been applied for in situ film growth studies. A variety of analytical techniques such as TEM, SEM, ERD, and RBS have been used to characterize the deposited film structures. The goal of the program is to create pin-hole-free amorphous carbon films and single-crystal diamond films with good adhesion to a variety of substrate materials.

Keywords: Plasma Processing, Carbon-Based Materials, Amorphous Films, Diamond

Materials Properties, Behavior, Characterization or Testing

395. Tritium and Decay Helium Effects on Crack Growth in Metals and Alloys FY 1989
$700,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
SNL Contacts: S. L. Robinson, (415) 294-2209, S. H. Goods, (415) 294-3274 and R. Moody, (415) 294-2622

The effects of tritium and decay helium on the mechanical properties and crack growth susceptibility of fcc alloys are presently being studied. These studies begin with tests in high pressure hydrogen gas and with tests on hydrogen precharged samples to determine the effects of applied stress, microstructure, and thermomechanical processing on hydrogen-induced failure. The fundamental effects of hydrogen (and tritium which is chemically similar) on the mechanisms that govern plastic flow and fracture are then defined with these results. Similar studies are underway in samples exposed to tritium, which decays to helium without inducing radiation damage, to determine the added effects of decay helium on failure properties. With preliminary results from these studies and theoretical analysis based on the Embedded Atom Method developed at Sandia, we are beginning to define the effects of helium on properties, crack growth susceptibility, and on the mechanisms of plastic flow and fracture.

Keywords: Metals: Ferrous and Non-Ferrous, Crystal Defects/Grain Boundaries, Fracture

396. Joining Science and Technology FY 1989
$400,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
SNL Contacts: M. I. Baskes, (415) 294-3226, J. A. Brooks, (415) 294-2051, K. W. Mahin, (415) 294-3582

We are directing considerable effort toward developing a science-based methodology for designing, analyzing, and optimizing welding processes in order to control weld geometry, distortion, and microstructure, thereby improving both the fundamental understanding of the complex welding process, and the performance of welded structures. The studies include modeling of heat transfer, coupling thermal and mechanical computer codes to allow simultaneous calculation of both temperature and stress as a function of time throughout the weld, and the modeling of microsegregation during weld solidification. The computer-generated results are being compared to experimental measurements temperature, residual stresses, and elemental segregation.

Additional welding metallurgy activities include the evaluation of alloy modifications to improve the weldability of specific alloys, the evolution of weld microstructure during solidification and cooling, the study of weldment cracking mechanisms, the weld microstructure property relationships, and analysis of joints in composite materials. In solid state welds, the current emphasis includes establishing specifications for weld evaluation and acceptance, and improved NDE techniques to verify weld quality. Alloy systems of current interest include austenitic and martensitic stainless steels (single phase and precipitation hardenable), powder processed alloys, and model alloy systems.

Keywords: Joining and Welding, NDE, Microstructure, Metals, Transformation, Solidification, Modeling

397. Composites: Characterization and Joining FY 1989
$150,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
SNL Contacts: D. L. Lindner, (415) 294-3306 and J. R. Springarn, (415) 294-3307

The stability, compatibility, and joining of polymer matrix composite materials are being investigated. The work focuses on graphite-fiber-reinforced composites and includes both thermosetting and thermoplastic matrix materials. The influence of matrix materials and post-cure thermal processing on adsorption sites and the coefficient of moisture expansion will be investigated. Condensible volatile materials in resins considered for space applications are being identified. Coatings for composite materials are under investigation to enhance stability for special design needs (e.g., mirrors). We are also developing coatings for the protection of composite materials in high temperature oxidizing environments. Thermoplastic matrix materials will be studied to determine the influence of matrix crystallinity upon performance. The influence of galvanic corrosion upon composite/metal joints is also under investigation to assess long-term storage effects.

Joining of composite materials is being studied and includes mechanical fasteners, adhesives and the welding of thermoplastics. Techniques are being developed to measure the fracture toughness of adhesive bonds and predict the strength of mechanically fastened joints.

Keywords: Composites, Joining and Welding, Fibers, Corrosion, Coatings

398. Compatibility, Corrosion, and Cleaning of Materials — FY 1989 $20,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
SNL Contacts: R. E. Stoltz, (415) 294-2162, H. R. Johnson, (415) 294-2822 and D. K. Ottesen, (415) 294-3687 and J. M. Hruby, (415) 294-2596

Examination of surfaces to determine compatibility, corrosion, and cleanliness is being carried out using state-of-the-art electroanalytical and spectroscopic means. Many potential problems exist during production and assembly of components if parts are not properly cleaned. However, it is difficult to quantify cleanliness and many parts have interiors inaccessible for examination by conventional methods. We have developed a unique technique using Fourier transform infrared spectroscopy that is capable of peering inside small diameter tubes or examining small diameter wires to identify wall-surface contamination. This method has been shown to be robust in a production environment and is being transferred to Rocky Flats.

Keywords: Compatibility, Corrosion, Cleaning, FTIR

399. Tritium-Metal Interaction — FY 1989 $350,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
SNL Contacts: A.E. Pontau, (415) 294-3159 and M. E. Malinowski, (415) 294-2069

The interactions of tritium gas with metals is characterized by a number of experimental techniques including tritium imaging and nuclear reaction ion micro-beam analysis. Tritium imaging is the real time, two-dimensional detection of tritium in the near surface region of metals. Developed at SNLL, imaging is a non-contact technique, and is based on the detection of secondary electrons created by the primary beta decay electrons. Imaging is sensitive to the equivalent of submonolayer quantities of tritium and is being used in tritium grain boundary segregation studies, metal tritide imaging work, and surface diffusion studies using a technique which combines tritium imaging and laser desorption. This unique technique, called "TILDE" (Tritium Imaging following Laser Desorption), will be used in upcoming experiments to measure long-range tritium movement on well-characterized metal surfaces.

Hydrogen isotope and helium depth distribution in metals are determined from nuclear reaction analysis techniques. A microbeam facility has been constructed and operated with ion beams of $\leq 10\ \mu m$ spatial resolution.

Keywords: Metals: Ferrous and Non-Ferrous, Surface, Defects/Grain Boundaries, Tritium

400. <u>Measurement of Multilayer Thin Film Structures</u> <u>FY 1989</u>
$60,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
SNL Contact: B. E. Mills, (415) 294-3230

Beta backscatter methods are commonly used to measure thicknesses of thin layers (micrometers) on substrates. Experience has shown that this technique cannot be used for the measurement of multilayer structures. We have extended the utility of the method through the use of beta sources of two different energies. We have demonstrated that data from such measurements can be used to determine layer thicknesses in a two-layer thin film structure on a substrate. We have used the method to determine the extent of intermetallic interlayer formation between protective metal overlayers on reactive metal substrates as a result of thermal and aging effects.

Keywords: Instrumentation and Technique Development, Films

401. <u>Helium in Metal Tritides</u> <u>FY 1989</u>
$200,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
SNL Contacts: W. A. Swansiger, FTS 234-2496, S. E. Guthrie, FTS 234-2360 and D. F. Cowgill, (505) 844-7480

The evolution of helium in metal tritides is being studied by NMR, gas volumetry and dilatometry techniques. NMR measurements carried out over the past year are a continuation of prior work on the determination of helium densities in bubbles of aged Pd through the observation of the solid, liquid, gas phase transitions of the helium trapped in the bubbles. Initial tests have been completed on a sensitive gas sampling system to measure in real time the evolution of helium from metal tritides. Changes in the phase behavior of Pd tritide as a function of He bubble content have been determined by gas volumetry and correlated to measurements of physical size changes due to the dilation of the metal lattice with the evolution of bubbles.

Keywords: Helium, Metal Tritides

402. Analysis of Defects and Interfaces in Metals — FY 1989 $300,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
SNL Contacts: T. C. Lowe, (415) 294-3187, S. H. Goods, (415) 294-3247

Fundamental understanding of deformation and failure processes near interfaces is being developed through crystal plasticity modeling. Initially, we have analyzed the effects that cavities at grain boundaries have on ductility and strength. Experiments performed on polycrystalline copper containing grain boundary cavities have shown that ductility decreases with decreasing strain rate. Similar decreases in ductility were not observed in samples without grain boundaries cavities. Companion crystal plasticity calculations are underway to explain the effects of strain rate on ductility. Initial calculations have shown inhomogeneous distributions of crystallographic slip and stress near the cavities. The dependence of these distributions upon strain rate is being analyzed.

Keywords: Fracture, Metals: Ferrous and Non-Ferrous, Interfaces, Composites

Instrumentation and Facilities

403. New Spectroscopy — FY 1989 $50,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
SNL Contacts: D. L. Lindner, (415) 294-3306, M. C. Nichols, (415) 294-2906 and B. E. Mills, (415) 294-3230

New spectroscopic techniques are being developed for special applications. For example, a micro-fluorescence spectrometer is being assembled. This unit permits the examination of very small areas for elemental composition and do it in an automated way to provide coverage of large areas with high resolution.

Keywords: Spectroscopy, Elemental Composition

404. <u>Tritium Facility Upgrade for Materials Characterization and Testing</u> <u>FY 1989</u>
$500,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
SNL Contacts: S. H. Goods, (415) 294-3274 and S. L. Robinson, (415) 294-2209

Exposure to tritium is now known to degrade the performance of many structural and containment materials. Materials research needs in the Tritium Research Laboratory have driven the acquisition of new analytical techniques and equipment and the upgrading of existing experimental test equipment. New capabilities being developed include, quantitative ^{3}He mass spectrometry for characterizing helium concentrations resulting from tritium decay, and induction heating capability for rapid thermal cycling of small tritium charged metallic specimens. A new high-pressure T_2 thermal charging and quench facility is yielding precise measurement of tritium solubility as a function of pressure and temperature in a variety of materials. A new Auger spectrometry system allows us to analyze surface compositions. Computerized data acquisition has been added to the servohydraulic mechanical test frame. Characterization of fracture phenomena is facilitated by a modern scanning electron microscope. These capabilities contribute to the characterization and prediction of tritium-induced degradation phenomena in containment materials.

A new laboratory system is being developed to permit accurate determinations of tritium/material phases for materials under consideration as potential tritium solid storage media. Under computer control, the system will provide variations in pressure (.01 atm to 20 atm with better than .001 atm resolution) and temperature (-80°C to 200°C with .1°C stability) to determine the pressure, concentration, temperature (PCT) diagrams for the materials under study. Careful gas inventory using standard volumetric procedures allows better than 1 microgram resolution for tritium and the site permits a nominal limitation of 3 grams of tritium which dictates the upper bound for samples of host material. The additional provision of an ultra-high vacuum system and inexpensive quadrapole mass spectrometer permits a degree of sample preparation and characterization prior to PCT study.

Keywords: Spectrometer, Tritium Charging, Mechanical Testing, Scanning Electron Microscopy

405. New Analytical Techniques FY 1989
$50,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
SNL Contacts: D. L. Lindner, (415) 294-3306, M. C. Nichols, (415) 294-2906 and B. E. Mills, (415) 294-3230

New spectroscopic and analytical techniques are being developed for special applications. For example, we have developed a system for chemically selective X-ray microtomography. We are employing this technique to image 3D elemental distributions in a variety of materials and structures.

Keywords: X-ray Tomography, Chemical Analysis

406. New High Resolution Electron Microscopy Facility FY 1989
$200,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
SNL Contacts: G. J. Thomas, (415) 294-3224, M. J. Mills, (415) 294-3018

A new high resolution transmission electron microscope laboratory is now operational. It includes an intermediate voltage high resolution microscope, sample preparation and photoprocessing facilities, and computational facilities for image simulations and image processing. It will be utilized to determine the atomistic structures of a number of material systems, including (a) metal-metal interfaces, such as grain boundaries, (b) defect structures in undeformed and deformed metals and alloys, (c) helium-induced defect evolution in metal tritides, and (d) semiconductor-oxide interfaces. These studies are important to gas transfer technologies and to semiconductor device fabrication.

Keywords: High Resolution Electron Microscopy, Interfaces, Grain Boundaries, Tritides, Semiconductors

Lawrence Livermore National Laboratory

Materials Preparation, Synthesis, Deposition, Growth or Forming

407. Inorganic Aerogels FY 1989
$600,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
LLNL Contact: L. W. Hrubesh, (415) 423-1691/FTS 543-1691

The approach is to perform a controlled hydrolysis of metal alkoxides such that the partially hydrolyzed chemical can be limited from further condensing reactions by using an appropriate buffer solvent. Subsequently, this pre-hydrolyzed chemical can either be diluted to make low density sol-gels, or directly gelled to achieve higher densities. Aerogels are obtained by super-critical solvent extraction of the wet gels.

We have successfully applied this approach to make silica aerogels starting with partially hydrolyzed tetramethoxysilane (TMOS). We have made transparent, monolithic silica aerogels with dimensions of 2.5 cm x 4.5 cm x 40 cm at selected densities over the range of 0.01 to 0.65 gms/cc.

This material has unusual optical and thermal properties due to its ultrafine microstructure. Its applications include target material for direct drive laser fusion experiments, thermally insulating window glass, and as collector material for hyper-velocity microparticle capture.

Keywords: Inorganic Aerogels, Sol-Gel, Laser Fusion Targets

408. Photoactivated Catalysis on Aerogels FY 1989 $80,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
LLNL Contact: C. A. Colemenares, (415) 422-6352/FTS 532-6352

A low density SiO_2 aerogel (50-100 mg/cm^2) doped with 0.45 wt% uranyl ions (UO_{2++}) was found to be photochemically active for the production of hydrocarbons from various gas sources. The energy source was a 1000-W Mercury-Xenox, solar-simulator lamp, which illuminated fine particles of aerogel suspended in a fluidized bed using the reaction-gas mixture. Experiments with a $2H_2$:1CO gas mixture produced mostly methane, ethylene, ethane, and propane. Products from a 1 H_2:1 C_2H_4 mixture were methane, ethane, propane, butane, pentane, hexane, and some unidentified products; while mostly ethylene with small amounts of methane were formed from a 1 H_2:1 C_2H_6 gas mixture. Europium and cerium-doped SiO_2 aerogels have been prepared and we are in the process of evaluating them.

Basic studies of the energy transfer mechanisms have been initiated. We are using fast optical spectroscopic techniques, as well as ultraviolet and x-ray photoelectron spectroscopies to carry out these studies.

Keywords: Photoactivation, Silicon Dioxide

409. Synthesis Project (Explosives) FY 1989
$250,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
LLNL Contact: C. L. Coon, (415) 422-6311/FTS 532-6311

Strict guidelines were developed pertaining to energy, density, sensitivity, and stability to use in the selection of specific target molecules that appear to possess improved properties for energetic materials. We have designed synthetic routes to these compounds which are reasonable and not lengthy, and we have identified key reactions which required further development and have outlined a systematic study of these reactions so as to (1) develop entirely new synthetic procedures, and (2) optimize reaction conditions. This approach has resulted in the synthesis of a series of target materials which contain two fused 5-, 6-, and 7-membered rings related to, and including, Bicyclo-HMX. Several of these materials, such as K-6 and HK-55, are in the process of being scaled up to pound quantities for further characterization and evaluation as useful energetic materials. The success of this synthetic effort was made possible by the development of (1) a new procedure for fusing 5-, 6-, and 7-membered rings, (2) new nitrolysis procedures involving $N_2O_5/HNO_3/$ trifluoromethanesulfonic anhydride, and (3) a new procedure for the replacement of alkyl groups with nitro groups using $N_2O_5/HNO_3/TFAA$. Several of these new nitramine compounds have been selected for scaleup to prepare pounds quantities for further characterization and performance studies.

