

ENERGY MATERIALS COORDINATING COMMITTEE (EMaCC)

Fiscal Year 1988

June 30, 1989



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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Office of Basic Energy Sciences
Division of Materials Sciences
Washington, D.C. 20545**

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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, Batteries and Fuel Cells, Radioactive Waste Containment, and Superconductivity (established in FY 1987). 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 four 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 1988 and describes the materials research programs of various offices and divisions within the Department.

The Chairman of EMaCC for FY 1988 was Henry F. Walter; the Executive Secretary was Joseph B. Darby, Jr. The compilation of this report was assisted by QuesTech, Inc.

Joseph B. Darby, Jr.
Division of Materials Sciences
Chairman of EMaCC, FY 1989

**MEMBERSHIP LIST
DEPARTMENT OF ENERGY
ENERGY MATERIALS COORDINATING COMMITTEE**

<u>Organization</u>	<u>Representative</u>	<u>Phone No.</u>
CONSERVATION AND RENEWABLE ENERGY		
<u>Energy Utilization Research</u>		
Energy Conversion and Utilization Technologies	Stanley M. Wolf, CE-12 David Mello, CE-12	586-1514 586-9345
<u>Buildings and Community Systems</u>		
Building Systems Building Equipment	Peter Scofield, CE-131 John Ryan, CE-132 Ronald Fiskum, CE-132 Danny C. Lim, CE-132	586-9193 586-9130 586-9130 586-9130
<u>Industrial Programs</u>		
Waste Energy Reduction Improved Energy Productivity	Scott Richlen, CE-141 Matthew McMonigle, CE-142	586-2078 586-2082
<u>Transportation Systems</u>		
Heat Engine Propulsion	Robert B. Schulz, CE-151	586-8051
<u>Energy Storage and Distribution</u>		
Electric Energy Systems Energy Storage	Russell Eaton, CE-32 Albert R. Landgrebe, CE-32 Eberhart Reimers, CE-32	586-1506 586-1483 586-4563
<u>Solar Heat Technologies</u>		
Solar Thermal Technology Solar Buildings Technology	Brian G. Volintine, CE-331 Frank Wilkins, CE-331 John Goldsmith, CE-332 Mary-Margaret Jenior, CE-332	586-1739 586-1684 586-8779 586-2998

MEMBERSHIP LIST (Continued)

<u>Organization</u>	<u>Representative</u>	<u>Phone No.</u>
<u>Solar Electric Technologies</u>		
Wind/Ocean Technologies	William Richards, CE-351	586-5540
Photovoltaic Energy Technology	Morton B. Prince, CE-352	586-1725
<u>Renewable Energy</u>		
Biofuels and Municipal Waste Geothermal Technology	Michael Gurevich, CE-341 Raymond LaSala, CE-342	586-6104 586-4198
ENERGY RESEARCH		
<u>Basic Energy Sciences</u>		
Materials Sciences	Iran L. Thomas, ER-13	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	Ryszard Gajewski, ER-16	353-5995
<u>Health and Environmental Research</u>		
Physical and Technological Research	Gerald Goldstein, ER-74	353-5348
<u>Fusion Energy</u>		
Reactor Technologies	Theodore C. Reuther, ER-533	353-4963
NUCLEAR ENERGY		
<u>Program Support</u>		
Safety QA and Safeguards	Benjamin C. Wei, NE-46	353-3927

MEMBERSHIP LIST (Continued)

<u>Organization</u>	<u>Representative</u>	<u>Phone No.</u>
<u>Remedial Action and Waste Technology</u>		
Waste Treatment Projects	Henry F. Walter, NE-24	353-5510
<u>Uranium Enrichment</u>		
Advanced Technology Projects and Technology Transfer	Arnold P. Litman, NE-35	353-5777
<u>Civilian Reactor Development</u>		
Advanced Reactor Programs Technology Support Programs	J. Edward Fox, NE-451 Andrew Van Echo, NE-462	353-3985 353-3930
<u>Space and Defense Power Systems</u>		
Defense Energy Projects and Special Applications	William Barnett, NE-522	353-3097
<u>Naval Reactors</u>	Robert H. Steele, NE-60	557-5561
CIVILIAN RADIOACTIVE WASTE MANAGEMENT		
<u>Facilities Siting and Development</u>		
Siting and Facilities Technology	Mark Frei, RW-22	586-3217
<u>Systems Integration and Regulations</u>		
Systems Development	Tien Nguyen, RW-322	586-2797

MEMBERSHIP LIST (Continued)

<u>Organization</u>	<u>Representative</u>	<u>Phone No.</u>
DEFENSE PROGRAMS		
<u>Defense Waste and Byproducts</u>		
R&D and Byproducts	Ken Chacey, DP-123	353-4970
<u>Weapons Research, Development and Testing</u>		
Weapons Research	A. E. Evans, DP-242.2	353-3098
Inertial Fusion	Carl B. Hilland, DP-243	353-3687
FOSSIL ENERGY		
<u>Management, Planning, and Technical Coordination</u>		
Technical Coordination	James P. Carr, FE-14	353-6519

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 1988 Budget Summary Table for materials activities in each of the programs within the DOE is presented on page 7.

**FY 1988 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.)

	<u>FY 1988</u>
<u>Energy Conservation</u>	\$ 31,749,000
Office of Energy Utilization Research	6,889,000
Office of Buildings and Community Systems	483,000
Office of Industrial Programs	3,200,000
Office of Transportation Systems	21,177,000
<u>Renewable Energy</u>	\$ 33,997,300
Office of Energy Storage and Distribution	7,626,300
Office of Solar Heat Technologies	4,020,000
Office of Solar Electric Technologies	20,900,000
Office of Renewable Energy Technologies	1,451,000
<u>Office of Energy Research</u>	\$210,331,763
Office of Basic Energy Sciences	177,486,000
Office of Health and Environmental Research	364,000
Office of Fusion Energy	11,377,410
Small Business Innovation Research Program	21,104,353
<u>Office of Nuclear Energy</u>	\$125,718,000
Office of Remedial Action and Waste Technology	2,285,000
Office of Uranium Enrichment	17,462,000
Office of Civilian Reactor Development	36,771,000
Office of Space and Defense Power Systems	2,200,000
Office of Naval Reactors	67,000,000*

* Approximate

**FY 1988 BUDGET SUMMARY TABLE FOR
DOE MATERIALS ACTIVITIES (Continued)**

	<u>FY 1988</u>
<u>Office of Civilian Radioactive Waste Management</u>	\$ 12,833,000
Office of Systems Integration and Regulations	711,000
Office of Civilian Radioactive Waste Management/ Yucca Mountain Project (OCRWM/YMP)	11,767,000
Sandia National Laboratories: Brittle Fracture Technology Program	355,000
<u>Office of Defense Programs</u>	\$ 50,995,250
Office of Waste Research and Development	9,750
Office of Weapons Research, Development, and Testing	50,985,500
<u>Office of Fossil Energy</u>	\$ 7,028,000
Office of Technical Coordination	6,902,000
Office of Coal Technology	126,000
 TOTAL	 \$472,652,313

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 1988 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 in the second part of the report.