Keywords: Explosives, Chemical Synthesis, Weapons

410. Synthesis and Reactivity of Transition Metal Fluorocarbon Complexes FY 1989
$150,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
LLNL Contact: Robert D. Sanner, (415) 423-3875/FTS 543-3875

The synthesis of $(CF_3)AuL$ ($L=PMe_3,PEt_3,PPh_3$) from $(CF_3)AuCl$ and $Cd(CF_3)_2$ was developed. These linear gold(I) compounds readily add excess halogen to form the predominantly *trans* square planar gold(III) dihalides, (CF$_3$)AuXU2(L) ($X=Br,I$). The use of stoichiometric (or less) halogen leads to a significant quantity of $(CF_3)_2AuX(L)$ ($L=PMe_3,PEt_3$) which is shown to arise from trifluoromethyl/halogen ligand exchange between $(CF_3)AuL$ and $(CF_3)AuX_2(L)$. No evidence for ligand exchange is found when $L=PPh_3$. $(CF_3)_2AuI(L)$ ($L=PMe_3,PEt_3$) may also be prepared in 80 percent yield from the *cis* oxidative addition of trifluoromethyl iodide to $(CF_3)AuI$; experiments with the radical scavenger galvinoxyl suggest a radical chain mechanisms for this CF_3I addition. Close examination of the ^1H and ^{19}F NMR spectra for the new square planar complexes reveals that downfield shifts occur for both nuclei when a *cis* halide is changed from Br to I; a *trans* halide causes an upfield shift upon this substitution. The cadmium reagent is, in general, ineffective for the preparation of Au(III) complexes since reduction to $(CF_3)AuL$ usually occurs. However, treatment of $(CF_3)_2AuI(PMe_3)$ with $Cd(CF_3)_2$ in the presence of excess CF_3I leads to the high yield synthesis of the tris(trifluoromethyl) species $(CF_3)_3AuPMe_3$.

Keywords: Fluorocarbons

411. Sputtering (Plutonium Alloys) FY 1989 $100,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
LLNL Contact: H. F. Rizzo, (415) 422-6369/FTS 532-6369

The triode sputtering process provides a versatile, controllable deposition environment in which kinetic and energetic bombardment effects can be studied. Sputtered metal atom fluxes as high as 1 x 10^{17} atoms/cm^2-s, which allow deposition rates as high as 400Å/s, can simultaneously be bombarded by ionized or neutral noble gas atoms at fluxes up to 1 x 10^{17} atom/cm^2-s with energies between 20 and 1000 eV. The triode "split-target" configuration was used to synthesize wide ranges of Pu-solute compositions in the Pu-Ce, Pu-Sc, and Pu-Yb systems to determine how these specific elements influenced the stability of Pu-rich alloys. This project was terminated in FY89.

Keywords: Sputtering, Actinides

412. Organic Aerogels FY 1989 $200,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
LLNL Contact: R. W. Pekala, (415) 422-0152/FTS 532-0152

Organic aerogels have been produced from the base catalyzed, aqueous reaction of resorcinol with formaldehyde. The aerogels have a microstructure composed of interconnected colloidal-like particles with diameters of 30-200 Å, cell sizes of less than 1000 Å, and surface areas of 400-900 m^2/g. This microstructure is retained even after carbonization at 1100°C.

Keywords: Organic Aerogels, Sol-Gel, Laser Fusion Targets

413. Polymer Coating and Foam Development FY 1989 $1,000,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
LLNL Contact: S. A. Letts, (415) 423-2681/FTS 543-2681

Low-density polymer foam is needed to act as a wick to liquid DT in a spherical shell configuration for direct-drive laser fusion targets. The foam must be porous, low-density (0.05 g/cc), uniform density, and have a pore size less than one micron to provide sufficient capillary pressure to hold the DT. Carbonized resorcinol-formaldehyde foam was chosen as the foam that best meets laser target requirements. Resorcinol-formaldehyde foam is made by a condensation polymerization in aqueous solution followed by a supercritical drying. The foam is finally carbonized in an inert atmosphere. The foam material is characterized for cell size by SEM TEM and freeze-fracture TEM. Uniformity is measured by X-ray radiography. The foam was tested for hydrogen wettability, the effects of DT exposure and thermal contraction measured from room temperature to 20K. Plasma polymer coatings are used as the ablator layer in direct-drive laser fusion targets. The effect of polymerization process variables on coating composition and properties is being studied. The electronic properties of the plasma generator are also being studied.

Keywords: Polymer Foams, Low-Density Materials, Laser Fusion Targets, Plasma Polymer Coatings

414. Atomic Engineering

FY 1989
$100,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
LLNL Contact: Troy W. Barbee, Jr., (415) 423-7796/FTS 543-7796

Thin film deposition processes were understood to be "atom by atom" in nature very early in the development of the appropriate synthesis technologies. This understanding undoubtedly resulted in a leap of imagination to a time when the atomic positions of chemically specific species necessary to achieve a scientific result, or to fulfill a technologically significant need, could be theoretically determined and then experimentally realized—in a word, *engineered*. Hence, "Atomic Engineering" requires that we know which atoms go in which places for a given reason, and further that we be able to achieve physically the desired result in a systematic and reproducible manner. In this research program the extension of multilayer technology to "Atomic Engineering" by synthesis of equilibrium and metastable structure materials on an atomic layer by atomic layer basis is addressed. The program goals are: (1) experimentally investigate the dependence of deposited material structure on individual layer thicknesses (i.e., the transition from layering to compound formation); (2) to apply this knowledge to the synthesis of materials of scientific and technological significance; (3) to use the techniques developed to produce samples allowing investigation of dimensionality limitations on cooperative phenomena in condensed matter.

Keywords: Thin Films, Multilayer Technology

Materials Structure and Composition

415. Theory of the Structure and Dynamics of Molecular Fluids FY 1989 $300,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
LLNL Contact: D. F. Calef, (415) 422-7797/FTS 532-7797

We have been developing and applying the methods of modern statistical mechanics to study the behavior of molecular fluids, especially under the high density and temperature conditions experienced by reacting explosive molecules. We are completing a computer code to calculate liquid mixture structures. The program calculates a complete set of thermodynamic properties using more realistic intermolecular potentials than any other currently available. The output of this program will also be used in calculating reaction "transition state volumes" and solvation dynamics. We are also developing molecular dynamic models for phase separations and carbon coagulation.

Keywords: Molecular Fluids, Prediction Behavior Modeling

416. Site-Specific Chemistry Using Synchrotron Radiation FY 1989 $197,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
LLNL Contact: Joe Wong, (415) 423-6385

This experimental program employs X-ray absorption spectroscopy (XAS) utilizing intense synchrotron radiation as a light source to probe the local atomic and electronic structure (chemical bonding) of materials with a view of gaining better understanding of their physico-chemical properties. A number of materials have been investigated. These include (a) metal-doped beta boron thermoelectric materials, (b) rare-earth metal ions substitution in YBa2Cu307 (YBC), (c) site selective detection with optical EXAFS, (d) interface structure of near-monolayer of Hf on a Pt/C layer and (e) solute pairing in solution-hardened fcc Cu alloys and (f) Cr3+ ions in fluoride laser crystals. These various studies serve to establish a new experimental capability at LLNL to enhance our basic understanding of materials and their processing from the point of view of site-specific chemistry in terms of bond distance, central atom coordination, valence site symmetry and coordination geometry.

Keywords: Site-Specific Chemistry, Superconductors

417. Capillary Structures (in Foams) FY 1989 $100,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
LLNL Contact: R. W. Hopper, (415) 423-2420/FTS 543-2420

Real foam structures are compared with models in terms of their geometrical features and their material correlation function. Scattering behavior is analyzed theoretically. The shape evolution of viscous bodies under the influence of surface tension is analyzed theoretically. Mechanical properties of foams are studied analytically and by computer modeling. Replica carbon foams of varied, but controlled structures and densities are made for mechanical properties measurements.

Keywords: Foams, Structure

418. Plutonium Pyrochemical Research FY 1989 $160,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
LLNL Contact: O. H. Krikorian, (415) 422-8076/FTS 532-8076

The emphasis of this study has been to determine thermodynamic data for Pu-Si compounds, because Si is an important constituent of Pu residual wastes and the data are needed to aid in developing pyrochemical processing methods for plutonium recovery. An approximate ΔH°_{f298} value has been determined for Pu_5Si_3 through a study of exchange reactions of selected metal silicides with molten plutonium. The reactions were carried out by arc-melting. Results show that Pu_5Si_3 is intermediate in stability between V_3Si and Mo_3Si, and has a ΔH°_{f298} of -52 ±13 kJ/g-atom. Estimates of ΔH°_{f298} for the higher plutonium silicides are: Pu_3Si_2 -54, PuSi -60, Pu_3Si_5 -58, and $PuSi_2$ -56 kJ/g-atom with uncertainties of ±18 kJ/g-atom. The plutonium silicides are found to be more stable than both the thorium and uranium silicides. Results of this study have been submitted for publication in the Journal of Nuclear Materials. No further work is planned at this time.

Keywords: Plutonium Silicides, Plutonium Thermodynamics, Pyrochemical Processing, Plutonium Residual Wastes

419. Electronic Structure in Superconducting Oxides FY 1989 $290,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
LLNL Contact: M. J. Fluss, (415) 423-6665/FTS 543-6665

We have designated three experimental task areas; materials synthesis and properties, electron structure, and thin films, all of which are guided and supported by a broad theoretical task in band structure, ligand field effects, and pairing mechanisms. The selection of these activity areas provides the basis for a flexible, but focused program which is contributing to the solution of critical problems in the search for an understanding of the oxide superconductors. Additionally, the thrust is sensitive to opportunities for utilization of the new superconductors in future LLNL programs and has explored processing and applications oriented activities.

Keywords: Superconductors, Electronic Structure, Positron Annihilation

420. Theory of Superconducting Oxides — FY 1989 — $450,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
LLNL Contact: A. McMahan, (415) 422-7198/FTS 532-7198

A variety of theoretical approaches have been used to study the nature of the charge carriers, the paring mechanism and the formation of a superconducting state in superconducting oxide materials. The properties of paired charge carriers of fractional charge in a superconducting mechanism were investigated as was the condensation of a two dimensional Bose-Coulomb gas. Calculations of the electronic structure of superconducting oxides were done based both on band theory and Hartree-Fock with configurational interactions. Both of these approaches suggested the importance of specific hole states in the superconducting mechanism. Results that directly describe laboratory experiments were obtained from the Hartree-Fock method for Mossbauer measurements and from linear combination of atomic and molecular orbitals in a cluster approach to describe electronic structure measurements made with positrons on several materials.

Keywords: Superconductors, Electronic Structure

421. A New Method for the Calculation of the Electronic Structure of Surfaces and Interfaces — FY 1989 — $150,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
LLNL Contact: A. Gonis, (415) 423-5836/FTS 543-5836

We have developed the formalism and associated computer codes for a new first-principles method for the calculation of the electronic structure of systems with reduced symmetry, such as surfaces and interfaces. In contrast to existing techniques, this new method treats exactly the semi-infinite extent of a surface or interface system. A version of the code has been extended to the calculation of self-consistent charge densities. Successful applications of the codes have been made to both model and ideal surfaces and grain boundaries in Cu, and the code is being further developed to be applicable to the study of realistic surfaces and interfaces, and adsorbates.

Keywords: Electronic Structure, Grain Boundary, Surface

Materials Properties, Behavior, Characterization or Testing

422. Nuclear Spin Polarization — FY 1989 — $1,100,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
LLNL Contact: P. C. Souers, (415) 422-1301/FTS 532-1301

The triton polarization memory time has proved to be too short in regular solid D-T and 95 percent molecular DT absorption of the D-T on silica aerogel foam shows promise of lengthening the memory time. Design of an adsorption column to purify DT has begun. A Raman spectrometer intended to measure small $J = 1$ T_2 levels in the DT is almost ready. Theory suggests that the deuteron should have a longer memory time and that triton-to-deuteron polarization may be possible. Electron spin resonance shows atom concentrations up to 1,000 ppm for use as pumpers in dynamic nuclear polarization. Heat spikes and a long electron relaxation time are negative findings. Design of a 0.5 K, 94 GHz polarization system, intended to be ready in 1992, has begun. This system will attempt polarization of the purified DT sample.

Keywords: Spin Polarization, Electron Spin Resonance

423. Measurement of Tritium Permeation Through Resistant Materials at Low Temperatures — FY 1989 — $90,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
LLNL Contact: Jon L. Maienschein, (415) 423-1816/FTS 543-1816

We measure tritium permeation by capturing, in liquid, tritium that permeates through a sample membrane. The liquid is subsequently analyzed by liquid scintillation counting. Because our apparatus is simple and inexpensive, we can run many replicates of each material for the lengthy periods that are required to reach steady-state permeation behavior. We therefore get an accurate measurement of the permeation rate. The high sensitivity of liquid scintillation counting allows us to measure very low permeation rates. In prior tests with many polycrystalline metals, including aluminum, beryllium, cadmium, copper, gold, iridium, lead, molybdenum, rhenium, silver, and tungsten, we showed that tritium transport along defects dominates the permeation process. Therefore, permeation measurements at higher temperatures cannot be extrapolated to low temperatures. We have made permeation measurements on single crystal copper, and have shown that they are consistent with extrapolation of high temperature results in the literature. We are currently preparing specimens of single crystal beryllium. Our data on single crystal beryllium will be the only true measurement in tritium permeation through that material, as all other data in the literature were taken with polycrystalline samples where transport along defects dominates the permeation rate. Future work will include measurements on other single crystal metals.

Keywords: Permeation, Tritium, Liquid Scintillation Counting

424. Pretransformation Behavior in Alloys FY 1989
$175,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
LLNL Contact: L. E. Tanner, (415) 423-2653/FTS 543-2653

Recent studies of displacive transformations indicate that vital information on their origins and mechanisms can be extracted from anomalous pretransformation behavior of the parent phase. Of particular interest is the evolution of atomic displacement modulations as the parent cools toward a martensitic transformation. Using the current generation of high-resolution structural probes, we are systematically examining microstructures in alloys from a variety of systems. Our primary experimental approach is with TEM and SAED at ambient temperature, as well as in situ at higher and lower temperatures. Elastic and inelastic neutron and X-ray scattering, Mössbauer spectroscopy and acoustic emission, and molecular dynamics simulation of a martensitic transformation are also being used to develop an understanding of pretransformation behavior.

Keywords: Metals: Ferrous and Non-Ferrous, Predictive Behavior Modeling

425. Interfacial Bonding in Multilayer X-ray Mirrors FY 1989
$25,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
LLNL Contact: A. F. Jankowski, (415) 423-2519/FTS 543-2519

A measurable improvement in the reflectivity of W/C multilayer X-ray mirrors has been developed through the fabrication of W/B_4C structures via planar magnetron sputter deposition. The cause of the improvement in performance is suspected to be structural in nature, specifically a reduction in interfacial roughness. The nature of carbon bonding in these thin film structures, the link to the presence of carbides—the source of interfacial roughness, is investigated using Auger Electron Spectroscopy with depth profiling.

Keywords: Films, Structure, Bonding, Reflectivity, X-ray Mirrors

426. ΔN=O Spectroscopy Using Multilayer Gratings FY 1989
$152,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
LLNL Contacts: T. W, Barbee, Jr., (415) 423-7796 and D. D. Dietrich, (415) 422-7868

Recent advances in normal incidence multilayer X-ray and extreme ultraviolet optics now make it possible to construct diffraction gratings in the wavelength range 40 to 800 Å which can be employed for precision measurements using normal incidence spectrometers. Normal incidence spectrometers have two important advantages in studying the spectra of foil-excited heavy ion beams from accelerators: (1) the sensitivity of normal incidence spectrometers is typically a factor of 10 or more higher than that of conventional grazing incidence spectrometers, and (2) it is possible to refocus normal incidence spectrometers so as to compensate for the Doppler width of the lines. An interesting candidate line for study by this technique is the $^{(1s)}1/2^{(2p)}(1/2)\ ^3P_0 \rightarrow {}^{(1s)}1/2^{(2s)}1/2^3S_1$ transition in helium-like ions. A precision measurement of this transition energy in highly-ionized atoms could provide the most precise test of QED effects in strong Coulomb fields. This transition has not been studied for $Z > 29$ because existing grazing incidence spectrometers are not sufficiently sensitive.

Keywords: Spectroscopy, Diffraction Gratings, X-ray Optics, UV Optics

427. Multilayer X-ray Optics Development FY 1989
$250,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
LLNL Contact: Troy W. Barbee, Jr., (415) 423-7796

Multilayers are vapor-deposited thin-film structures fabricated by sequential deposition of layers of compositionally-differing materials with individual layer thickens of from 0.10 to 50 nm. These in-depth microstructures are superlattices in terms of X-ray diffraction and may be applied as efficient-dispersion elements in the soft X-ray and extreme ultraviolet if of sufficient perfection. In this program, a strong effort has been directed to developing multilayer-optics instrumentation and optimized-material multilayers for specific spectral domains. During this period, synthesis of multilayers using materials expected to enhance multilayer stability was emphasized. Model calculations were performed and used as a basis for materials selection. Also, techniques for the synthesis of small period multilayers have been addressed.

Keywords: Multilayer-Optics, X-ray Optics

428. Thin Film X-ray Studies

FY 1989
$80,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
LLNL Contact: Troy W. Barbee, Jr., (415) 423-7796

Grazing incidence X-ray fluorescence studies of ultra thin copper films 0.1, 0.5, 1.0, 2.0, and 5.0 monolayers thick deposited on 500 Å thick tungsten were performed on BL 10-2, a 30 pole wiggler insertion device sources, at the Stanford Synchrotron Radiation Research Laboratory. It was demonstrates that EXAFS from these low surface concentration samples was easily obtainable. This will allow studies of interface formation and thin film nucleation and growth characteristics during growth.

Keywords: Multilayer-Optics, Diffraction Gratings, Microlithography, Thin Films

429. *In Situ* Reversed Deformation Experiments

FY 1989
$20,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
LLNL Contact: M. E. Kassner, (415) 523-2329/FTS 543-2329

There has been, in the past, only limited success by the general scientific community with *in situ* cyclic or reversed plastic deformation tests in the high-voltage transmission electron microscope (HVEM). This is due to problems associated with buckling of thin foils when an applied tensile or shear stress is reversed. Analysis has shown that dislocation movement can be reversed by tensile stressing in alternating perpendicular directions (i.e., 90° rotations of a tensile stress); thus, buckling of the foil can be avoided. A new design by the author for performing such X-Y in situ HVEM tests has provided preliminary success. The X-Y tests are designed to be performed on the 1-MeV HVEM located at the Metals Research Institute, Apeldoorn, The Netherlands, utilizing specimens that are prepared by techniques that will be developed by our research. The first set of FY 1986 tests demonstrated that *in situ* X-Y mechanical tests can be performed on thin (5-um) foils in which a "cyclic" micro structure exists. Special specimen-preparation procedures to accomplish this were quite successful. We have, therefore, provided the metallurgical community with an experimental procedure that is capable of observing fatigue at the atomic level. Single crystal experiments are currently underway.

Keywords: Metals, Structure, Mechanical Properties, Fatigue

430. Dislocation Microstructure of Aluminum and Silver Deformed to Large Steady-State Creep Strains

FY 1989
$90,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
LLNL Contact: M. E. Kassner, (415) 423-2329/FTS 543-2329

Large Strain Deformation experiments on pure polycrystalline silver between $0.16T_m$ and $0.30T_m$ confirm mechanical saturation; by dynamic recrystallization at $0.30T_m$ and by dynamic recovery at ambient temperature and below. Various rate-controlling mechanisms were considered. Stage IV hardening was observed at strain of about 0.50 and may be the result of the formation of very small subgrains ($\approx 1/4$ μm dia) whose boundaries have a relatively high misorientation.

The elevated temperature single crystal torsional deformation experiments on aluminum have confirmed "geometric-dynamic recrystallization" as the mechanism for the dramatic increase in high angle boundary area in heavily deformed polycrystalline aluminum.

Furthermore, large strain deformation of polycrystalline aluminum at elevated temperatures confirms "extended ductility." Initially, increased temperature results in increased torsional ductility due to dynamic recovery. However, eventually cavity-growth (initiated by grain boundary sliding) causes reduced ductility with increasing temperature. These mechanisms are consistent with the observed changes in ductility with strain-rate.

Keywords: Metals: Non-Ferrous, High-Temperature Behavior, Creep

431. Delayed Failure of Silver-Aided Diffusion Bonds

FY 1989
$190,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
LLNL Contact: M. E. Kassner, (415) 423-2329/FTS 543-2329

A very wide variety of non-weldable (by conventional fusion welding or brazing) or otherwise difficult-to-join metals can be very effectively joined by silver-aided diffusion bonding. The intermediate layer of silver is applied to the facing surfaces using planar magnetron sputter deposition. Joining of the silver interfaces is accomplished by applying pressure and elevated temperature (below the melting point of the metals). The tensile strengths of thin interlayer joints can be quite high (>700 MPa). However, delayed or creep failure is observed within a few months at stresses that are just 25 percent of this value. Experiments performed during the past year have confirmed that several distinct failure mechanisms can be rate controlling depending upon the strength and type of base metal used. For joints where there is significant time-dependent plasticity in the base metal, delayed tensile failure in the silver interlayer is controlled by creep in the base metal. When the base metal is non-yielding or exhibits a very low creep rate, tensile stress rupture is controlled by a mechanism within the silver interlayer (e.g., coupled cavity growth). For joints subject to in-plane shear stresses, delayed failure is controlled by the steady-state creep of the silver interlayer. When uranium is used as a base metal, stress corrosion cracking has been observed at the silver-uranium interface if the bonds are stressed in high relative humidity environments.

Keywords: Metals, Bonding Agents, Diffusion, Creep, Joining and Welding

432. Constitutive and Failure Behavior of Metals at High Rates of Tensile Strain FY 1989 $290,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
LLNL Contact: W. H. Gourdin, (415) 422-8093/FTS 532-8093

The model correctly describes the interplay between temperature and strain rate and provides a good description of the stress-strain behavior for strain rates between 10^{-3} and $10^{4}s^{-1}$ and temperatures between 25°C and 400°C. Ring studies of electrodeposited and previously shock loaded copper have been performed, and both show a larger flow stress than the finest grain sized OFE copper. Electrodeposited coppers also display a significantly reduced elongation to failure. The expanding ring experiment has been moved to a new facility, and the necessary redesign has resulted in a more stable and more easily aligned apparatus.

Keywords: Metals, Expanding Rings, Constitutive Properties, Failure, High Strain-Rate

433. Theoretical and Experimental Studies of Solid Combustion Reactions FY 1989 $190,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
LLNL Contact: J. B. Holt, (415) 422-8003/FTS 532-8003

A mathematical model for condensed-phase combustion involving a sequential reaction mechanism was derived. The model accounts for the evolution of the concentrations of the reactants and intermediate species, as well as the temperature and includes the effects of melting. This model will be applied to thermite-type combustion which involves sequential reactions. Precise methods to measure temperature profiles at the combustion front and to observe propagation instabilities have been developed. Temperature profiles of the $Ti + C \rightarrow TiC$ reactions were measured and the raw experimental data was smoothed so that both 1st and 2nd derivatives could be calculated. From this data it should be possible to define the kinetic constants and the mechanism of reaction.

Keywords: Combustion, Reactions, Mathematical Modeling

434. Fracture Behavior of Refractory Metals and Alloys in Liquid Actinides

FY 1989
$100,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
LLNL Contact: J. S. Huang, (415) 422-5645/FTS 532-5645

Deformation and fracture behaviors of Nb and Ta metals and alloys in liquid U are studied using slow-rate tensile testing at high temperatures. The interaction between the metals and liquid actinide are studied with optical and scanning electron microscopy, and electron microprobe analysis. The results indicate that Nb and Nb-based alloys remain ductile in liquid U, while Ta and Ta-based alloys are severely embrittled. The embrittlement in Ta and Ta alloys is associated with a very fast grain boundary penetration of U. The difference between Nb and Ta is currently related to the difference in mutual solubility between the U-Ta system and the U-Nb system.

Keywords: Deformation, Fracture, Actinide, Solubility, Refractory Metals

435. Modeling and Experimental Measurement of Residual Stress

FY 1989
$160,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
LLNL Contact: E. Flower, (415) 423-1572/FTS 543-1572

Our goal is to further understand the evolution of residual stresses in metal components and to determine strengths and limitations of measurement techniques. We have used the finite-element codes NIKE2D and NIKE3D to predict the evolution of residual stresses in metal components. We have compared the effectiveness of neutron and X-ray diffraction, as well as acoustoelastic and blind hole drilling, for measuring these stresses. We are also reviewing recent literature to determine if improved techniques of measuring residual stresses could be developed. We have gained confidence in the principle of the diffraction technique but have recognized that measurements with neutrons or X-rays are severely limited if they are confined to the surface. From the literature review, we find that this limitation is being overcome with higher energy X-ray sources and with energy-dispersive diffraction.

Keywords: Metals, Predictive Behavior Modeling, Mechanical Properties

436. Failure Characterization of Composite Materials FY 1989 $117,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
LLNL Contact: Scott E. Groves, (415) 422-1331

The primary objective of this research is to characterize the three-dimensional failure response of continuous fiber graphite epoxy composite materials. This effort includes the development of a new failure criterion, generation of the three-dimensional failure data, and an investigation of the dynamic strength behavior. This research represents a continuation of an ongoing project initiated in mid FY87. The primary effort to date has centered on the development of the necessary experimental techniques required to generate the complex failure response of these materials. A biaxial test system has been developed for applying tension, torsion, and internal pressure to 2-inch diameter composite tubes. This system has been successfully used to obtain the biaxial failure surface for T300/F263 graphite epoxy with a [0.45,-45,90]s orientation. Future work will characterize the failure response for Toray 1000, Hitco 900, and Hercules IMe fibers which will be matrixed with a DER332/2403 resin derivative. The new failure criterion is written in terms of the elastic strain invariants and will utilize the concepts of multipolar continuum mechanics to model the complex global failure mechanisms.

Keywords: Composite Materials, Fibers, Failure Testing

437. Surface Modification to Reduce Abrasion and Friction FY 1989 $100,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
LLNL Contact: Herman R. Leider, (415) 423-1884/FTS 543-1884

We have shown that hair-like ceramic fibers can effectively protect surfaces from abrasion by hard particles entrained in flowing gases over a useful range of air flow. The limits for which such structures are effective can be defined by a simple model of impact failure. In principal, the range of conditions over which ceramic "hair" will protect surfaces can be extended by using higher strength materials, either larger diameter fibers of a given material, or other intrinsically stronger materials. Ceramic hair, if attached to a substrate by ceramic or metallic bonding could be very useful at relatively high temperatures. If hair structures at higher fiber packing density becomes available, better performance could be expected.

Keywords: Abrasion, Carbon Fibers, Ceramics, Fibers, Protective Coatings

438. <u>Numerical Modeling of Crack Growth</u> FY 1989
$145,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
LLNL Contact: R. A. Riddle, (415) 523-7541/FTS 543-7541

Thermal stresses are a common cause of failure in glass and other brittle solids. These failures are typically associated with crack growth. In order to solve thermal stress cracking problems a J integral post processor has been implemented for use with finite element codes NIKE2D and TOPAZ2D. Based on a thermal stress analysis of a cracked body subjected to temperature boundary conditions, the tendency for catastrophic crack growth may be predicted. Crack extension from an existing crack is predicted based on a critical energy release rate (a J integral value), which in turn is related to a critical stress intensity factor. This J Integral post-processor has been the subject of a thorough verification and has been used in conjunction with an experimental effort to measure critical stress intensity factors for stressed glass plates under Mode I and Mode II loading.

Keywords: Crack Growth, Deformation, Predictive Behavior Modeling, Metals: Ferrous and Non-Ferrous, Glass Ceramics

439. <u>Interfaces, Adhesion, and Bonding</u> FY 1989
$600,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
LLNL Contact: Wayne E. King, (415) 423-6547

The influence of interfaces on materials properties is controlled by mechanisms that are operative over the range of length scales from atomic to macroscopic dimensions. Detailed determination of the operative mechanisms requires theory validated by comparable experiments. Theoretically, 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. Currently, it is not possible to predict atomic relaxations using the RSMST (because of the large computational resources that would be required) so we have coupled this method with the semi-empirical embedded atom method (EAM) which uses modified two-body potentials with molecular dynamics, molecular statics, or Monte Carlo techniques to determine atomic rearrangements. These methods are at present limited to metallic systems; however, the extension of one or both methods to metal/ceramic interfaces appears to be possible.

Our experimental effort will produce results that are directly comparable with theoretical calculations. Consequently, our initial investigations will treat planar metal/metal interfaces and metal/ceramic interfaces (in anticipation of improvements in the theory) of well defined misorientations relative to the perfect crystal. 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 recently demonstrated at the Max-Planck-Institut, Institut für Werkstoffwissenschaft, Stuttgart, W. Germany (MPI). Initially, bicrystals will be obtained through a collaboration with MPI. An ultra-high-vacuum diffusion bonding machine will be developed in parallel with the proposed research project (in collaboration with Sandia National Laboratories-Livermore) for installation at LLNL. Some special interfaces, such as the Σ5 tilt grain boundary in Au, can be obtained by vapor deposition; however, these interfaces are suitable only for structural studies. We have selected systems for investigation that exhibit interesting properties, e.g., the Ag/Ni systems shows limited solubility while Ag readily bonds with Ni in the UHV Bonding Machine.

Keywords: Interfaces, Bonding, Electronic Structure

Device or Component Fabrication, Behavior or Testing

440. IC Protective Coatings — FY 1989 $720,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
LLNL Contact: R. A. Riddle, (415) 523-7541/FTS 543-7541

We are developing coatings which are designed to protect the memory of ICs against intrusion and their architecture against reverse engineering. These materials must be capable of preventing easy access. We have fielded the first two generations of these materials. Current development efforts are devoted to the third and fourth generation coatings.