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, superconductors, 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:

	<u>FY 1988</u>
1. <u>Energy Conservation</u>	\$31,749,000
a. Office of Energy Utilization Research	\$ 6,889,000
(1) Energy Conversion and Utilization Technologies Division	6,889,000
b. Office of Buildings and Community Systems	483,000
(1) Building Systems Division	483,000
c. Office of Industrial Programs	\$ 3,200,000
(1) Improved Energy Productivity Division	1,414,000
(2) Waste Energy Reduction Division	1,786,000
d. Office of Transportation Systems	\$21,177,000
2. <u>Renewable Energy</u>	\$33,997,300
a. Office of Energy Storage and Distribution	\$ 7,626,300
(1) Energy Storage	4,451,300
(2) Electric Energy Systems	3,175,000
b. Office of Solar Heat Technologies	\$ 4,020,000
(1) Solar Buildings Technology Division	2,080,000
(2) Solar Thermal Technology Division	1,940,000
c. Office of Solar Electric Technologies	\$20,900,000
(1) Photovoltaic Energy Technology Division	20,900,000
d. Office of Renewable Energy Technologies	\$ 1,451,000
(1) Geothermal Technology Division (GTD)	645,000
(2) Biofuels and Municipal Waste Technology Division	806,000

OFFICE OF ENERGY UTILIZATION RESEARCH

	<u>FY 1988</u>
<u>Office of Energy Utilization Research - Grand Total</u>	\$6,889,000
<u>Energy Conversion and Utilization Technologies Division (ECUT)</u>	\$6,889,000
<u>Materials Preparation, Synthesis, Deposition, Growth or Forming</u>	\$2,950,000
Solid Lubricants Deposited From the Gas Phase	75,000
Engineered Tribological Surfaces	750,000
Modeling of Hard Coatings for Tribological Systems Operating Under Extreme Conditions	0
Abrasion and Impact Resistant Coatings	0
Coordination of ECUT Plastics Recycling and Reuse Efforts	0
Surface Roughness Wear Model for Ceramics	78,000
Assessment of the Economic Potential of Plastics Reuse	10,000
Laser Surface Modifications of Ceramics	125,000
Plasma-Assisted Sintering of Ceramics	94,000
Ion Implantation of Ceramics	345,000
Compositionally Modified Ceramics	342,000
Injection Molding of Electrosterically-Stabilized Oxide Suspensions in an Aqueous Medium	25,000
Assessment of the State of the Art in Machining and Surface Preparation of Ceramics	0
Microporous Ceramics	150,000
Chemical Vapor Deposition of Ceramic Composites	150,000
Thin-Wall Hollow Ceramic Spheres from Slurries	203,000
Strain Tolerant Ceramic Fibers from Liquid Crystal Polymer Precursors	55,000
Synthesis of SiC Whisker - MoSi ₂ Matrix Composites for Elevated Temperature Applications	100,000
Assessment of Curing and Joining of Polymers	15,000
Separation of Impurities from Molten Metals Using MHD Forces	100,000
Additives for High-Temperature Liquid Lubricants	55,000
IAD of TiN and Cr ₂ O ₃	100,000
Self-Lubricating Ceramic Surfaces	100,000
Surface Laser Treatment of Partially Stabilized Zirconia (PSZ)	78,000

OFFICE OF ENERGY UTILIZATION RESEARCH (Continued)

	<u>FY 1988</u>
<u>Materials Structures and Composition</u>	<u>\$1,735,000</u>
Mechanisms of Adherence at Ceramic Joints	150,000
Modeling of Boron-Effect in Ni ₃ Al	650,000
Predictions of Ordered Intermetallics	275,000
Predictions of Super-Strong Liquid Crystal Polymers	50,000
Predictions of Polymer Decompositions	135,000
Influence of Electronic Structure on Ordered Intermetallics	0
Liquid Crystalline Polymers Assessment	0
	(25,000 in FY 1985)
Thermosetting Resins with Reversible Crosslinks	100,000
Biobased Polymers	150,000
Assessment of DoD/NASA Thermal Insulation Technology	0
The Role of Inert Gas Entrapped in Rapidly Solidified Materials	225,000
<u>Materials Properties, Characterization, Behavior or Testing</u>	<u>\$ 895,000</u>
Ordered Metallic Alloys for High Temperature Applications	440,000
Measurements of Grain Boundary and Surface Energies of Metals and Ceramics	25,000
Effects of Laser Machining of Silicon Nitride	15,000
Friction and Wear Research and Development	415,000
<u>Device or Component Fabrication, Behavior or Testing</u>	<u>\$1,309,000</u>
Development of a Wear Model for Lubricated Sliding of Ceramics	114,000
Lubrication Research and Development	760,000
Energy-Efficient Gear-Lubrication Model	50,000
Modeling of Solid Ceramic Joints	0
	(175,000 in FY 1986)
Electromagnetic Joining of Ceramics - Laboratory Proof of Concept	25,000
Development of Tests for Ceramic-Ceramic and Ceramic-Metal Joints	30,000
Nondestructive Evaluation (NDE) of Ceramic Joints	80,000

OFFICE OF ENERGY UTILIZATION RESEARCH (Continued)

FY 1988

Device or Component Fabrication, Behavior or Testing (continued)

Assessment of Energy Applications of High Temperature Superconductors	135,000
Advanced Laser Fluorescence Measurements of Lubricant Film Behavior in a Diesel Engine	65,000
Ring/Cylinder Modeling	0
Effect of Cycle-to-Cycle Variations on Instantaneous Friction Torque	50,000

Instrumentation and Facilities \$ 0

Assessment of X-Ray Methods for Investigations of Ceramic Wear Surfaces	0
Thin Film Thermocouples for Heat Engines	0

(100,000 in FY 1987)

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 (ECUT)

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 Program is found in two projects, the Materials Project and the Tribology Project. The Tribology Project is managed by Argonne National Laboratory (ANL) and the Materials Project by the Oak Ridge National Laboratory (ORNL). 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 Project is in the areas of intermetallic compounds, ceramic-ceramic and ceramic-metal attachments, surface modifications of ceramics, recovery and reuse of plastic scrap, ceramic coatings, and materials structures theory. Materials research in the Tribology Project 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 Project.

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.
 - 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 Al₂O₃ and of B₂O₃ on steel were prepared and shown to have outstanding adherence and friction and wear reduction properties.
3. Modeling of Hard Coatings for Tribological Systems Operating Under Extreme Conditions¹ - DOE Contact D. Mello, (202) 586-9345; George Washington University Contact Bruce Kramer, (202) 676-8237
 - Work based on Kramer's Thermomechanical-Mechanical Theory for tool wear, and predictions for increased wear resistance.
 - Theory confirmed for several coatings on carbide inserts, predictions not confirmed for coatings on tool steels. Softening and deformation of the steel substrate below the coating, due to frictional heating during cutting, was determined to be the cause of coating failure.
 - TiC, TiN, ZrC, ZrN, HfC, HfN coatings on T-15 High Speed Cutting Tool Steel inserts produced wear lifetimes 3 to 10 times that of uncoated tool steel.
4. Abrasion and Impact Resistant Coatings¹ - DOE Contact D. Mello, (202) 586-9345; LLNL Contact William Steele, (415) 423-2949
 - Development and testing of innovative wear resistant coatings constructed by anchoring high density mat of very fine, hard filaments or "hairs" into surface of bulk matrix, at near vertical angles.

¹This project is concluding in FY 1988.

- Tests established that dense mat of 2 to 5 micron diameter carbon fibers embedded in the surface of any epoxy matrix provided complete protection to the matrix in a sandblast tester (which completely destroyed unprotected specimens).
 - Future tests are focusing on metal matrices, and on C, B, SiC, Al₂O₃, and ZrO fibers.
 - An initial *in situ* test of a polyvinyl chloride pipe lined with an 8 mm carbon fiber coating in a simulated industrial oil shale retort flow line resulted in failure at the coating due to shearing by fly ash and silica particles. Large pressure drops also occurred.
5. Coordination of ECUT Plastics Recycling and Reuse Efforts - DOE Contact Stanley M. Wolf, (202) 586-1514; Plastics Institute of America Contact Mike Curry or Al Spaak, (201) 420-5552
- Study of various methods for recycling or recovering value from post-consumer plastic wastes.
 - Transfer of technology.
6. 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 is being transferred to interested industries.
7. Assessment of the Economic Potential of Plastics Reuse - DOE Contact Stanley M. Wolf, (202) 586-1514; ORNL Contact Randall Curlee, (615) 576-4864
- Study of the economic viability of plastics reuse and the institutional incentives and barriers impacting market acceptance of recycle technologies.

8. Laser Surface Modifications of Ceramics - DOE Contact Stanley M. Wolf, (202) 586-1514; North Carolina State University Contact Jagdish Narayan, (919) 737-7874
 - Investigation of the effects induced by pulsed laser irradiation of thin films of metals deposited onto surfaces of ceramics.
 - Work has expanded from silicon carbide to silicon nitride materials and high temperature superconducting films.
9. Plasma-Assisted Sintering of Ceramics - DOE Contact Stanley M. Wolf, (202) 586-1514; Northwestern University Contact D. Lynn Johnson, (312) 492-3537
 - Investigation of the acceleration of sintering of ceramics via plasmas.
 - Equipment building stage complete, tests in progress.
10. Ion Implantation of Ceramics - DOE Contact Stanley M. Wolf, (202) 586-1514; ORNL Contact Carl McHargue, (615) 574-4344; Georgia Institute of Technology Contact Joe Cochran, (404) 894-6104; Universal Energy Systems Contact Peter Pronko, (513) 426-6900, ext. 113
 - Exploration of the effects of ion implantation on strength, fracture toughness, hardness, friction coefficient, and wear rates of ceramics.
 - Current work is on ion implantation into TiB_2 , ZrO_2 , Al_2O_3 , SiC , and Si_3N_4 .
11. Compositionally Modified Ceramics - DOE Contact Stanley M. Wolf, (202) 586-1514; ORNL Contact Rodney McKee, (615) 574-5144
 - Synthesis and characterization of layered structures of aluminum oxide and titanium oxides.
 - Study of the mechanics and mechanical behavior of the system
 - Development of superconducting films.

12. Injection Molding of Electrosterically-Stabilized Oxide Suspensions in an Aqueous Medium - DOE Contact Stanley M. Wolf, (202) 586-1514; University of Washington Contact Ilhan Aksay, (206) 543-2625
 - Attempts to produce a ceramic oxide suspension suitable for higher speed injection molding but using an aqueous solvent and minimum organic additives.
 - Approach is to adsorb polymer onto surface of submicron particle in suspension.
 - Concentrating on alpha-Al₂O₃.
13. Assessment of the State of the Art in Machining and Surface Preparation of Ceramics - DOE Contact Stanley M. Wolf, (202) 586-1514; ORNL Contact Dave Stinton, (415) 574-4556 and Ted Besmann, (615) 574-6852
 - Assessment of the current state of the art in the technologies of machining and surface preparation of ceramics.
 - Formulate recommendations for the need for further research and development, concluding in FY 1988.
14. Microporous Ceramics - DOE Contact Stanley M. Wolf, (202) 586-1514; LBL Contact Arlon Hunt, (415) 486-5370
 - Development of process to produce controlled porosity materials with tailored thermal, optical, and physical characteristics.
 - Determination of the properties of the finished material as related to the preparation technique.
15. Chemical Vapor Deposition of Ceramic Composites - DOE Contact Stanley M. Wolf, (202) 586-1514; ORNL Contact Ted Besmann, (615) 574-6852
 - Production of toughened ceramic matrix coatings via simultaneous chemical vapor deposition of dispersoid and matrix phases.
 - Development of silicon nitride-boron nitride coatings prepared from dichlorosilane, boron trichloride, and ammonia.

16. Thin-Wall Hollow Ceramic Spheres from Slurries - DOE Contact Stanley M. Wolf, (202) 586-1514; Georgia Institute of Technology Contact A. T. Chapman, (404) 894-4815; ORNL Contact David McElroy, (615) 574-5976
 - Development of a technique for producing thin-wall hollow ceramic spheres in the .1-5 mm diameter range using conventional dispersions of ceramic powders (slurries).
 - Initial work on Al_2O_3 and $\text{Al}_2\text{O}_3\text{-Cr}_2\text{O}_3$ with emphasis on materials as potential thermal insulations.
 - Measurement of thermal properties of beds of above materials for potential use as thermal insulations.

17. Strain Tolerant Ceramic Fibers from Liquid Crystal Polymer Precursors -DOE Contact Stanley M. Wolf, (202) 586-1514; University of Tennessee Contact Jack Fellers, (615) 974-5345; Collaborating ORNL Contact Mark Janney, (615) 574-4281
 - Attempt to demonstrate the feasibility of a ceramic reinforcing fiber with some amount of plastic strain tolerance.
 - Initial approach is to produce a microfibrillated liquid crystal polymer precursor fiber which will covert to a ceramic fiber with a "bundle of sticks" microstructure.

18. Synthesis of SiC Whisker - MoSi_2 Matrix Composites for Elevated Temperature Applications - DOE Contact Stanley M. Wolf, (202) 586-1514; LANL Contact Frank Gac, (505) 667-5452
 - Examination of SiC whisker- MoSi_2 matrix composites for potential elevated temperature structural applications in oxidizing environments.

19. Assessment of Curing and Joining of Polymers² - DOE Contact Stanley M. Wolf, (202) 586-1514; ORNL Contacts Ron Bradley, (615) 574-6094 and Paul Phillips, (615) 974-5304
 - Assessment aimed at identifying ECUT role, if any, in support of base technologies of curing and joining of polymers.

²This project will conclude in FY 1988.