Keywords: IC Protection, Protective Coatings

441. Characterization of Solid-State Microstructures in High Explosives by Synchrotron X-ray Tomography — FY 1989 $50,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
LLNL Contact: W. C. Tao, (415) 423-0499/FTS 543-0499

After demonstrating the feasibility of using 3D Microtomography to study pore distributions in materials with similar X-ray absorption coefficients as high explosives (HE), we have successfully applied the non-invasive techniques to characterize the detailed microstructures in HMX single crystals and a composite formulation consisting of fuel (RDX, NG/TA), oxidizer ($NaNO_3$), and metallic additives (aluminum). Due to cancellation of two dedicated runs at the Stanford Synchrotron Research Lab, we have performed the experiments using a conventional X-ray source coupled with the analytical software and data acquisition hardware developed for 3D Microtomography. Although the exposure time is lengthened and the spatial resolution is decreased slightly, we were able to resolve the topographical features of the HMX single crystal, the tomographical structure at a depth equal to 25 percent of the crystal thickness, and identify the aluminum and pore distribution in the composite mixture. The inability to probe the bulk of the HMX crystal for microstructural defects is due to beam hardening and penumbral blurring, both inherent technical inefficiency in a conventional X-ray source. With an intense source of monochromatic and tunable X-ray beam, such as that from a Synchrotron facility, we will be able to image the bulk crystal. The composite formulation examined supposedly was non-porous with the 5 μm aluminum dispersed evenly throughout the matrix. From our results, we found that the aluminum was not dispersed below a 50 μm scale, and the composition has approximately 5 percent porosity. This provided insights into the degree of mixing and wetting between components in the composite formulation as related to the formulation methodology. To further test our experimental capability, we designed a phantom matrix using the X-ray absorption coefficients for HMX,. with a complex integration of defect structures (pores, aluminum, orthorgonal microcracks, density gradients), and subjected this phantom for 3D Tomography analysis. Using a well characterized Synchrotron beam profile and the radiometric deconvolution techniques of our analytical software, we were able to reproduce the image of the phantom with minimal loss in structural resolution. This again demonstrates the capability of 3D Microtomography for examining defect microstructures in high explosives. These results were presented at the 9th Detonation Symposium at Portland, Oregon. The next phase of the research involves studying the correlation between microstructural defects and initiation sensitivity. Two experimental methods will be employed in this phase of the study: microphotography and infrared emission mapping. Coupled with both streak and frame cameras, ultrafast microphotography allows us to examine a single crystal under shock loading with a spatial and temporal resolution of 1 micron and 1 nsec, respectively. Measuring the infrared emission vs. time yields information on the mechanism of Hot-Spot formation and dissipation.

Keywords: Synchrotron, X-ray, High Explosive, Single Crystal, Initiation Sensitivity, Defect Microstructure, Non-Destructive Characterization

442. <u>Optical Diagnostics of High Explosives Reaction Chemistry</u> <u>FY 1989</u>
$175,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
LLNL Contact: S. F. Rice, (415) 423-3258/FTS 543-3258

This research effort falls into two general technical areas: (1) high pressure deflagration of high explosives within a diamond anvil cell coupled with single shot coherent anti-Stokes Raman spectroscopy (CARS) designed to measure the pressure dependence of rapid decomposition and product formation and (2) using the spectral properties of Mie scattering to study time dependence and shock intensity sensitivity of the generation of sub-micron carbon particles in reacting high explosives and other energetic materials.

Progress has continued in both areas from FY 1988. We have extended the burn rate curve of nitromethane to 40 GPa and have observed an interesting deuterium isotope effect on these rates in CD_3NO_2. Preliminary work has begun to extend this technique to HMX, RDX, and TATB. Seven shots were conducted on the scattering properties of shocked benzene. The timescales of the production of carbon particles as well as light absorbing molecular transients has been identified.

Keywords: Reaction Zone Chemistry, High Explosive Carbon Particle Formation, Time Resolved Diagnostics

Instrumentation and Facilities

443. Scanning Tunneling Microscope — FY 1989 $165,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
LLNL Contact: W. Siekhaus, (415) 422-6884/FTS 532-6884

Scanning tunneling microscopy and spectroscopy in air were used to study the structure of surfaces and of molecules adsorbed on surfaces. Carbon films deposited as antifriction coatings were shown to be a mixture of graphitic and diamond-like material. The structure of sulfur adsorbed on single crystal molybdenum and rhenium (via the dissociation of H_2S) were determined, and in the case of molybdenum it was shown by measuring the height variation of the adsorbed sulfur atoms that sulfur atoms are located in bridge sites only, and not alternately in bridge sites and four-fold sites—a fact difficult to determine by LEED techniques. Double stranded DNA from calf-thymus adsorbed on the basal plane of graphite was imaged with a resolution sufficient to resolve the helical structure and moreover the minor and major groove, the DNA helix. This was achieved without coating the adsorbed DNA.

Keywords: Instrumentation and Technique Development, Surface, Structure

444. Scanning Tunneling Microscopy (STM) and Atomic Force Microscope (AFM) as a Detector

FY 1989
$20,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
LLNL Contact: W. Siekhaus, (415) 422-6884/FTS 532-6884

Based on our STM design, we have built and are operating now an atomic force microscope using a tungsten needle as the touching and deflecting element, and measuring the deflection of the needle by fiber-optical techniques. The instrument performs both as STM and AFM with angstrom resolution.

Keywords: Optical Components, Instrumentation and Technique Development, Defects, NDE

445. Tritium Facility Upgrade

FY 1989
($11,900,000)*

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
LLNL Contact: G. M. Morris, (415) 423-1770/FTS 543-1770

The Tritium Facility Upgrade (TFU) consists of three line items: (1) a new 5,700 square foot office addition along with modification of 2,000 square feet of the existing facility, (2) a Vacuum Effluent and Recovery System (VERS) designed to recover over 90 percent of the existing routine stack emissions, (3) a Secondarily Contained Tritium System (SCOTS) which replaces the existing low and high pressure systems with a modern totally secondarily contained system. This is designed to capture and then recover via VERS any accidental spill when handling large quantities of tritium.

Presently, the office addition is complete and has received final DOE acceptance. VERS design and construction is complete and is presently in the final acceptance testing phase. SCOTS is in final design stage with construction approximately 80 percent complete. Scheduled project completion is in February 1990.

Keywords: Facilities, Tritium

*Line-Item Construction Project: not included in subtotal or total.

446. Decontamination and Waste Treatment Facility (DWTF) FY 1989
($7,700,000)*

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
LLNL Contact: R. Quong, (415) 422-7093/FTS 532-7093

Construction of the DWTF is scheduled to be completed by year-end 1992. The project started in FY86; through FY89, 19 percent of the $41.3 million authorized funds has been expended. Title 2 final design is complete. A draft environmental impact statement (DEIS) has been prepared and issued for public comment. Applicable permits (RCRA and Air Quality) have been submitted and have undergone initial review by the regulatory agencies. The progress of the environmental documentation and permits has been slowed by an ongoing internal review of the DWTF by the Laboratory. Some changes in the facility design is anticipated. The DWTF is a line-item construction project comprising seven new buildings (88,000 square feet of new building space) plus a full complement of treatment equipment including a rotary kiln incinerator system. The facility will occupy a 6-acre site within the laboratory, replace existing outmoded facilities, and will greatly diminish the need for off-site treatment and disposal of waste generated by the laboratory.

Keywords: Facilities, Waste Treatment

Los Alamos National Laboratory

Materials Preparation, Synthesis, Deposition, Growth or Forming

447. Actinide Alloy Development FY 1989
$1,350,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
LANL (Contract No. W-7405-ENG-36) Contact: D. C. Christensen, (505) 667-2345/ FTS 843-2345

The aim of this project is the development and characterization of fabrication processes and the study of new alloys of plutonium. Research involves casting, thermomechanical working, and stability studies. Measurements of resistivity, thermal expansion and bend ductility are made to evaluate fabrication processes and alloy stability.

Keywords: Radioactive Materials, Plutonium Alloys, Ductility, Thermal Expansion, Electrical Resistivity, Stability

*Line-Item Construction Project: not included in subtotal or total.

448. Plutonium Oxide Reduction FY 1989
$150,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
LANL (Contract No. W-7405-ENG-36) Contact: D. E. Peterson, (505) 667-5181/ FTS 843-5181

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

449. Ion-Beam Implantation FY 1989
$200,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
LANL (Contract No. W-7405-ENG-36) Contact: D. V. Duchane, (505) 667-6887/ FTS 843-6887

Ion implantation is being explored as a means for surface modification of a variety of materials. This technique has been proven effective at modifying the surface structure of materials to a depth of about one micron. Improved surface hardness and corrosion resistance are but two of the expected benefits.

Keywords: Ion Implantation, Surface Modification, Corrosion Tribology

450. Electroplating Low Atomic Number Materials FY 1989
$100,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
LANL (Contract No. W-7405-ENG-36) Contact: D. V. Duchane, (505) 667-6887/ FTS 843-6887

Aqueous solutions presently limit the metals that can be electroplated. This project is looking at electroplating low-atomic-number metals (aluminum and beryllium) by using non-aqueous plating baths. These new baths include solvents and fused salts. Applications include weapons components and inertial confinement fusion (ICF) target fabrication.

Keywords: Electroplating, Aluminum, Beryllium, Coatings, Metals

451. Liquid Crystal Polymer Development FY 1989
$200,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
LANL (Contract No. W-7405-ENG-36) Contact: D. V. Duchane, (505) 667-6887/ FTS 843-6887

Conventional liquid crystal polymers possess high strength in only one direction. Working with theoretical physicists, an attempt are being made to synthesize a liquid crystal polymer with strength in three dimensions. This will be a unique polymer with a number of possible applications. Low to medium molecular weight polymers have been synthesized.

Keywords: Liquid Crystal Polymers

452. Surface Property Modified Plastic Components FY 1989
$50,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
LANL (Contract No. W-7405-ENG-36) Contact: D. V. Duchane, (505) 667-6887/ FTS 843-6887

The surface properties of plastic components can be modified by a solvent infusion process. This process may be used to improve the biocompatibility properties of such plastics as acrylics and silicones.

Keywords: Acrylics, Silicones, Polymers, Surface Properties

453. Low-Density, Microcellular Plastic Foams FY 1989
$300,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
LANL (Contract No. W-7405-ENG-36) Contact: D. V. Duchane, (505) 667-6887/ FTS 843-6887

Microstructural polyolefin foams with densities between 0.01 g/cc and 0.2 g/cc are manufactured by a nonconventional foaming process. Foams are open-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 25um down to the 1um range depending on the process. Composite foams are being produced with submicron cell sizes while maintaining structural properties.

Keywords: Foams, Polyolefins, Polyurethanes, Silicones, Polyesters

454. Target Coatings FY 1989
$400,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
LANL (Contract No. W-7405-ENG-36) Contact: D. V. Duchane, (505) 667-6887/FTS 843-6887

Single and multilayer metallic and nonmetallic thin-film coatings, smooth and uniform in thickness are being prepared. Substrates are planar and nonplanar and made of metal, glass, or plastic. Coatings may be bulk density or fractional bulk density and may also be free standing.

Keywords: Coatings and Films, Physical Vapor Deposition

455. Physical Vapor Deposition and Surface Analysis FY 1989
$700,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
LANL (Contract No. W-7405-ENG-36) Contact: D. V. Duchane, (505) 667-6887/FTS 843-6887

Physical vapor deposition and 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 plating of aluminum and rare earth oxides onto various substrates for corrosion resistance to gases and liquid plutonium, deposition of oriented AlN onto various substrates is accomplished to enable nondestructive evaluation of materials, 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

456. Chemical Vapor Deposition (CVD) Coatings FY 1989
$200,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
LANL (Contract No. W-7405-ENG-36) Contacts: J. R. Laia and D. W. Carroll, (505) 667-3239/FTS 843-3239

Chemical vapor deposition (CVD) techniques are used to deposit thin-film and bulk coatings of a wide variety of elements and compounds. Coatings are deposited by the following techniques: conventional flow-by, fluidized-bed, plasma-assisted, and chemical vapor infiltration. To support and enhance our basic CVD program, efforts are underway to study the fundamental nature of the CVD process, including *in-situ* diagnostics in the gas phase just above the substrate and modeling efforts to predict gas flows, reactor design, and chemical behavior within the CVD systems. Another collaborative effort at Los Alamos is attempting to synthesize organometallic precursors to deposit coatings at temperatures <300°C. Substrates coated by the CVD technique range from particles 2.0 μm diameter to infiltrations of fabrics a square meter in area.

Applications include nuclear and conventional weapons, space nuclear reactor systems (fuels and structural components), inertial confinement fusion program, high temperature engine and structural components for advanced high-performance aircraft, hard/wear resistant coatings (tribological), corrosion resistant coatings, coatings of complex geometries, near-net-shape fabrication, heat-pipe structures, precision CVD of ultra-thin, freestanding shapes.

Keywords: Chemical Vapor Deposition, Coatings (metal and ceramic)

457. Synthesis of Metallic Glasses — FY 1989 $75,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
LANL (Contract No. W-7405-ENG-36) Contact: A. Mayer, (505) 667-1146/FTS 843-1146

Synthesis of amorphous alloys by electrodeposition is presently possible only with the iron group metals alloyed with metalloids such as phosphorus. In collaboration with the Los Alamos Center for Materials Science, we are investigating the feasibility of synthesizing other metallic glasses by electrochemical and chemical reduction techniques. We have had encouraging results in depositing amorphous coating of cobalt-tungsten and nickel-tin-phosphorus alloys by electrodeposition. We have also produced small quantities of amorphous cobalt-boron alloy powders by a chemical reduction technique from aqueous solutions. Applications include: hard coatings, corrosion-resistant coatings, coatings for weapons physics experiments and inertial confinement fusion components, and possibly biomedical applications.

Keywords: Metallic Glasses, Amorphous Alloys, Electrodeposition, Metals

458. Polymers and Adhesives — FY 1989 $803,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
LANL (Contract No. W-7405-ENG-36) Contact: D. A. Hemphill, (505) 667-8335/ FTS 843-8335

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 to 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, high strength reinforced composites, cushioning materials, and high-explosive compatible adhesives, potting materials, and castable loaded thermoplastics.

Keywords: Adhesives, Composites, Plastics, Polymers, Weapons Design, Weapons Engineering, Integrated Contractors

459. Tritiated Materials FY 1989
$511,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
LANL (Contract No. W-7405-ENG-36) Contact: D. H. W. Carstens, (505) 667-5849/ FTS 843-5849

Advanced research and development efforts are focused on tritiated metals and other materials with the emphasis on Li(D,T) (salt) and other metal tritides. New methods for preparing, fabricating, and containing such compounds are under investigation. We are also developing laser-Raman techniques for *in situ* measurements or deuterium-tritium gas mixtures, and kinetic studies of hydrogen-metal interactions.

Keywords: Tritium, Metal Tritides, Li(D,T), Tritiated Materials, Radioactive Materials

460. Salt Fabrication FY 1989
$379,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
LANL (Contract No. W-7405-ENG-36) Contact: D. H. W. Carstens, (505) 667-5849/ FTS 843-5849

Development and evaluation of new fabrication and containment processes for Li(D,T) (salt). Research topics include development of hot pressing, machining techniques for salt compacts, new containment methods, and studies of radiation induced growth and outgassing.

Keywords: Tritium, Hydrides, Machining, Radioactive Materials, Near-Net-Shape Processing

461. Slip Casting of Ceramics FY 1989
$150,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
LANL (Contract No. W-7405-ENG-36) Contact: G. F. Hurley, (505) 667-9498/ FTS 843-9498

We are slip casting many ceramics including alumina, magnesia, and thoria. The technology uses colloidal chemistry and powder characterization theory along with materials engineering. Bodies so formed are used in many energy technologies including nuclear reactors. Development problems include processing of powder to yield satisfactory sintering and shrinkage. Success may lead to improved materials with superior strength. We are now investigating the use of this technology to form thermal-shock-resistant bodies from transformation-toughened ceramic alloys.

Keywords: Ceramics, Microstructure, Strength, Sintering Refractory Liners, Thoria, Transformation Toughened Ceramics, Thermal Shock

462. Whisker Growth Technology FY 1989
$120,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
LANL (Contract No. W-7405-ENG-36) Contact: P. D. Shalek, (505) 667-6863/ FTS 843-6863

Silicon carbide whiskers are grown by a vapor-liquid-solid process which produces very long fibers. Research on this program is directed towards optimizing this process to grow whiskers of appropriate length for use in staple yarns and subsequent woven cloths. These materials are to be used as oriented reinforcement to give high strength epoxy matrix composites.

Keywords: Whiskers, Yarns, Polymer Matrix Composites

463. New Hot Processing Technology FY 1989
$300,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
LANL (Contract No. W-7405-ENG-36) Contact: H. Casey, (505) 667-4365/FTS 843-4365

Hot pressing techniques are used to consolidate bodies of materials such as Al_2O_3, ZrO_2, UO_2, B_4C, copper, aluminum, and carbon. Applications are for Los Alamos and other national laboratory programs, and include armor, ceramic components for nuclear reactor meltdown experiments, nuclear shielding, and filters.

Keywords: Ceramics, Metals, Composites, Microstructure, Hot Pressing, High Temperature Service, Nuclear Reactors, Filters, Hot Isostatic Pressing

464. Glass and Ceramic Coatings | FY 1989 $40,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
LANL (Contract No. W-7405-ENG-36) Contact: R. E. Honnell, (505) 667-5432/ FTS 843-5432

Components employing ceramic-metal seals, metallizing, and insulating coatings are fabricated for various groups associated with accelerator technology. Novel material applications are used to solve difficult electrical problems. Ceramic coated metals have been investigated for liquid metal containment.

Keywords: Enamels, Ceramic Coatings, Metals, Radiation Effects, Accelerator Technology

465. Cold Pressing, Cold Isostatic Pressing and Sintering | FY 1989 $10,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
LANL (Contract No. W-7405-ENG-36) Contact: G. F. Hurley, (505) 667-9498/ FTS 843-9498

Cold pressing and cold isostatic pressing are used to consolidate ceramic and metal powders to support laboratory programs. Materials processed include UO_2, ThO_2, Al_2O_3, Y_2O_3, and MgO. End uses include plutonium processing hardware and fluxes, simulated fuel pellets, high temperature resistant ceramics for nuclear reactors.

Keywords: Cold Pressing, Sintering, Ceramics

466. Plasma-Flame Spraying Technology | FY 1989 $185,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
LANL (Contract No. W-7405-ENG-36) Contact: H. Casey, (505) 667-4365/FTS 843-4365

Free-standing shapes and metallic and ceramic coatings are fabricated by plasma spraying. Materials examined recently include Fe_3O_4, Al_2O_3, tungsten, and LiF, among others. Parts of this work involve investigation of ultrasonic-assisted densification to produce high density coatings. 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

467. Rapid Solidification Technology FY 1989
$100,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
LANL (Contract No. W-7405-ENG-36) Contact: H. Casey, (505) 667-4365/FTS 843-4365

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

468. Superplastic Forming FY 1989
$150,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
LANL (Contract No. W-7405-ENG-36) Contact: H. Casey, (505) 667-4365/FTS 843-4365

Superplastic forming of titanium and uranium alloys is being investigated. Demonstration components made with titanium alloys will be completed. Fine grained Uranium alloy (2mm grain size) has been shown to exhibit superplasticity and will be evaluated in biaxial forming.

Keywords: Superplastic Forming, Near-Net-Shape, Titanium, Uranium Alloys

469. Microwave Sintering/Processing FY 1989
$120,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
LANL (Contract No. W-7405-ENG-36) Contact: J. D. Katz, (505) 667-1424/FTS 843-1424

In this program, techniques of bonding and sintering ceramics are being investigated. Materials under study include Al_2O_3, B_4C and TiB_2 as well as ceramic composites such Al_2O_3-SiC platelets. The method involves the use of 2.45 GHz microwaves which couple directly to the area in which the heat is needed. It has potential technical advantages related to heat distribution effects and a cost advantage because only the part is heated. Problems to be investigated include the control of the heating and its effect on microstructure.

Keywords: Ceramics, Sintering, Microwave Sintering, RF Heating

470. Predictions of Super Strong Polymers FY 1989
$565,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
LANL (Contract No. W-7405-ENG-36) Contact: Flonnie Dowell, (505) 667-8765/ FTS 843-8765

Advanced, first-principles, microscopic, molecular statistical-physics theories have been originated and developed into mathematical models that have been used to predict (with the aid of computer-based modeling) new molecular structures most likely to form super strong polymers. These candidate molecules are being chemically synthesized and will be experimentally characterized. The theoretical work is continuing with emphasis on the prediction of other mechanical and dynamic properties, solvent effects, and processing conditions.

Keywords: Super Strong Polymers, Modeling

471. High Energy Storage Material FY 1989
$200,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
LANL (Contract No. W-7405-ENG-36) Contact: D. V. Duchane, (505) 667-6887/ FTS 843-6887

A recently developed copolymer of vinyl fluoride/trifluorethylene has dielectric properties which may make it useful in extremely high density energy storage applications. Capacitors made using this polymer may be able to store up to 50 times the energy of Mylar capacitors of similar dimensions. Synthesis routes to this copolymer and variations of it, and processing techniques are being developed. Applications involving electrical energy storage and rapid delivery of electrical power are being evaluated.

Keywords: Energy Storage, Capacitors, Polymeric Insulators/Dielectrics

472. Synthesis of Ceramic Coatings FY 1989
$30,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
LANL (Contract No. W-7405-ENG-36) Contact: C. P. Scherer, (505) 665-3202/ FTS 855-3202

The objective of this effort is to synthesize Ceramic Films for liquid metal containment. Organic and aqueous solvents are of interest, but initial efforts have focused on nonaqueous. Film materials of interest include erbia, yttria, and magnesia.

Keywords: Ceramic Coatings, Sol Gel

473. Laser Surface Treatment of Materials FY 1989
$250,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
LANL (Contract No. W-7405-ENG-36) Contact: D. V. Duchane, (505) 667-6887/ FTS 843-6887

Laser surface treatment of metals such as stainless steel and titanium coated stainless steel is being investigated. An excimer laser is used to briefly melt the top micron layer of the material. During this time diffusion and/or ion mixing takes place resulting in a change in surface properties without a deterioration of bulk properties.

Keywords: Laser Surface Treatment, Stainless Steel, Titanium Diffusion

Materials Structure or Composition

474. Actinide Surface Properties FY 1989
$700,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
LANL (Contract No. W-7405-ENG-36) Contact: D. C. Christensen, (505) 667-2556/ FTS 843-2556

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

475. Neutron Diffraction of Pu and Pu Alloys FY 1989
$237,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
LANL (Contract No. W-7405-ENG-36) Contact: A. C. Lawson, (505) 667-8844/ FTS 843-8844

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

476. Surface, Material and Analytical Studies — FY 1989 — $175,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
LANL (Contract No. W-7405-ENG-36) Contact: W. C. Danen, (505) 667-4686/FTS 843-4686

Studies are underway in three key areas: surface and interfacial structures and properties, explosives dynamics, and laser-based isotopic analysis. Current investigations in surface and interfacial studies include: surface modification, HTSC composition and structure, and the use of MeV ion beams. In explosives chemistry, we are using real-time optical- and mass-spectral methods to probe the early-time dynamics of detonation. Analytical studies have centered on the use of resonance ionization mass spectrometry to eliminate isobaric interferences in the measurement of high-dynamic range isotope ratio measurements.

Keywords: Surface, Explosives, Interfaces

Materials Properties, Behavior, Characterization or Testing

477. Mechanical Properties of Plutonium and Its Alloys — FY 1989 — $450,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
LANL (Contract No. W-7405-ENG-36) Contact: M. Stevens, (505) 667-4414/FTS 843-4414

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

478. Phase Transformations in Pu and Pu Alloys — FY 1989 — $450,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
LANL (Contract No. W-7405-ENG-36) Contact: M. Stevens, (505) 667-4414/FTS 843-4414

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

479. Isobaric Expansion of Actinides FY 1989
$200,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 3098
LANL (Contract No. W-7405-ENG-36) Contact: R. Mulford, (505) 667-3543/FTS 843-3543

The V-T relationships in liquid actinide elements are determined by isobaric expansion measurements at high temperatures to 8000K. The facility developed for this work can be used to study other hazardous materials.

Keywords: Radioactive Materials, Plutonium Alloys, Thermal Expansion, Equation of State

480. Plutonium Shock Deformation FY 1989
$350,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 3098
LANL (Contract No. W-7405-ENG-36) Contact: M. J. Reisfeld, (505) 667-1375/ FTS 843-1375

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

481. Nondestructive Evaluation FY 1989
$500,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
LANL (Contract No. W-7405-ENG-36) Contact: M. Mathieson, (505) 667-6404/ FTS 843-6404

Development of nondestructive evaluation technology that produces qualitative estimates of material properties. Use of tomographic techniques to enhance radiographic inspection. In-process ultrasonic probing of ceramic sintering methods. Flash and cine radiography of dynamic and ultra-fast events.

Keywords: Nondestructive Evaluation, Radiography, Ultrasonic Microscopy, Tomography, Cine Radiography, Ceramic Sintering Processes

482. Powder Characterization FY 1989
$50,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
LANL (Contract No. W-7405-ENG-36) Contact: G. J. Vogt, (505) 667-5813/FTS 843-5813

Synthesis and processing of ceramic or metal powders critically depends on the physical characterization of the starting powders being used. Typical starting powders include commercial powders of thoria, silicon nitride, magnesia, alumina, tungsten, copper, and tungsten carbide. In the past year, considerable effort has been given to characterizing commercially prepared high-T_c precursor powders and superconducting 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: Metal Powder, Ceramic Powder, Particle Size, Superconducting Powder, X-ray Diffraction, Surface Area

483. Shock Deformation in Actinide Materials FY 1989
$200,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
LANL (Contract No. W-7405-ENG-36) Contact: M. Stevens, (505) 667-4414/FTS 843-4414

Measurement of shock-wave profiles in uranium, plutonium, and plutonium alloys. Use of soft-shock recovery test to examine the microstructural changes occurring during shock deformation. Measurement of spall strength in actinide materials and examination of fracture surfaces.

Keywords: Actinides, Shock Deformation, Microstructure, Spall Strength

484. Dynamic Mechanical Properties of Weapons Materials FY 1989
$225,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
LANL (Contract No. W-7405-ENG-36) Contact: P. Armstrong, (505) 667-4889/FTS 843-4889

Measurements of dynamic stress-strain and fracture behavior of materials used in the earth penetrator weapon. Development of plastic constitutive relations. Microstructural characterization of as-fabricated components.

Keywords: Dynamic, Strength, Fracture, Microstructure

485. Dynamic Testing of Materials for Hyper-Velocity Projectiles — FY 1989 $280,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
LANL (Contract No. W-7405-ENG-36) Contact: G. T. Gray, III, (505) 667-4665/ FTS 843-4665

Soft-recovered shock-wave deformation and spall testing of high density materials. Microstructural characterization of shock-deformed materials and fractography on spall fracture surfaces. Dynamic and quasi-static compression and tension tests.

Keywords: Shock Deformation, Spall Strength, Microstructure, Strength

486. Mechanical Properties — FY 1989 $300,000

DOE Contact: R. J. Gottschall, (301) 353-3428/FTS 233-3428
LANL (Contract No. W-7405-ENG-36) Contact: M. G. Stout, (505) 667-6750/FTS 843-6750

Basic Studies of mechanical properties of metals. Multi-axial testing on pure metals and alloys. Measurement and prediction of texture development and its effect on stress-strain behavior. Constitutive model development and implementation in large-scale computer calculations. Correlation with microstructural characterization.

Keywords: Mechanical Properties, Texture, Strength, Microstructure, Constitutive Modeling

487. Radiation Damage in High-Temperature Superconductors — FY 1989 $281,000

DOE Contact: R. J. Gottschall, (301) 353-3428/FTS 233-3428
LANL (Contract No. W-7405-ENG-36) Contact: K. E. Sickafus, (505) 667-3457/ FTS 843-3457

High-temperature oxide superconductors are exposed to various kinds of radiation to determine the nature and extent of damage from atomic displacements and absorption of ionizing energy. Results are correlated with atomic resolution structural measurements and with changes in electrical and magnetic properties.

Keywords: High-Temperature Superconductors, Radiation Damage, Atomic Displacements, Ionization Damage, Properties, Atomic Resolution

488. Structural and Superconducting Ceramics FY 1989
$595,000

DOE Contact: R. J. Gottschall, (301) 353-3428/FTS 233-3428
LANL (Contract No. W-7405-ENG-36) Contact: J. J. Petrovic, (505) 667-0125/ FTS 843-0125

Program goals are to conduct fundamental investigations of interfaces in important structural ceramic composites, to develop an understanding of metastable and topologically-disordered structures produced in high-temperature superconductors by irradiation, and to study the role of irradiation on strength, fracture, and interfacial properties of structural ceramics.

Keywords: Superconducting Ceramics, Structural Interfaces, Irradiation

Device or Component Fabrication, Behavior or Testing

489. Radiochemistry Detector Coatings FY 1989
$200,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
LANL (Contract No. W-7405-ENG-36) Contact: D. V. Duchane, (505) 667-6887/ FTS 843-6887

Physical vapor deposition of metallic and nonmetallic coatings is employed for preparation of radiochemical detectors.

Keywords: Coatings and Films, Physical Vapor Deposition, Radiochemical Detectors

490. Target Fabrication FY 1989
$1,500,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
LANL (Contact No. W-7405-ENG-36) Contact: D. V. Duchane, (505) 667-6887/ FTS 843-6887
KMS Fusion, Inc., Contact: Timothy Henderson, (313) 769-8500, ext. 302
LLNL Contact: W. Hatcher, (415) 422-1100

Hydrocarbon polymer (CH) is applied by plasma polymerization to glass microspheres to act as an ablator. These targets represent a unique fabrication capability that combines micromachining, plasma etching, and plasma polymerization. The targets are filled with a deuterium-tritium gas mixture during the process of making the glass microspheres. The targets are irradiated with a laser or particle beam to produce a fusion burn for various military and energy applications. Other techniques are classified.

Keywords: Inertial Fusion, Target Fabrication

491. Filament Winder — FY 1989 $150,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 3098
LANL (Contract No. W-7405-ENG-36) Contact: E. Eaton, (505) 667-5261/FTS 843-

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

492. Polymeric Laser Rods — FY 1989 $150,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 3098
LANL (Contract No. W-7405-ENG-36) Contact: D. V. Duchane, (505) 667-6887/ FTS 843-6887

Polymeric-host dye laser rods are currently being developed for use in solid state dye lasers having a tunable wavelength output. Organic laser dyes are incorporated into the polymeric matrix by *in situ* polymerization of the dye/monomer mixture in a controlled process. The rod blanks are then machined down to the appropriate size (1 cm dia. x up to 20 cm length). The ends are either polished using conventional lapping techniques or diamond-tool machined to produce optically flat surfaces.

The polymeric-host dye laser rod is considered to be the first "disposable" type laser rod. Cost per rod is less than $150 compared to $5,000 or more for conventional or more exotic rods such as Nd-Glass or Nd-YAG, etc.

Keywords: Laser, Dye Laser

493. <u>High Energy Density Joining Process Development</u> <u>FY 1989</u>
$410,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
LANL (Contract No. W-7405-ENG-36) Contact: H. Casey, (505) 667-4365/FTS 843-4365

Microcomputer technology and signal analysis are used for process control, together with multiaxis, programmable component manipulation for high-voltage electron beam welding. A high voltage electron beam welder has been modified and a spectrometer obtained for beam/target interaction studies. A high-voltage electron beam welder is now operational for fabrication of products in the fissile material area.