- Concentration on technologies that would help US auto makers deploy lighter weight polymeric components in future vehicles.
20. Separation of Impurities from Molten Metals Using MHD Forces - DOE Contact Stanley M. Wolf, (202) 586-1514; ORNL Contact David O. Hobson, (615) 574-5109
- Theoretical and experimental proof-of-concepts.
 - W, pyrex beads removal from Hg.
 - SiC, Al₂O₃ removal from molten Al.
 - Computer modeling of MHD forces for optimization.
21. Additives for High-Temperature Liquid Lubricants³ - 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.
22. IAD of Tin and Cr₂O₃³ - DOE Contact D. Mello, (202) 586-9345; NRL Contact Fred Smidt, (202) 767-4800
- Films of TiN and Cr₂O₃ will be 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.
23. Self-Lubricating Ceramic Surfaces³ - 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 (BaF₂/CaF₂ + Ag or Sn, MoS₂, WS₂ and TaS₂) into ZrO₂ and Al₂O₃ substrates to obtain self-lubricating low friction and wear characteristics.

³This is a new project that was initiated at the end of FY 1988.

24. Surface Laser Treatment of Partially Stabilized Zirconia (PSZ) - DOE Contact D. Mello, (202) 586-9345; Illinois Institute of 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.

Materials Structures and Composition

25. Mechanisms of Adherence at Ceramic Joints - DOE Contact Stanley M. Wolf, (202) 586-1514; ORNL Contact Mike Santella, (615) 574-4805; Carnegie-Mellon University Contact Dick Fruehan, (412) 268-2677
- Investigations of the mechanisms of adherence at ceramic-metal joints.
 - Developed novel thinning procedure for TEM analysis of joints which led to realization of sub-micron scale of features.
 - Develop thermodynamic models to predict reaction of ceramics with liquid metal alloys.
26. Modeling of Boron-Effect in Ni₃Al - DOE Contact Stanley M. Wolf, (202) 586-1514; LANL Contact Jeff Hay, (505) 667-2097; Virginia Polytechnic Institute and State University Contact Diana Farkas, (703) 961-4742
- Computer modeling of the interfacial properties of Ni₃Al and the role of solute atoms such as B in preventing brittle fracture at grain boundaries.
 - Modeling of electronic properties, interatomic potentials, atomistic simulation, and crack propagation.
27. Predictions of Ordered Intermetallics - DOE Contact Stanley M. Wolf, (202) 586-1514; Imperial College of London Contact David Pettifor, 1-589-5111, ext. 5756 (England); ORNL Contact Don Nicholson, (615) 574-5873
- Develop and experimentally verify models for predicting ordered intermetallic alloys with cubic ordered crystal structures.
 - Initial approach based on structure maps.

28. Predictions of Super-Strong Liquid Crystal Polymers - DOE Contact Stanley M. Wolf, (202) 586-1514; LANL Contact Flonnie Dowell, (505) 667-8765
- Originate and develop advanced, first-principles, microscopic, molecular statistical-physics theories into mathematical models to predict new molecular structures most likely to form liquid crystal polymers.
 - Chemical synthesis and experimental characterization of liquid crystal polymers.
29. Predictions of Polymer Decompositions - DOE Contact Stanley M. Wolf, (202) 586-1514; ORNL Contact Bill Thiessen, (615) 574-4973
- Develop computer models at the atomic/molecular level to guide the development and optimization of polymers.
 - Discover how to tailor polymers to allow recovery of value from waste plastics by approaches based on molecular decomposition and/or rearrangements.
30. Influence of Electronic Structure on Ordered Intermetallics - DOE Contact Stanley M. Wolf, (202) 586-1514; Carnegie-Mellon University Contact T. B. Massalski, (412) 578-2708
- Identification of phenomenological correlations between the electronic structure and the ordering temperature and stacking arrangement in ordered intermetallics.
 - Initiation of electronic-level calculations to explain the correlations in terms of valence electronic energies as functions of the atomic arrangements in various stacking sequences.
31. Liquid Crystalline Polymers Assessment⁴ - DOE Contact Stanley M. Wolf, (202) 586-377; University of Tennessee Contact Paul Phillips, (615) 974-5304
- Identification of research activities currently underway in the area of liquid crystalline polymers.
 - Define research program to augment knowledge base.

⁴Assessment will be completed in FY 1988.

32. Thermosetting Resins with Reversible Crosslinks - DOE Contact Stanley M. Wolf, (202) 586-1514; Polytechnic of New York Contact Giuliana Tesoro (718) 643-5244
 - Development of thermosetting resins with "reversible crosslinks."
 - Feasibility shown in FY 1986 in epoxy with disulfide crosslink.
 - Production of plastics with the strengths, toughnesses, temperature capabilities, and corrosion resistances typical of thermoset resins but which can be easily reprocessed like a thermoplastic.
33. Biobased Polymers - DOE Stanley M. Wolf, (202) 586-1514; SERI Contact Helena Chum, (303) 231-7249
 - Exploration of the potential of innovative polymers from biomass, as well as biobased materials in general, for the production of inexpensive materials at a substantial overall energy savings.
 - Formulation of a research program for the development of biobased materials: biomass-derived plastics, innovative bioprocessing, and biotechnology-produced lightweight materials.
34. Assessment of DoD/NASA Thermal Insulation Technology - DOE Contact Stanley M. Wolf, (202) 586-1514; University of Kentucky Contact Alan Fine, (606) 257-3713
 - Assessment of the possibilities of technology transfer of specialized concepts from aerospace and other government programs to energy conservation applications in the civilian sector.
35. 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; University of Wisconsin Contact T. F. Kelly, (608) 263-1073
 - Ni-20Fe-20Cr with and without 2Mo and varying C (3 levels) processed by centrifugal atomization in flowing He gas into powders containing entrapped He.
 - Significant strengthening of several RSMs containing He.

Materials Properties, Characterization, Behavior or Testing

36. Ordered Metallic Alloys for High Temperature Applications -DOE Contact Stanley M. Wolf, (202) 586-1514; ORNL Contact Chain Liu, (615) 574-4459; NC State Contact Carl Koch, (919) 737-7340; Columbia Contact John Tien, (212) 280-5192; University of Tennessee Contact Ben Oliver, (615) 974-5326; Rensselaer Polytechnic Institute Contact Norm Stoloff, (518) 266-6436
- Development and determination of properties of ductile long-range ordered alloys mainly based on aluminides and silicides.
 - Main applications in high temperature service in steam turbines, heat engines, and heat exchangers.
37. Measurements of Grain Boundary and Surface Energies of Metals and Ceramics - DOE Contact Stanley M. Wolf, (202) 586-1514; ORNL Contact Ron Bradley, (615) 574-6094
- Experimental measurements of grain boundary and surface energies of metals and ceramics.
 - Measurements to be made in India using US Held Rupe funds (formerly PL 480 funds).
 - Efforts to establish long term effort in progress.
38. Effects of Laser Machining of Silicon Nitride - DOE Contact Stanley M. Wolf, (202) 586-1514; University of Southern California Contact Steve Copley, (213) 743-6223
- Elucidate the mechanisms of the reduction of strength but increase of Weibull moduli of laser machined versus diamond ground bend bars of silicon nitride.
 - Hope to learn how to increase strength and Weibull modulus at same time.

39. Friction and Wear Research and Development - DOE Contact D. Mello, (202) 586-9345; ORNL Contact Peter Blau, (615) 574-5377

- Measurements of the wear and friction coefficients for room-temperature, unlubricated sliding of alumina/silicon-carbide-whisker composites and zirconia-toughened alumina-matrix composites.
- Testing of low-temperature, unlubricated low-friction properties of diamond sliding on titanium diboride and on alternate materials.
- Measurement of friction and wear properties of high-temperature superconducting materials.
- Investigation of the effect of wear-debris particle conglomerates on the frictional behavior of high-temperature wear materials.
- Development of a "friction microprobe" for the measurement of friction coefficients of individual micrometer-sized constituent phases on the bearing surfaces of engineering materials.
- Measurement of unlubricated and lubricated sliding-friction coefficients of ceramics at temperatures up to 1000°C for a range of bearing loads.

Device or Component Fabrication, Behavior or Testing

40. 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.

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

- The low friction P-6 subfraction of 600N oil, identified in earlier studies, will be analyzed, and its constituent compounds will be tested for friction and wear performance.

- 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).
42. 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, is being developed and validated.
43. Modeling of Solid Ceramic Joints⁵ - DOE Contact Stanley M. Wolf, (202) 586-1514; The Norton Company Contact Don Patten, (617) 393-5962
- Development of finite element models of stress states in and around solid joints between a ceramic and a ceramic or metal part for specific geometries.
 - Initial modeling work on butt-on-butt in cylindrical and rectangular cross sections complete.
 - Experimental verifications of models in progress.
44. Electromagnetic Joining of Ceramics - Laboratory Proof of Concept - DOE Contact Stanley M. Wolf, (202) 586-1514; QuesTech, Inc., Contact Richard Silberglitt, (703) 760-1043; NRL Contact Dave Lewis, (202) 767-2131
- Develop methods for joining ceramic materials to one another by microwave-induced heating of the joint interface.
 - Work to date on alumina, mullite, and silicon nitride to themselves.

⁵This project will conclude in FY 1988.

45. Development of Tests for Ceramic-Ceramic and Ceramic-Metal Joints - DOE Contact Stanley M. Wolf, (202) 586-1514; ORNL Contact Artie Moorhead, (615) 574-5153
- Develop test specimens for measurement of strength and fracture toughness of ceramic-ceramic and ceramic-metal joints.
 - Fabricate and test brazed fracture toughness specimens for comparison with theoretical data generated by finite models.
46. Nondestructive Evaluation (NDE) of Ceramic Joints⁶ - DOE Contact Stanley M. Wolf, (202) 586-1514; ORNL Contact Bob McClung, (615) 574-4466
- Investigation of methods for non-destructive evaluation of ceramic joints in order to increase body of knowledge concerning properties and characteristics that affect serviceability of the joints.
 - Most work to date on acoustic techniques.
47. Assessment of Energy Applications of High Temperature Superconductors - DOE Contact Stanley M. Wolf, (202) 586-1514; ORNL Contact Steinar Dale, (615) 574-4829
- Object was to evaluate potential applications of high-temperature superconductors in energy-conserving systems.
 - Economic evaluations will be made on most promising applications, based on mature technologies.
 - Final report should provide definition for ECUT role in future superconductor research.

⁶This project will conclude in FY 1988.

48. Advanced Laser Fluorescence Measurements of Lubricant Film Behavior in a Diesel Engine⁷ - 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.
49. Ring/Cylinder Modeling⁸ - DOE Contact D. Mello, (202) 586-9345; Compu-Tec Engineering Contact Larry Brombolich, (314) 532-4062
- A PC-based computer model, the RING code, which predicts the effect of cylinder-bore distortions and operational variables on oil consumption, emission, friction and wear in internal-combustion engines has been developed and partially validated.
50. 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.
 - Final phase will use IFT measurements for *in situ* engine evaluation of new low-friction solid-lubricant coatings and surfaces developed in the tribology program.

⁷This is a new project that was initiated in the final quarter of FY 1988.

⁸This project is concluding in FY 1988.

Instrumentation and Facilities

51. Assessment of X-ray Methods for Investigations of Ceramic Wear Surfaces⁹ - DOE Contact D. Mello, (202) 586-9345; Virginia Polytechnic Institute and State University Contact Charles Houska, (703) 961-5652
 - Determine the potential of X-ray diffraction and fluorescence methods for nondestructive analyses of the near-surface wear regions of ceramics.

52. Thin Film Thermocouples for Heat Engines¹⁰ - DOE Contact D. Mello, (202) 586-9345; NIST-Gaithersburg Contact Ken Kreider, (301) 921-3281
 - Demonstration of the feasibility of a materials system and fabrication technique for measuring temperature inside the combustion chamber of ceramic insulated engines using thin film thermocouples.
 - Thin film thermocouple on ceramic substrate successfully tested in an engine in FY 1987.

⁹Assessment will be completed in FY 1988.

¹⁰This project will be completed in FY 1988.

OFFICE OF BUILDINGS AND COMMUNITY SYSTEMS

	<u>FY 1988</u>
<u>Office of Buildings and Community Systems - Grand Total</u>	\$483,000
<u>Building Systems Division</u>	\$483,000
<u>Materials Properties, Behavior, Characterization or Testing</u>	\$483,000
Unguarded Thin Heater Tester	200,000
Heat Flux Transducer Calibration Design	45,000
Variable R/Switchable Surface Analysis	30,000
Moisture Specimen Test Procedures	25,000
Recommended R-Levels - ZIP Program	30,000
CFC Foam Characterization	45,000
Foam Insulation Research	108,000

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 and building energy performance standards. Specific objectives include providing the technology to:

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

Building Systems Division

The goal of this Division is to provide a scientific and technical basis (including model standards) for reducing the use of energy in residential and commercial buildings by 35 percent by the year 2000 from that used in 1975, while maintaining existing levels of human comfort, health and safety. The Division's primary objectives are to support research that advances the scientific and technical options for increased energy efficiency in buildings, to promote the substitution of abundant fuels for scarce fuels in buildings, and to promulgate standards for increased efficiency of energy use. To accomplish a portion of this, the Building Materials Program seeks to increase the knowledge base concerning the physical, chemical and mechanical properties of building materials that determine their thermal energy performance effectiveness, durability, safety, and health impacts; 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 of materials; and to provide technical assistance, advice and data to organizations that develop consensus standards for the performance characteristics of materials. The DOE contact is Peter Scofield, (202) 586-9193.