Real-time diagnostics of laser welding efficiency are thus under investigation. Plasma effects on laser welding efficiency are being studied. Photodiode, acoustic, light-spectral and electron current measurements have been made and are being correlated with high speed cinematography and resultant weld geometry.

Keywords: Welding, Laser, Electron Beam, Diagnostics

494. <u>Arc Welding Process Development</u> <u>FY 1989</u>
$150,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
LANL (Contract No. W-7405-ENG-36) Contact: H. Casey, (505) 667-4365/FTS 843-4365

Video monitoring and Varistraint testing have been established as techniques to investigate crack susceptibility of gas-tungsten-arc welds. Emphasis is directed toward dissimilar metal welds between 304L stainless steel and Inconel 625.

Keywords: Welding, Hot Cracks, Stainless Steel, Inconel, Varistraint, Video

495. <u>Solid State Bonding</u> <u>FY 1989</u>
$20,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
LANL (Contract No. W-7405-ENG-36) Contact: H. Casey, (505) 667-4365/FTS 843-4365

Initial experimentation has been conducted on aluminum solid state bonding for seamless ICF targets. A new system has been procured to evaluate bond load modulation and ion bombardment cleaning. Bonding technique optimization will be investigated. Emphasis on aluminum and beryllium will continue with primary application to pure fusion experiments.

Keywords: Joining and Welding, Solid State Bonding, Sputtering

OFFICE OF FOSSIL ENERGY

The mission of the Fossil Energy Program is to develop technologies that will increase domestic production of oil and gas or that will permit the Nation to shift from oil or gas to more abundant coal. Specifically, the Fossil Energy role is to develop technologies to support the following objectives:

- Provide a capability to convert coal to liquid and gaseous fuels;
- Increase domestic production of coal, oil, and gas;
- Ensure that current and new facilities that burn coal can do so in an economically viable and environmentally acceptable manner; and
- Allow more efficient and more economically attractive utilization of fossil energy resources.

The Fossil Energy activity includes fourteen major programs, which are grouped under seven program offices. One of these seven is the Advanced Research and Technology Development Program of the Office of Technical Coordination, which is the central point of contact for inquiries from universities concerning the Fossil Energy program.

Project execution and technical monitoring are administered in five energy technology centers and selected national laboratories.

Office of Technical Coordination

Fossil Energy AR&TD Materials Program

The objectives of the Advanced Research and Technology Development program are to assess and identify long-range advanced research needs in coal processing, fossil fuels utilization and extraction, materials, components, and instrumentation; to provide oversight of ongoing advanced research in fossil energy so as to ensure balance and proper priorities; to initiate and fund projects involving new, exploratory concepts or goal-oriented basic research; to manage the Materials Research and University Coal Research programs; and to provide policies for, and overview of, Fossil Energy-supported university activities. The Advanced Research and Technology Development program also is designed to provide an effective communications channel between the Fossil Energy program and academic institutions; to encourage these institutions to become involved in programs related to the DOE Fossil Energy mission; and to manage programs concerned with providing an adequate technical base for development of commercial construction materials and instrumentation for Fossil Energy pilot plants and demonstration plants.

The program supports workshops to identify research needs in all fossil energy technologies and manages selected training programs for faculty and students at Energy Technology Centers. The acronym PF designates that the project was provided funds in prior years.

Materials Preparation, Synthesis, Deposition, Growth or Forming

496. Fundamental Study of Aluminizing and Chromizing Processes — FY 1989 $0 (PF)

DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735

Ohio State University (Contract No. DE-AC05-84OR21400, Martin Marietta Energy Systems, Inc., Subcontract No.19X-SB154C) Contact: R. A. Rapp, (614) 292-6178

The purpose of this work is to conduct a study of aluminizing and chromizing of iron-base alloys which will lead to a fundamental understanding of these processes. Halide-activated processes will be studied. The work will provide the ability to specify pack compositions and conditions that will assure the deposition of corrosion-resistant coatings. The work will also provide specifications such as coating thickness, diffusion zone thickness, and elemental concentrations for corrosion-resistant coatings.

Keywords: Alloys, Corrosion, Coatings

497. Development of Iron Aluminides — FY 1989 $333,000

DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735

Oak Ridge National Laboratory (Contract No. DE-AC05-840R21400, Martin Marietta Energy Systems, Inc.) Contact: C. G. McKamey, (615) 574-6917/FTS 624-6917

The objective of this project is to develop low-cost and 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 conversion systems.

Keywords: Alloys, Aluminides

498. Development and Evaluation of Advanced Austenitic Alloys FY 1989 $260,000

DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735

Oak Ridge National Laboratory (Contract No. DE-AC05-84OR21400, Martin Marietta Energy Systems, Inc.) Contact: R. W. Swindeman, (615) 574-5108/FTS 624-5108

Alloys based on modifications to four groups of alloys will be developed on the basis of attributes required for advanced steam cycle superheater service. The four alloy groups studied include modified type 316 stainless steel, modified type 310 stainless steel, modified high nickel (alloy 800H) steels, and aluminum-containing steels. The bases for the alloy design include long-term strength and stability. Strength will be developed by control of chemical composition, and stability will be assured by suppression of inter-metallic and other embrittling phases by the addition of elements that promote austenitic stabilization. Added strength will be achieved through the precipitation of fine carbides, nitrides, or phosphides that stabilize dislocation networks, prevent grain boundary migration, and resist coarsening during long service under constant and varying load conditions. Metallurgical tools used in these studies will include optical microscopy, electron microscopy, and microhardness measurements.

Creep-rupture data on alloys will be gathered in the temperature range 600° to 760°C for times from 10 to 10,000 h. The effects of mechanical and thermal cycles will be examined, and results from testing will be used to establish cumulative damage models. Multiaxial stress testing, notched-bar stress-rupture testing, and creep crack-growth testing will be undertaken for constant and variable load conditions to verify cumulative damage models.

Evaluation of the weldability of alloys will include a specialized technique on a device called a Sigmajig, which evaluates the hot cracking tendency of the weldments. Ranking of alloys is by the extent of cracking as a function of applied load and plate thickness. Weldments in the alloys produced as tubing will be evaluated against requirements of the ASME BPV Code Sections I and IX, which involve bend testing, tensile testing, and metallography. Additional evaluation will be based on varestraint and circular groove tests. Other tests not required by the Code may be identified during the course of this work, and those tests will be included as appropriate. The development of a suitable filler metal is an important part of this work. Oak Ridge National Laboratory will work with university and industrial subcontractors in this development.

Keywords: Steam Cycle, Materials, Mechanical Properties, Austenitics

499. <u>Evaluation of the Fabricability of Advanced Austenitic Alloys</u> <u>FY 1989</u>
$144,000

DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735

Babcock & Wilcox (Contract No. DE-AC05-84OR21400, Martin Marietta Energy Systems, Inc., Subcontract No. 72X-SB775C) Contact: S. E. LeBeau, (216) 821-9110

The purpose of this work is to evaluate the fabricability, weldability, and surface treatments of advanced austenitic tubing for superheater applications. The problem of the fabrication of tubing from alloys containing controlled amounts of minor element additions and surface treatments of the tubing for optimum strength and corrosion resistance is examined in this activity.

Keywords: Austenitics, Alloys, Tubing

500. <u>Consolidation of Rapidly Solidified Aluminide Metal Powders</u> <u>FY 1989</u>
$175,000

DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735

Idaho National Engineering Laboratory (Contract No. DE-AC07-76ID01570) Contacts: J. E. Flinn and R. N. Wright, FTS 583-8127

The purpose of this project is to determine the most effective means of, and associated parameters for, consolidating rapidly solidified nickel-iron aluminide powders. Three consolidation techniques will be explored for the rapid solidification process (RSP) powders: hot extrusion (baseline), hot isostatic pressing (HIP), and dynamic (i.e., explosive) methods. The investigation of these consolidation techniques will emphasize the influence of pressure, temperature, and time on RSP structures. Structure/property assessments will be performed on the consolidated materials. In particular, thermal stability, mechanical properties, and oxidation response will be determined. The RSP aluminide powders and extrusions will be obtained from outside sources. Limited atomization investigations will be performed at the Idaho National Engineering Laboratory to assess RSP parameters for the aluminide powders.

Keywords: Aluminides, Powders, Consolidation of Powder

501. Investigation of Electrospark Deposited Coatings for Protection of Materials in Sulfidizing Atmospheres FY 1989

$50,000

DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735

Westinghouse Hanford Company (FWP ERT0001) Contact: R. N. Johnson, (509) 376-0715

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

502. Vapor-Liquid-Solid SiC Whisker Process Development FY 1989

$200,000

DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735

Los Alamos National Laboratory (Contract No. W-7504-eng-36) Contact: P. D. Shalek, (505) 667-6863/FTS 843-6863

The purpose of this study is to optimize an existing Los Alamos whisker growth process to produce alpha-phase silicon nitride (alpha-Si_3N_4) whiskers and beta-phase silicon carbide (beta-SiC) whiskers of uniform size, optimum strength, and in quantities suitable for composite use.

Keywords: Ceramics, Whiskers, Composites

503. Sol-Gel Synthesis of Ceramics FY 1989

$75,000

DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735

Idaho National Engineering Laboratory (Contract No. DE-AC07-761D01570) Contact: R. M. Neilson, FTS 583-8274

The purpose of this activity is to investigate techniques for fabricating sol-gel derived films of $YBa_2Cu_3O_{7-x}$ based superconducting ceramics.

Keywords: Ceramics, Superconducting, Film

504. Fabrication of Fiber-Reinforced Composites by Chemical Vapor Infiltration (CVI)
FY 1989
$190,000

DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735

Oak Ridge National Laboratory (Contract No. DE-AC05-84OR21400, Martin Marietta Energy Systems, Inc.) Contacts: D. P. Stinton, (615) 574-4556/FTS 624-4556

The purpose of this task is to develop a ceramic composite having higher than normal toughness and strength yet retaining the typical ceramic attributes of refractoriness and high resistance to abrasion and corrosion. The desired toughness and strength are on the order of 20 MPa-$m^{1/2}$ and 350 MPa, respectively. In addition, a practical process capable of fabricating simple or complex shapes is desired. The ceramic fiber-ceramic matrix composites are fabricated by infiltrating low-density fiber structures with vapors, which deposit as solid phases on and between the fibers to form the matrix of the composite. The goal is to demonstrate that a ceramic composite can be prepared using materials of high interest to the fossil energy community. SiC fibers and matrices of SiC and Si_3N_4 have been identified as being most promising. Fiber dimensions, geometry, packing density, binder type and concentrations, and other processing variables have been evaluated experimentally. Important variables of the CVI process, such as temperature, gas composition, flow rate, pressure, etc., are being systematically altered to maximize matrix density and to obtain a microstructure consistent with the goal of fabrication of high-toughness high-strength ceramic composites.

Keywords: Composites, Fiber-Reinforced, Ceramics

505. Characterization of Fiber-CVD Matrix Interfacial Bonds
FY 1989
$140,000

DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735

Oak Ridge National Laboratory (Contract No. DE-AC05-84OR21400, Martin Marietta Energy Systems, Inc.) Contact: R. A. Lowden, (615) 574-7714/FTS 624-7714

The purpose of this task is to optimize the strength and toughness of fiber-reinforced ceramic composites by tailoring the strength of the bonds between the fiber and the matrix. Methods must first be developed to characterize the fiber-matrix bond strengths in fiber-reinforced ceramic composite systems. Coating or pretreatment processes can then be utilized to tailor the fiber-matrix bonding within various composite systems and to optimize the strength and toughness of the composite.

Keywords: Composites, Ceramics, Fiber-Reinforced, Interfaces

506. Microwave Sintering of Ceramics FY 1989
$200,000

DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735

Oak Ridge National Laboratory (Contract No. DE-AC05-84OR21400, Martin Marietta Energy Systems, Inc.) Contacts: M. A. Janney and H. D. Kimrey, (615) 574-4281/FTS 624-4281

The purpose of this activity is to conduct research and development on the microwave processing of new ceramics. The heating and sintering of yttria-stabilized zirconia, the electrolyte for the monolithic fuel cell design, is being studied.

Keywords: Ceramics, Microwave Sintering

507. Development of Advanced Fiber Reinforced Ceramics FY 1989
$192,000

DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735

Georgia Institute of Technology, Georgia Tech Research Institute (Contract No. DE-AC05-84OR21400, Martin Marietta Energy Systems, Inc., Subcontract No. 19X-43369C) Contact: T. L. Starr, (404) 894-3678

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

508. Modeling of Fibrous Preforms for CVD Infiltration FY 1989
$50,000

DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735

Georgia Institute of Technology, Georgia Tech Research Institute (Contract No. DE-AC05-84OR21400, Martin Marietta Energy Systems, Inc., Subcontract No. 19X-55901C) Contact: T. L. Starr, (404) 894-3678

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. Chemical vapor deposition (CVD) has demonstrated considerable promise as a technique for fabrication of fiber-reinforced ceramic composites. Unidirectional and cloth-reinforced composites of SiC fibers in a SiC matrix have shown good strength and exceptional strain tolerance. However, results have been inconsistent with the fabrication of randomly oriented short-fiber composites. A critical problem has been the inability to consistently fabricate fibrous preforms with both high fiber loading and a permeability suitable for infiltration. A better understanding of the fundamental parameters controlling preform fabrication and CVD infiltration of such preforms is needed to guide further development. The proposed 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. Initially, the model will be developed for preforms containing only one type of fiber, but extension to mixed fiber and fiber-particle blends is planned.

Keywords: Ceramics, Composites, Modeling

Materials Structure and Composition

509. Analytical Characterization of Coal Surfaces and Interfaces FY 1989
$300,000

DOE Contacts: J. D. Hickerson, FTS 723-5721 and E. E. Hoffman, (615) 576-0735/ FTS 626-0735

Oak Ridge National Laboratory (DE-AC05-88OR21400, Martin Marietta Energy Systems, and Inc.) Contact: E. L. Fuller, (615) 574-4959/FTS 624-4959

The objective of this task is to provide analytical characterization of coal surfaces and interfaces between coal and various included minerals for the purpose of assisting the Pittsburgh Energy Technology Center in its research on coal characterization and cleaning. Particular emphasis is given to the chemical binding of the detrimental elements, including sulfur, nitrogen, mineral matter, etc. The distribution of these elements in various coals, and particularly the chemical and structural characterization of interfaces in coals are major tasks in the research.

Keywords: Coal Surfaces, Interfaces

Materials Properties, Behavior, Characterization or Testing

510. Transfer Model Predicting Thermomechanical Behavior of Refractory Linings to Industry FY 1989
$65,000

DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735

Tennessee Center for Research and Development (Contract No. DE-AC05-84OR21400, Martin Marietta Energy Systems, Inc., Subcontract No. 41X-SB628V) Contact: B. J. George, (615) 675-9505

The purpose of this activity is to develop user-friendly and intelligent computer-based software for the prediction of thermomechanical behavior of refractory lining systems. The user-friendly software system is anticipated to enable users to have access to design guidelines and to develop preliminary refractory designs, to perform finite element analyses for final designs, and to facilitate the modification of existing or the addition of new capabilities through a modular program structure.