Materials Properties, Behavior, Characterization or Testing

53. 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.
54. Heat Flux Transducer Calibration Design - DOE Contact Peter Scofield, (202) 586-9193; ORNL Contact David McElroy, (615) 574-5976
 - Laboratory study of calibration of imbedded heat flux transducers to produce accurate relation of millivolt signal to heat flux for use in large scale simulator.
55. 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.
56. Moisture Specimen Test Procedures - DOE Contact Peter Scofield, (202) 586-9193; NJIT Contact Erv Bales, (201) 596-3010
 - Study to use the thin heater and moisture measurement techniques to define a procedure for measuring and analyzing moisture interactions.
57. Recommended R-Levels - ZIP Program - DOE Contact Peter Scofield, (202) 586-9193; NIST Contact Steve Petersen, (301) 975-6136
 - Provide recommendations for R-values in residences for insulation zones in the USA.
 - Document the ZIP computer program that was used to select the recommended R-value levels.
58. CFC Foam Characterizations - 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.

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

- Freon-blown rigid urethane foam is studied for changes due to diffusional effects as insulation ages.
- Experimental measurements of gas permeability through cell wall materials.
- Investigation of new concepts which reduce overall thermal conductivity of foam material.

OFFICE OF INDUSTRIAL PROGRAMS

	<u>FY 1988</u>
<u>Office of Industrial Programs - Grand Total</u>	\$3,200,000
<u>Improved Energy Productivity Division</u>	\$1,414,000
<u>Materials Preparation, Synthesis, Deposition, Growth or Forming</u>	\$ 614,000
Composite Cathode Material Development	218,000
Cerox Inert Anode Material	150,000
Corrosion Resistant Amorphous Metallic Films	246,000
Investigation of Material for Inert Electrodes in Aluminum Electrodeposition Cells	0
<u>Materials Properties, Behavior, Characterization or Testing</u>	\$ 800,000
Diagnostic Sources of Current Inefficiency in Industrial Molten Salt Electrolytic Cells by Raman Spectroscopy	0
Expand and Control Inert Electrode Cell Operating Conditions	800,000
<u>Waste Energy Reduction Division</u>	\$1,786,000
<u>Materials Preparation, Synthesis, Deposition, Growth or Forming</u>	
Microwave Sintering of β -Alumina for Use in the Sodium Heat Engine	0
<u>Materials Properties, Behavior, Characterization or Testing</u>	\$ 940,000
Advanced Heat Exchanger Material Technology Development	825,000
Assessment of Strength Limiting Flaws in Ceramic Heat Exchanger Components	50,000
National Laboratory Support to Assessment of Strength Limiting Flaws in Ceramic Heat Exchanger Components	65,000

OFFICE OF INDUSTRIAL PROGRAMS (Continued)

	<u>FY 1988</u>
<u>Device or Component Fabrication, Behavior or Testing</u>	\$ 846,000
Ceramic Composite Heat Exchanger for the Chemical Industry	0
HiPHES System Design Study for Energy Production from Hazardous Wastes	302,000
HiPHES System Design Study for Energy Production from Hazardous Wastes	174,000
HiPHES System Design for an Advanced Reformer	195,000
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

60. Composite Cathode Material Development - DOE Contact M. J. McMonigle, (202) 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.
61. Cerox Inert Anode Material - DOE Contact M. J. McMonigle, (202) 586-2082; EL TECH Contact Tom Gilligan, (216) 357-4066
 - Evaluation of factors controlling costing formation, characteristics and stability when CeO_2 is added to molten cryolite.
62. Corrosion Resistant Amorphous Metallic Films - DOE Contact William Sonnett, (202) 586-2389; JPL Contact Edward Cuddihy, (818) 354-3188
 - Development of magnetron sputtering of MoCrB and TiCrPC on carbon steel to provide corrosion resistant surface.
63. Investigation of Material for Inert Electrodes in Aluminum Electrodeposition Cells - DOE Contact M. J. McMonigle, (202) 586-2087; MIT Contact J. S. Haggarty, (617) 253-3300
 - Generation of ultra pure powders and single crystals of candidate ceramic inert anodes using laser units and testing via pendant droplet technique.

Materials Properties, Behavior, Characterization or Testing

64. Diagnostic Sources of Current Inefficiency in Industrial Molten Salt Electrolytic Cells by Raman Spectroscopy - DOE Contact M. J. McMonigle, (202) 586-2087; MIT Contact D. R. Sadoway, (617) 253-3300
- Analysis of molten salts with Raman Spectroscopy to determine bath chemistry during electrolysis.
65. Expand and Control Inert Electrode Cell Operating Conditions - DOE Contact M. J. McMonigle, (202) 586-2087; PNL Contact Larry Morgan, (509) 375-3874
- Development of cermets for inert anodes and testing of attachment techniques for TiB_2 stable cathode.

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

66. 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

67. 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 corrosive waste stream constituents on candidate ceramic materials.
 - Development of advanced wet forming techniques for monolithic ceramic components.
68. 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.
69. 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.

Device or Component Fabrication, Behavior or Testing.

70. Ceramic Composite Heat Exchanger for the Chemical Industry - DOE Contact S. Richlen, (202) 586-2078; Babcock & Wilcox Contact W. Parks, (804) 522-5260
- Design and field test of non-recuperative process heat exchanger for the chemical industry.
 - Evaluation of composite systems in processing environment.
71. 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.

72. HiPHES System Design Study for Energy Production from Hazardous Wastes - DOE Contact S. Richlen, (202) 586-2078; Babcock & Wilcox Contact W. Parks, (804) 522-5260
- Development of preliminary design for high pressure heat exchange system (HiPHES) to produce heated pressurized air to a turbine.
 - Identification of critical material and design problems.
73. HiPHES System Design Study for an Advanced Reformer - DOE Contact S. Richlen, (202) 586-2078; Stone & Webster Engineering Corp. Contact J. Williams, (617) 589-7197
- Development of preliminary design for high pressure heat exchange system (HiPHES) for an advanced convective reformer.
 - Identification of critical material and design problems.
74. Ceramic Components for Stationary Gas Turbines in Cogeneration Service - DOE Contact J. Eustis, (202) 586-2098
- Develop ceramic composite components for stationary gas turbines used in cogeneration systems.

OFFICE OF TRANSPORTATION SYSTEMS

	<u>FY 1988</u>
<u>Office Of Transportation Systems - Grand Total</u>	\$21,177,000
<u>Materials Preparation, Synthesis, Deposition, Growth or Forming</u>	\$ 5,465,000
Silicon Carbide Powder Synthesis	80,000
Turbomilling of SiC	130,000
Sintered Silicon Nitride	200,000
Si ₃ N ₄ Powder Synthesis	305,000
Processing of Monolithics	305,000
Dispersion Toughened Si ₃ N ₄	371,000
Dispersion Toughened Si ₃ N ₄	550,000
Composite Development	560,000
Advanced Composites	149,000
Dispersion Toughened Oxide Composites	325,000
Transformation Toughened Ceramics Processing	346,000
Development of Toughened Ceramics	150,000
Injection Molded Composites	0
Low Expansion Ceramics	153,000
Active Metal Brazing PSZ-Iron	210,000
TiB ₂ Whiskers	131,000
Advanced Processing	1,000,000
Advanced Processing	500,000
<u>Materials Properties, Behavior, Characterization or Testing</u>	\$ 4,293,000
Ceramic Component Design Technology	100,000
Microstructural Modeling of Cracks	69,000
Adherence of Coatings	20,000
Dynamic Interfaces	182,000
Advanced Statistics Calculations	190,000
Physical Properties	75,000
Translucence Effects	20,000
Project Data Base	100,000
Characterization of Transformation-Toughened Ceramics	100,000
Fracture Behavior of Toughened Ceramics	210,000
Cyclic Fatigue of Toughened Ceramics	210,000