Keywords: Refractory Linings, Software, Stress

511. Mechanical Properties and Microstructural Stability of Advanced Austenitic Alloys FY 1989
$125,000

DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735

Cornell University, Materials Science and Engineering Department (Contract No. DE-AC05-84OR21400, Martin Marietta Energy Systems, Inc., Subcontract No. 19X-27488C) Contact: Che-Yu Li, (607) 256-4349

The purpose of this project is to rank the strengths and metallurgical stabilities of advanced austenitic alloys at temperatures ranging from 650° to 760°C. Mechanical testing of the steels consists of relaxation experiments (24 h duration each) that cover stresses producing deformation rates from about 10^{-3} to 10^{-9}/sec. The precipitate or dislocation microstructure of the steels in the grain boundary and matrix regions is being studied to determine the role of strain-time history on the stability of the microstructure. The relaxation data will be correlated with constant-load creep data provided by Oak Ridge National Laboratory and analyzed in terms of deformation mechanisms to determine relative contributions of grain boundary and matrix deformations. The most promising alloys from the screening test will be included in relaxation tests at 700°C to determine optimum heat treatments for strength and metallurgical stability.

Keywords: Steam Cycle, Microstructure, Mechanical Properties

512. Investigation of the Weldability of Ductile Aluminides — FY 1989 $75,000

DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735

Colorado School of Mines, Center for Welding Research (Contract No. DE-AC05-84OR21400, Martin Marietta Energy Systems, Inc., Subcontract No. 19X-27421C) Contact: G. R. Edwards, (303) 273-3773

The purpose of this project is to study the weldability of nickel-iron 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. This project is a cooperative effort of Oak Ridge National Laboratory and Colorado School of Mines.

Keywords: Joining and Welding, Materials Characterization

513. Corrosion Studies of Iron Aluminides — FY 1989 $50,000

DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735

University of Tennessee (Contract No. DE-AC05-84OR21400, Martin Marietta Energy Systems, Inc. Subcontract No. 41B-07685C) Contact: R. A. Buchanan, (615) 974-4858

The objective of this project is to investigate the aqueous corrosion of iron aluminides based on Fe_3Al. The effort will provide basic corrosion information over a wide range of pH values for each of several experimental iron aluminide compositions and will allow comparisons to be made among iron aluminide compositions, as well as with other corrosion-resistant materials of interest to fossil energy systems.

Keywords: Alloys, Aluminides, Corrosion

514. Fireside Corrosion Tests of Candidate Advanced Austenitic Alloys, Coatings, and Claddings FY 1989
$15,000

DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735

Foster Wheeler Development Corporation (Contract No. DE-AC05-84OR21400, Martin Marietta Energy Systems, Inc., Subcontract No. 86X-SA187C) 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 will be examined. The variables affecting coal ash corrosion and the mechanisms governing oxide breakdown and corrosion penetration will be evaluated. Corrosion rates of the test alloys will be determined as functions of temperature, ash composition, gas composition, and time. The parameters influencing corrosion rates will be identified and correlated with past data for high temperature alloys.

Keywords: Austenitics, Alloys, Corrosion

515. Microstructural Studies of Advanced Austenitic Steels FY 1989
$35,000

DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735

University of Southern California (Contract No. DE-AC05-84OR21400, Martin Marietta Energy Systems, Inc., Subcontract No. 19X-SA663C) Contact: J. A. Todd, (213) 743-4966

The purpose of this project is to develop a thorough understanding of the metallurgical factors contributing to degradation of austenitic alloys in advanced steam power boilers under long-term, high-temperature operating conditions. Among the phenomena that are studied are: (1) precipitation of massive intermetallic phases, and (2) coarsening of fine carbide precipitates that are important for strengthening. This work will also aim at a thorough understanding of the kinetics of precipitation and aging processes is needed to predict long-term performance of these alloys.

Keywords: Alloys, Austenitics, Degradation

516. <u>Joining Techniques for Advanced Austenitic Alloys</u> <u>FY 1989</u>
$37,000

DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735

University of Tennessee (Contract No. DE-AC05-84OR21400, Martin Marietta Energy Systems, Inc., Subcontract No. 41B-07685C) Contact: C. D. Lundin, (615) 874-5310

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 and Welding

517. <u>Corrosion and Mechanical Properties of Alloys in FBC and Mixed-Gas Environments</u> <u>FY 1989</u>
$320,000

DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735

Argonne National Laboratory (Contract No. W-31-109-eng-38) Contact: K. Natesan, (312) 972-5103/FTS 972-5103

The purposes of this task are to: (1) develop corrosion information in the temperature range 400° to 750°C in mixed-gas atmospheres containing O, S, and Cl by use of internally cooled tube specimens of selected commercial materials, (2) evaluate mechanisms of the formation and breakaway behavior of protective scales on base metals and weldments exposed to atmospheres containing O, S, and Cl; (3) experimentally evaluate the uniaxial creep rupture behavior of selected high-chromium alloys and weldments exposed to complex gas mixtures, (4) establish the synergistic effects of stress and environment on the materials behavior, (5) develop corrosion rate expressions on the basis of experimental data for long-term extrapolation to component design lives, and (6) correlate the creep properties such as rupture life, rupture strain, and minimum creep rate with the chemistry of exposure environment, temperature, and alloy chemistry.

Additional objectives of this project are to: (1) experimentally evaluate the high-temperature corrosion behavior of iron- and nickel-base alloys in gas environments with a wide range of oxygen, sulfur, and carbon potentials, (2) develop corrosion information in the temperature range 400° to 750°C in mixed-gas atmospheres using internally cooled tube specimens of selected commercial materials, (3) evaluate deposit-induced corrosion behavior of heat-exchanger and gas-turbine materials after exposure to multicomponent gas environments, and (4) develop corrosion rate expressions, based upon experimental data, for long-term extrapolation to component design lives.

Keywords: Corrosion, Gasification, Creep Rupture, Fluidized Bed Combustion

518. Development of Surface Treatments and Modifications to Produce Corrosion-Resistant Oxide Scales — FY 1989 $195,000

DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735

Oak Ridge National Laboratory (Contract No. DE-AC05-84OR21400, Martin Marietta Energy Systems, Inc.) Contact: J. H. DeVan, (615) 574-4451/FTS 624-4451

The purpose of this task is to develop protective oxide scales on Cr_2O_3- and Al_2O_3-forming iron-based alloys in mixed oxidant (O_2, SO_2, H_2S, H_2O) environments for coal-related applications at 600° to 800°C. Specific objectives include: (1) the development of protective oxide scales by modifying oxide chemistry and microstructure to reduce the transport of sulfur through the scale, (2) the formation of a sulfur-diffusion barrier (i.e., SiO_2 layer) under or above the protective oxide scale to minimize the sulfur attack, (3) the study of the effects of alloy chemistry, oxide morphology, and temperature on the breakdown of protective oxide scales, and (4) the examination of methods to limit internal sulfidation. The mechanical performance and adherence of oxide scales in mixed oxidant gases will be studied by impinging tungsten carbide particles on the oxide within a scanning electron microscope under controlled temperature and environmental conditions.

Keywords: Corrosion, Iron-Based, Mixed Gas, Scales

519. Investigation of the Effects of Microalloy Constituents, Surface Treatment, and Oxidation Conditions on Development and Breakdown of Protective Oxide Scales — FY 1989 $110,000

DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735

Battelle Columbus Laboratories (Contract No. DE-AC05-84OR21400, Martin Marietta Energy Systems, Inc., Subcontract No. 86X-57444C) Contact: I. G. Wright, (614) 424-4377

The objectives of this program are: (1) to gain an improved understanding of the effects of alloying constituents present at low levels on the development and mode of breakdown of protective oxide scales in conditions representing those encountered in combustion and gasification processes, and (2) to achieve better control over the growth of scales which will contribute to improvements in long-term high-temperature corrosion resistance of heat exchanger and heat recovery materials.

Keywords: Corrosion, Oxides, Scales

520. Investigation of the Effects of Microalloy Constituents, Surface Treatment, and Oxidation Conditions on Development and Breakdown of Protective Oxide Scales — FY 1989 — $50,000

DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735

Case Western Reserve University (Contract No. DE-AC05-84OR21400, Martin Marietta Energy Systems, Inc., Subcontract No. 86X-95900C) Contact: K. M. Vedula, (216) 368-4211

The focus of the current program is to obtain a better understanding of material behavior in fossil energy environments. The particular emphasis is on the effects of reactive element additions on the protectiveness of oxide scales formed in sulfidizing/oxidizing atmospheres. Iron-based alloys, including Fe-25Cr and Fe-25Cr-20Ni which are Cr_2O_3 formers and Fe-25Cr-6Al which is an Al_2O_3 former, are the base alloys for this investigation. Conventional alloying as well as ion-implantation are the techniques for incorporating the reactive elements into the base alloys.

Keywords: Corrosion, Oxides, Scales

521. Investigation of the Effects of Microalloy Constituents, Surface Treatment, and Oxidation Conditions on Development and Breakdown of Protective Oxide Scales — FY 1989 — $139,000

DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735

Universal Energy Systems, Inc. (Contract No. DE-AC05-84OR21400, Martin Marietta Energy Systems, Inc., Subcontract No. 86X-95901C) Contact: V. Srinivasan, (513) 426-6900

The main objective of this program is to develop a comprehensive basic understanding of the effects of additions of microalloy constituents and the surface conditions on the nucleation, growth and breakdown of protective oxide scales in the mixed oxidant environments relevant to coal utilization and conversion technologies. The alloys of primary interest are ferritic and austenitic steels with adequate high temperature mechanical strength. Model alloy systems of such compositions that will develop protective chromia or alumina scales will be used. The scope of this program includes the study of the influence of the type and concentration of microalloying additions, the surface pretreatments, the method of incorporation of the microalloy constituents, the temperature and the partial pressures of oxygen and sulfur on the formation and degradation of scales. The temperature range of present interest is between 500° and 700°C. A variety of analytical tools will be used to characterize the scale and the substrate as a function of time of exposure to understand the distribution and chemical status of reactants in the pre- and post-exposed samples, so that degradation mechanism can be understood. Thermogravimetric and scales thickness measurements will be used to describe the kinetics under isothermal and cyclic conditions.

Keywords: Corrosion, Oxides, Scales

522. Molten Salt-Induced Corrosion of Iron Aluminides — FY 1989, $32,000

DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735

University of Cincinnati (Contract No. DE-AC05-84OR21400, Martin Marietta Energy Systems, Inc. Subcontract No. 19X-SD169V) Contact: R. Y. Lin, (513) 556-3116

The purpose of this project is to evaluate the molten salt-induced hot corrosion of nickel iron and iron aluminides. The use of nickel iron aluminides in fossil energy conversion and utilization systems requires resistance to mixed sulfidation/oxidation attack and severe corrosion in the presence of molten salts at elevated temperatures.

Keywords: Corrosion, Salts, Aluminides

523. A Study of Erosive Particle Rebound Parameters — FY 1989, $122,000

DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735

University of Notre Dame (Contract No. DE-AC05-84OR21400, Martin Marietta Energy Systems, Inc. Subcontract No. 19X-91236C) Contact: T. H. Kosel, (219) 239-5642

This research project is designed to provide a systematic investigation of the effects of materials properties and experimental variables on the rebound directions and velocities of erodent particles. The general approach is to develop computer models for the impact of spherical and angular particles, and to compare the predictions with experimental measurements of both single and multiple impact rebound parameters.

Keywords: Erosion and Wear, Particles

524. Studies of Materials Erosion in Coal Conversion and Utilization Systems

FY 1989
$250,000

DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735

Lawrence Berkeley Laboratory (Contract No. DE-AC03-76SF00098) Contact: A. V. Levy, (415) 486-5822/FTS 451-5822

The erosion of materials surfaces by small solid particles carried in gas and liquid streams is being investigated. The materials are tested over a range of conditions that simulate portions of the operating environments of containment surfaces in coal gasification, liquefaction, and fluidized-bed combustion processes. The effects of the materials properties, microstructures, and compositions on their erosion behavior are determined. The effects of elevated temperature corrosion in combination with the erosion are studied to determine the mechanisms and rates of the combined surface degradation modes.

Keywords: Corrosion, Erosion and Wear

525. In-Situ Scanning Electron Microscopy Studies of Erosion and Erosion-Corrosion

FY 1989
$195,000

DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735

Oak Ridge National Laboratory (Contract No. DE-AC05-84OR21400, Martin Marietta Energy Systems, Inc.) Contact: J. R. Keiser, (615) 574-4453/FTS 624-4453

This project involves the evaluation of erosion and erosion-corrosion of alloys using microscopic techniques. Selected alloys will be subjected to single particle impacts both with and without a flowing corrosive gas stream. The degradation of the alloys will be followed by examination of the alloy surfaces with a scanning electron microscope. This technique should provide direct evidence of the erosion and erosion-corrosion modes of materials degradation in these systems.

Keywords: Erosion and Wear, Corrosion, Metals, Alloys

526. Solid Particle Erosion in Turbulent Flows Past Tube Banks FY 1989
$0 (PF)

DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735

University of California, Berkeley, Department of Mechanical Engineering (Contract No. DE-AC05-84OR21400, Martin Marietta Energy Systems, Inc., Subcontract No. 19X-55936C) Contact: J. A. C. Humphrey, (415) 642-6460

The purpose of this investigation is to improve the understanding of erosion processes in gas streams. To fully understand erosion processes caused by particles entrained in gas streams, the fluid dynamic behavior of the particulates must be understood. Laboratory experiments have generally focused on erosive particles interacting with materials under carefully controlled flow conditions (particle velocity and impact angle). This project should aid attempts to correlate the results of the carefully controlled laboratory experiments with the experience of plant systems.

Keywords: Materials, Erosion and Wear, Particle, Gas Streams

527. Study of Particle Rebound Characteristics and Material Erosion at High Temperatures FY 1989
$ 110,000

DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735

University of Cincinnati (Contract No. DE-AC05-84OR21400, Martin Marietta Energy Systems, Inc., Subcontract No. 19X-89628C) Contact: W. Tabakoff, (513) 475-2849

The purpose of this effort is to investigate the erosion processes and fluid mechanics phenomena that occur in fluidized-bed combustors, coal-fired boilers, cyclones, pumps, turbines, valves, and other coal combustion systems. The overall objective is to develop a quantitative model that will facilitate the prediction of erosion in systems operating in particle-laden environments. This investigation will at first be limited to ductile target materials. The experimental study of the impact and rebound characteristics will be performed with selected solid particles, possibly Al_2O_3 and SiO_2. The target materials will be selected according to present and anticipated materials needs of coal combustion systems.

Keywords: Erosion and Wear, Corrosion, Metals, Alloys

528. Development of Nondestructive Evaluation Techniques and the Effect of Flaws on the Fracture Behavior of Structural Ceramics FY 1989
$315,000

DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735

Argonne National Laboratory (Contract No. W-31-109-eng-38) Contacts: W. A. Ellingson, (312) 972-5068/FTS 972-5068 and J. P. Singh, (312) 972-5132/FTS 972-5132

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 will be studied, and correlations between NDE results and failure of specimens will be established.

Additional work will: (1) establish correlations between the composition, microstructure, and mechanical properties of structural ceramics (Si_3N_4 and SiC) with well-defined flaws, and (2) provide information which will be used to relate mechanical properties to non-destructive evaluation (NDE) results. The work will include fabricating specimens of Si_3N_4 and SiC with controlled flaws and measuring their mechanical properties (fracture stress, fracture toughness and elastic modulus). Microstructures of the fracture surface will be evaluated in order to locate the critical flaws. Information obtained from these studies will help control processing of structural ceramics to result in improved mechanical properties. Furthermore, correlation of mechanical properties with NDE results will provide additional information which will help verify the ability of NDE to detect failure-initiating flaws.