OFFICE OF TRANSPORTATION SYSTEMS (Continued)

FY 1988

Materials Properties, Behavior, Characterization or Testing (continued)

Rotor Materials Data Base	100,000
Ceramic Corrosion Evaluation AGT	100,000
Ceramic Durability Evaluation AGT	75,000
Environmental Effects in Toughened Ceramics	47,000
High Temperature Tensile Testing	200,000
Standard Tensile Test Development	120,000
Fracture Toughness Determination of Thin Coatings	55,000
Non-Destructive Evaluation	160,000
Ceramic Component NDE Technology	100,000
Computed Tomography	90,000
Nuclear Magnetic Resonance Imaging	160,000
NDE of Advanced Ceramics by Synchrotron Computer Tomography	100,000
Life Prediction	1,000,000
Life Prediction	500,000
Spectroscopic Characterization	70,000
Surface Adsorption	70,000
Thermodynamics of Surfaces	70,000
<u>Technology Transfer and Management Coordination</u>	\$ 1,222,000
Standard Reference Materials	270,000
Technology Transfer Assessment, Support Contracts, IEA Management and Coordination	87,000 865,000
<u>Device or Component Fabrication or Testing</u>	\$10,198,000
Metal-Ceramic Joints AGT	0
Metal-Ceramic Joints AGT	0
Ceramic-Ceramic Joints AGT	0
Advanced Coating Technology AGT	40,000
Advanced Coating Technology	150,000
Wear Resistant Coatings	248,000

OFFICE OF TRANSPORTATION SYSTEMS (Continued)FY 1988Device or Component Fabrication or Testing (continued)

Wear Resistant Coatings	244,000
Thick Thermal Barrier Coatings	246,000
Thick Thermal Barrier Coatings	145,000
Sliding Seal Materials for Diesel	75,000
High Temperature Solid Lubricant Coatings	50,000
Advanced Turbine Technology Applications Project (ATTAP, AGT-100)	4,500,000
Advanced Turbine Technology Applications Project (ATTAP, AGT-101)	4,500,000

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 nonpetroleum 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 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 of the following Office of Transportation Systems material projects.

Materials Preparation, Synthesis, Deposition, Growth or Forming

75. Silicon Carbide Powder Synthesis - 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 improved, sinterable silicon carbide powder with submicron particle size, narrow distribution, high surface area, and high purity using a plasma torch system that is scalable, environmentally acceptable, amenable to doping, and low-cost (<\$20/lb).
76. Turbomilling of SiC - 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
- Perform a feasibility study to determine the potential of turbomilling as a means of reducing particulate impurities in SiC whiskers.
 - Evaluate the effect of turbomilling variables on 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.
77. Sintered Silicon Nitride - 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.
78. Si_3N_4 Powder Synthesis - 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.

79. Processing of Monolithics - 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.
 - Develop processes that can be scaled most readily to high production rates.
80. Dispersion Toughened Si₃N₄ - 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.
81. Dispersion Toughened Si₃N₄ - 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.
82. Composite Development - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact D. Ray Johnson, (615) 576-6832; Norton Contact C. A. Ebel, (508) 393-5950
- Develop fully dense Si₃N₄ matrix SiC whisker composites utilizing the ASEA HIP (hot isostatic pressure) process.
83. Advanced Composites - 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
- Optimize the sintering procedure to densify composites of silicon nitride containing silicon carbide whiskers.

84. Dispersion Toughened Oxide Composites - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contacts D. Ray Johnson, (615) 576-6832 and T. N. Tieg, (615) 574-5173
- Development and characterization of SiC whisker-reinforced oxide composites with emphasis on pressureless sintering and control of the whisker-matrix interface properties.
85. Transformation Toughened Ceramics Processing - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact P. F. Becher, (615) 574-5157; Norton Contact Giulio A. Rossi, (508) 393-6600
- 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.
86. Development of Toughened Ceramics - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact D. Ray Johnson, (615) 576-6832; Ceramtec 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.
87. Injection Molded Composites - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contacts D. Ray Johnson, (615) 576-6832 and M. A. Janney, (615) 574-4281
- Develop alternate processes for complex shape formation of ceramic matrix composites that will reduce the binder removal time and increase the yield of high-reliability fired parts.
88. Low Expansion Ceramics - 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.

89. Active Metal Brazing PSZ-Iron - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contacts D. Ray Johnson, (615) 576-6832 and M. L. Santella, (615) 574-4805
- Develop brazing processes for joining ceramic components to nodular cast iron for adiabatic diesel application.
90. TiB₂ Whiskers - 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 TiB₂ whiskers, TiB₂-coated alpha-SiC whiskers, consolidate SiC matrix composites, and test in air above 1200°C.
91. Advanced Processing - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact R. L. Beatty, (615) 574-4536; Norton Contact S. D. Hartline, (508) 393-5828
- Development of new and/or improved ceramic processing tasks and in-process inspections that will eliminate many of the sources of strength-limiting flaws in structural ceramics, e.g., organic material in the powder, powder agglomerates, foreign inclusions, large grains.
92. Advanced Processing - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact R. L. Beatty, (615) 574-4536; GTE Contact Les Bowen, (617) 466-2536
- Development of new and/or improved ceramic processing tasks and in-process inspections that will eliminate many of the sources of strength-limiting flaws in structural ceramics, e.g., organic material in the powder, powder agglomerates, foreign inclusions, large grains.

Materials, Properties, Behavior, Characterization or Testing

93. 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.
94. Microstructural Modeling of Cracks - 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
- Investigate and develop models for fracture of cracks with realistic geometry under arbitrary stress states.

95. Adherence of Coatings - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact C. J. McHargue, (615) 574-4344; University of Tennessee Contact J. Sproul, (615) 974-5327
 - Conduct studies on adherence of coatings deposited on substrates subjected to ion beam mixing.
96. Dynamic Interfaces - 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 generic understanding of the friction and wear behavior of material interfaced between monolithic ceramics and ceramic-coated alloys in which the materials experience motion, as in adiabatic diesel engines.
97. Advanced Statistics Calculations - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact D. Ray Johnson, (615) 576-6832; GE Contact C. A. Johnson, (518) 387-6421
 - Develop advanced statistical techniques for describing and characterizing frequency distributions of strength in realistic cases of multiple and time-dependent distributions.
98. Physical Properties - 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.
99. Translucence Effects - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact D. L. McElroy, (615) 574-5976; Ricardo-ITI Contact Thomas Morel, (312) 789-0003/4
 - Evaluate the effects of translucence in diesel engines where ceramics are being considered for heat barrier applications.
100. Project Data Base - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contacts D. Ray Johnson, (615) 576-6832 and B. L. Booker, (615) 574-5113
 - Develop a comprehensive computer data base containing the experimental data on properties of ceramic materials generated in the overall program effort.