Keywords: Nondestructive Evaluation, Ceramics, Flaws, Fracture

529. Joining of Silicon Carbide Reinforced Ceramics FY 1989
$175,000

DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735

Idaho National Engineering Laboratory (Contract No. DE-AC07-76ID01570) Contact: B. H. Rabin, FTS 583-0058

The purpose of this project is to identify and to develop techniques for joining silicon carbide fiber-reinforced composite materials. Primary emphasis will be on composite materials with either a silicon nitride or a silicon carbide matrix; lesser emphasis will be placed on silicon carbide fiber-reinforced silica. The work will investigate oxynitride and oxide glass joining materials and joining techniques which promote the devitrification of these materials to produce glass-ceramics and joints which are both strong and tough.

Joining of composite matrix materials will be studied, and the resulting information applied to the joining of the fiber-reinforced composites. The joining material, surface preparation, heat treatments, methods of binder application, joining technique, and joint configuration will be considered during joint design and fabrication. Microstructural examination of the joints will be conducted to investigate wetting, microstructure, mass transfer, and process parameter effects. Limited mechanical testing of joints will be conducted. Thermal cycling and service environment scoping tests will be performed for selected composite joints. Practical joining techniques must be developed to fully realize the advantages of silicon carbide fiber-reinforced ceramic composite materials. Successful joining methods will permit the design and use of complex component shapes and the integration of component parts into larger structures.

Keywords: Joining and Welding, Ceramics, Composites

530. <u>Nondestructive Evaluation of Advanced Ceramic Composite Materials</u> <u>FY 1989</u>
$175,000

DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735

Idaho National Engineering Laboratory (Contract No. DE-AC07-76ID01570)
Contact: J. B. Walter, FTS 583-0033

The purpose of this project is to develop an effective capability for nondestructive evaluation of ceramic fiber reinforced ceramic composites. The response of selected samples of sintered composite materials consisting of SiC fibers in SiC and Si_3N_4 matrices to both ultrasonic and radiographic techniques will be investigated. Experimental techniques and signal processing algorithms will be developed for: (1) characterizing acoustic properties and sample morphology, including fiber size and distribution and the degree of bonding of the fibers to the matrix, (2) detecting flaws including cracks, porosity, fiber clusters, and bonding anomalies, and (3) detecting flaws in joints. The NDE techniques developed in this project will result in more effective and extensive use of advanced ceramic composite materials in fossil energy applications.

Keywords: Ceramics, Composites, Nondestructive Evaluation

531. Structural Reliability and Damage Tolerance of Ceramic Composites FY 1989
$150,000

DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735

National Institute of Standards and Technology (Contract No. DE-A105-80OR20679) Contact: E. R. Fuller, (301) 975-5795

The objective of this study is to characterize the high temperature failure mechanisms and factors that influence their operation with an aim toward improving the properties of structural ceramics, especially silicon carbide and silicon nitride based materials, for use in coal conversion applications.

Keywords: Ceramics, Glasses, Materials Characterization

532. Mechanical Properties of Ceramic Fiber-Ceramic Matrix Composites FY 1989
$74,000

DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735

North Carolina A&T State University (Contract No. DE-AC05-84OR21400, Martin Marietta Energy Systems, Inc., Subcontract No. 19X-SC423C) Contact: J. Sankar, (919) 334-7620

The purpose of this project is to expand the mechanical properties data base for composites fabricated by forced chemical vapor infiltration (CVI). Composites are currently being fabricated with continuous SiC fiber reinforcement, SiC whisker reinforcement, SiC platelet reinforcement, and continuous aluminosilicate fiber reinforcement. The mechanical properties vary with the type of reinforcement and with the type of coating utilized to control the fiber/matrix interfacial bond. The effect of the reinforcement type and interfacial bond on the tensile strength, thermal shock resistance, oxidation resistance, and tensile strength during cyclic loading are investigated.

Keywords: Ceramics, Composites, Mechanical Properties

533. Ceramic Catalyst Materials FY 1989
$100,000

DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735
Sandia National Laboratory (Contract No. DE-AC04-76DP00789) Contact: D. H. Doughty, FTS 844-1933

This project involves investigation of the role of ceramic materials properties in the activity and selectivity of novel catalytic materials. The research focuses on the relationship between the catalytic activity and the composition, structure, and acid/base character of the ceramic support material.

Keywords: Ceramics, Catalysts

Device or Component Fabrication, Behavior or Testing

534. *Materials and Components in Fossil Energy Applications* (Newsletter) FY 1989
$110,000

DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735
Battelle-Columbus Laboratories (Contract No. DE-AC05-84OR21400, Martin Marietta Energy Systems, Inc., Subcontract No. 11X-78931C) Contacts: E. E. Hoffman (DOE/ORO), (615) 576-0735/FTS 626-0735 and I. G. Wright (BCL), (614) 424-4377

The purpose of this task is to publish a periodic newsletter to address current developments in materials and components in fossil energy applications.

Keywords: Materials, Components

535. Assessment of Potential Applications of Ceramic Composites in Gas Turbines FY 1989
$ 0 (PF)

DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735
Babcock & Wilcox (Contract No. DE-AC05-84OR21400, Martin Marietta Energy Systems, Inc., Subcontract No. 87X-SA798V) Contact: W. P. Parks, (804) 522-6196

The purpose of this work is to review the materials requirements for direct coal-fired gas turbines or gas turbines for coal gasification combined cycle systems, to assess the state of technology for materials to meet those requirements, and to identify areas and components that require additional materials research and development and for which structural ceramic composites have potential applications.

Keywords: Gas Turbine Engines, Ceramics, Composites

536. Mechanisms of Galling and Abrasive Wear FY 1989
$50,000

DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735
National Institute of Standards and Technology (Contract No. DE-A105-83OR21322) Contact: L. K. Ives, (301) 975-6013

This project is directed to developing an understanding of the wear mechanisms of materials associated with valves in coal conversion systems. This work addresses the mechanical and chemical effects experienced in closure regions of valves in coal conversion systems. It includes theoretical considerations of chemical reactions and effects of the working media on valve closure materials. Measurements are being performed to determine the static and kinetic coefficients of friction of the various combinations of test materials.

Keywords: Erosion and Wear

537. Fabrication of Commercial-Scale Fiber-Reinforced Hot-Gas Filters by Chemical Vapor Deposition FY 1989
$149,000

DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735
3M Company (Contract No. DE-AC05-84OR21400, Martin Marietta Energy Systems, Inc., Subcontract No. 93X-SB482C) Contact: T. Kafka, (612) 736-1689

The purpose of this project is to scale-up the chemical vapor infiltration (CVI) process developed at Oak Ridge National Laboratory (ORNL) for fabricating ceramic fiber-ceramic matrix composites. The goal is to use this scaled-up CVI 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

538. Development of Ceramic Membranes for Gas Separation FY 1989
$130,000

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Oak Ridge Gaseous Diffusion Plant (Contract No. DE-AC05-84R21400, Martin Marietta Energy Systems, Inc.) Contact: D. E. Fain, (615) 574-9932/FTS 624-9932

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

539. Investigation of the Mechanical Properties of CVD Infiltrated Ceramic Composite Tubular Components FY 1989
$0 (PF)

DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735

Virginia Polytechnic Institute and State University (Contract No. DE-AC05-84OR21400, Martin Marietta Energy Systems, Inc., Subcontract No. 19X-SA946C) Contacts: K. L. Reifsnider and W. W. Stinchcomb, (703) 961-5316

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

540. Material Data Base Development for Refractories FY 1989
$78,000

DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735

Massachusetts Institute of Technology (Contract No. DE-AC05-84OR21400, Martin Marietta Energy Systems, Inc., Subcontract No. 19X-07862C) Contact: Oral Buyukozturk, (617) 253-7186

The objective of this task is to study the failure mechanisms of refractory-brick-lined coal gasification vessels under transient temperature loadings. A thermomechanical model, which includes cyclic multiaxial nonlinear constitutive law, temperature-dependent heat conduction, and temperature-dependent creep laws, has been developed for refractory brick and mortar. The model is implemented in a finite-element program for predicting the stress and strain distributions in brick-mortar linings during the heatup and cooldown cycles. Through simulation and parameter studies, design recommendations can be made for vessel configuration, material property combinations, and optimum heating schedules. The work under this activity is done in conjunction with the project to transfer a model predicting thermomechanical behavior of refractory linings to industry, as described above.

Keywords: Refractory Liners, Stress, Strain, Mechanical Behavior

541. Advanced Materials and Electrochemical Processes in High-Temperature Solid Electrolytes — FY 1989 $250,000

DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735
Pacific Northwest Laboratory (Contract No. DE-AC06-76RL01830) Contact: J. L. Bates, (509) 375-2579/FTS 444-2579

The objective of this research is (1) to identify, develop, and demonstrate advanced materials for use as alternative electrodes and current interconnections in solid oxide fuel cells, and (2) to develop an understanding of the synergistic effects of materials properties, structures, and compositions on electrochemical processes related to high-temperature solid electrolyte use in electrochemical cells.

Keywords: Fuel Cells, Electrochemical, Electrolytes

542. Gas Separations Using Inorganic Membranes — FY 1989 $200,000

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Oak Ridge National Laboratory (DE-AC05-88OR21400, Martin Marietta Energy Systems, Inc.) Contact: B. Z. Egan, (615) 574-6868/FTS 624-6868

The objective of this project is to explore the applicability of inorganic membranes to separate gases at high temperatures and/or in hostile process environments encountered in fossil energy conversion processes such as coal gasification. The program will seek to apply porous membrane technology developed for uranium enrichment to the separation of gases. The program could lead to the development of processes that would improve the economics of fossil energy conversion processes by significantly reducing gas cleanup and separation costs.

Keywords: Membrane, Gas Separation

543. Ceramic Fiber-Ceramic Matrix Hot Gas Filters FY 1989
$200,000

DOE Contacts: N. Holcombe, FTS 923-4829 and E. E. Hoffman, (615) 576-0735/ FTS 626-0735

Oak Ridge National Laboratory (DE-AC05-88OR21400, Martin Marietta Energy Systems, Inc.) Contact: D. P. Stinton, (615) 574-4556/FTS 624-4556

This task will develop ceramic fiber-ceramic matrix materials and fabrication techniques suitable for production of hot-gas cleanup filters. The technology developed will be transferred to industry via a research subcontract with an industrial organization (see project described above for the Fabrication of Commercial-Scale Fiber-Reinforced Hot-Gas Filters by Chemical Vapor Deposition) for the production of full-size candle filters.

Keywords: Ceramic Composites, Filters

544. Identification of Materials for Hot-Gas Filter Tubesheets FY 1989
$135,000

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Oak Ridge National Laboratory (DE-AC05-88OR21400, Martin Marietta Energy Systems, Inc.) Contact: R. W. Swindeman, (615) 574-5108/FTS 624-5108

The objectives of this work are: (1) to assess current tubesheet designs and blowback manifold materials for ceramic crossflow and ceramic candle filter; (2) to investigate alternative tubesheet designs; (3) to define the strength requirements for ceramic filter tubesheets in hot-gas cleanup systems based on design methodology developed at the Oak Ridge National Laboratory; (4) to collect and analyze data on commercial materials; (5) to collect and analyze data on advanced materials; and (6) to fabricate subsized components (tubesheets) out of the selected materials and characterize its mechanical properties across the thickness and carious orientations. This task is anticipated to result in the recommendation of a tubesheet materials for long-term operation in a high-efficiency hot-gas filter system.

Keywords: Filters, Tubesheets, Alloys

Instrumentation and Facilities

545. Management of the Fossil Energy AR&TD Materials Program FY 1989
$350,000

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Oak Ridge National Laboratory (Contract No. DE-AC05-84OR21400, Martin Marietta Energy Systems, Inc.) Contacts: R. R. Judkins, P. T. Carlson and D. N. Braski, (615) 574-4572/FTS 624-4572

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

546. Coal Conversion and Utilization Plant Support Services FY 1989
$45,000

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Oak Ridge National Laboratory (Contract No. DE-AC05-84OR21400, Martin Marietta Energy Systems, Inc.) Contact: J. R. Keiser, (615) 574-4453/FTS 624-4453

This task will provide screening data on the susceptibility to corrosion and stress-corrosion cracking of potential materials of construction, failure analyses and on-site examinations for coal conversion and utilization plants.

Keywords: Corrosion, Liquefaction, Failure Analysis

547. Assessment of Fossil Energy Materials Research Needs FY 1989
$50,000

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National Institute of Standards and Technology (Contract No. DE-A105-89OR21857) Contact: S. J. Dapkunas, (301) 975-6119

The purpose of this activity is to identify long-range materials research and development needs and opportunities as they impact evolving fossil energy technologies. The needs and opportunities that are identified shall be appropriate for future research on the Fossil Energy Advanced Research & Technology Development (AR&TD) Materials Program.

Keywords: Materials, Assessment, R&D Needs

548. Assessment of the Potential for Transfer of AR&TD Materials Program Technologies to Oil, Gas, and Shale Industries FY 1989
$ 0

DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735
Oak Ridge National Engineering Laboratory (Contract No. DE-AC05-84OR21400, Martin Marietta Engineering Systems, Inc.) Contact: P. T. Carlson, FTS 574-5135

The purpose of this assessment is to maximize the benefit of research on the AR&TD Materials Program, to enhance Department of Energy (DOE) research and development coordination efforts, and to provide possible materials technologies that could significantly benefit the oil, gas, and shale (OGS) industries. It is anticipated that this assessment will be useful as input into planning processes for the AR&TD Materials and Advanced Process Technology Programs, Office of Technical Coordination planning, information dissemination of AR&TD Materials Program research activities, and marketing and outreach activities.

Keywords: Oil, Gas, Shale, Materials

Office of Coal Technology

The Office of Coal Technology is responsible for management of cooperative agreements with industry to foster clean coal technology; for the conduct of research and development programs for coal combustion and conversion, embodying retrofit or near-or mid-term applications such as fluidized-bed combustion and surface coal gasification; and for environmental, health and safety technology integral to such coal combustion and conversion systems.

Division of Coal Conversion

Instrumentation and Facilities

549. Materials Technical Support for the Great Plains Coal Gasification Plant FY 1989
$0 (PF)

DOE Contacts: W. Miller, FTS 923-4827 and E. E. Hoffman, (615) 576-0735/FTS 626-0735
Oak Ridge National Laboratory (DE-AC05-88OR21400, Martin Marietta Energy Systems, Inc.) Contact: R. R. Judkins, (615) 574-4572/FTS 624-4572

This task provided materials technical support services to the Great Plains Coal Gasification Project, including support for technical issues related to materials performance in that plant. Activities included technical consultation, materials testing, recommendations of materials for use in the plant, welding techniques, corrosion and erosion analyses, and failure analyses.

Keywords: Technical Support, Materials

Division of Clean Coal Technology

Instrumentation and Facilities

550. Materials Technical Support for the Clean Coal Program FY 1989
$100,000

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Oak Ridge National Laboratory (DE-AC05-88OR21400, Martin Marietta Energy Systems, Inc.) R. R. Judkins, (615) 574-4572/FTS 624-4572 Contact: J. R. Keiser, (615) 574-4453/FTS 624-4453

This task is to provide materials technical support services to the projects on the Clean Coal Program which are being managed by the DOE Pittsburgh Energy Technology Center (PETC). The scope of the work will include assistance to PETC and the Clean Coal Program contractors on any technical issues related to materials performance on their projects. High-risk (in terms of materials degradation) areas will be identified to permit review and study that will minimize failures and thus protect U.S. Government interests in regard to schedules and costs. Emphasis of the project will be placed on prevention, rather than correction, of materials problems. Participation in project and design reviews will be a primary method used to assure that materials problems are avoided. Activities will also include technical consultation, materials testing, recommendations of materials, and failure analyses.

Keywords: Materials, Technical Support

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