101. Characterization of Transformation-Toughened Ceramics - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact D. Ray Johnson, (615) 576-6832; AMTL Contact J. J. Swab, (617) 923-5410
 - Determine the effect of time-at-temperature on toughened oxide ceramics especially zirconia and alumina zirconia materials.
 - Evaluate and characterize composite ceramics toughened by fibers, whiskers, or particulates.
102. Fracture Behavior of Toughened Ceramics - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contacts D. Ray Johnson, (615) 576-6832 and P. F. Becher, (615) 574-5157
 - Characterize the high-temperature strength and toughness of state-of-the-art structural ceramics for heat engine applications.
103. Cyclic Fatigue of Toughened Ceramics - 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 tensile and cyclic fatigue tests on a uniaxially loaded ceramic specimen at elevated temperatures.
 - Establish a data base for design and analysis applications.
104. Rotor Materials Data Base - 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.
105. Ceramic Corrosion Evaluation AGT - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact D. Ray Johnson, (615) 576-6832; NASA Contact Carl A. Stearns, (216) 433-5504
 - Determine the effects of fuel and ingested impurities on the most promising of the durability tested ceramic materials.

106. Ceramic Durability Evaluation AGT - DOE Contact Saunders 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.
107. Environmental Effects in Toughened Ceramics - 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
- Investigate effects of water vapor (in combustion gas from adiabatic diesel) on time-dependent strength of transformation-toughened ceramics.
108. High Temperature Tensile Testing - 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.
109. Standard Tensile Test Development - 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) 975-5772
- Development of tensile test standards for characterizing strength and creep behavior of ceramic specimens at elevated temperature.
110. Fracture Toughness Determination of Thin Coatings - 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).
111. Non-Destructive Evaluation - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contacts D. Ray Johnson, (615) 576-6832 and W. A. Simpson, (615) 574-4421
- Develop nondestructive evaluation (NDE) techniques for quantitative determination of conditions in ceramics that affect the structural performance using high-frequency ultrasonics and radiography.

112. 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.
113. Computed Tomography - 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.
114. Nuclear Magnetic Resonance Imaging - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact D. Ray Johnson, (615) 576-6832; Argonne National Lab Contact W. A. Ellingson, (312) 972-6068
 - 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.
115. NDE of Advanced Ceramics by Synchrotron Computer Tomography - 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.

116. Life Prediction - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact C. R. Brinkman, (615) 574-5106; Allison Gas Turbine Division Contact D. L. Vacarri, (317) 230-4313
 - Demonstrate that the useful life of ceramics used in either gas turbine or low heat-rejection diesel engines can be adequately predicted.
117. Life Prediction - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact C. R. Brinkman, (615) 574-5106; Garrett Auxiliary Power Division Contact J. R. Smyth, (602) 220-3360
 - Demonstrate that the useful life of ceramics used in either gas turbine or low heat-rejection diesel engines can be adequately predicted.
118. Spectroscopic Characterization - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact M. A. Janney, (615) 574-4281; University of Wisconsin Contact M. A. Anderson, (608) 262-2470
 - Develop an understanding of the critical characterization parameters for powders to be used as the starting materials for high-performance ceramics.
119. Surface Adsorption - 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.
120. Thermodynamics of Surfaces - 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.

Technology Transfer and Management Coordination

121. Standard Reference Materials - 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.
122. Technology Transfer Assessment, Support Contracts, IEA - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact D. Ray Johnson, (615) 576-6832
 - Facilitate the transfer of technology to private industry.
123. Management and Coordination - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact D. Ray Johnson, (615) 576-6832
 - Assess the ceramic technology needs for advanced automotive head engines, formulate technical plans to meet these needs, and prioritize and implement a long-range research and development program.

Device or Component Fabrication or Testing

124. Metal-Ceramic Joints AGT - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact D. Ray Johnson, (615) 576-6832; GTE Contact E. M. Dunn, (617) 466-2312
 - Develop analytical and experimental methods for designing and evaluating reliable silicon carbide to metal and silicon nitride to metal joints.
125. Metal-Ceramic Joints AGT - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact D. Ray Johnson, (615) 576-6832; Battelle Contact R. A. Schmidt, (614) 424-4396
 - Perform an analytical and experimental evaluation of joining ceramic oxides to ceramic oxides and ceramic oxides to metals.

126. Ceramic-Ceramic Joints AGT - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact D. Ray Johnson, (615) 576-6832; Norton Contact Donald O. Patten, Jr., (508) 393-5963
- Develop techniques for producing reliable silicon carbide/silicon carbide and silicon nitride/silicon nitride bonds and analytical modeling to predict the performance of these bonds under various environmental and mechanical loading conditions.
127. Advanced Coating Technology AGT - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact D. Ray Johnson, (615) 576-6832; GTE Contacts V. K. Sarin, (617) 890-8460 and H. J. Kim, (617) 466-2742
- Development of coating compositions and procedures that will yield long term adherence and reduce or eliminate contact-stress damage to silicon nitride, silicon carbide, or other ceramic materials when utilized in advanced gas turbine engines. Multiple/graded coatings will be applied by computer controlled CVD process.
128. Advanced Coating Technology - 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.
129. Wear Resistant Coatings - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact D. P. Stinton, (615) 574-4556, Caterpillar Contacts M. B. Beardsley, (309) 578-8514 and 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.
130. Wear Resistant Coatings - 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.

131. Thick Thermal Barrier Coatings - DOE Contact John 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.
132. Thick Thermal Barrier Coatings - DOE Contact John Fairbanks, (202) 586-8066; NASA Contact M. Murray Bailey, (216) 433-3416; Caterpillar Contact H. J. Larson, (309) 578-6549
 - Develop a thermal barrier coating with enhanced durability for application in advanced diesel engines.
133. Sliding Seal Materials for Diesel - DOE Contact John 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.
134. 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 Prah, (216) 368-2000
 - Develop and evaluate high temperature wear resistant coating systems for use in the range of 1000°C in diesel engines.
135. Advanced Turbine Technology Applications Project (ATTAP, AGT-100) - DOE Contact Saunders B. Kramer (202) 586-8012; NASA Contact Paul Kerwin, (216) 586-3409; General Motors, Allison Gas Turbine Div. Contact Phil Haley, (317) 230-2272
 - Develop an advanced technology base applicable to a competitive automotive gas turbine engine.
136. Advanced Turbine Technology Applications Project (ATTAP, AGT-101) - 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 technology base applicable to a competitive automotive gas turbine engine.

OFFICE OF ENERGY STORAGE AND DISTRIBUTION

	<u>FY 1988</u>
<u>Office of Energy Storage and Distribution - Grand Total</u>	\$7,626,300
<u>Energy Storage</u>	\$4,451,300
<u>Materials Preparation, Synthesis, Deposition, Growth or Forming</u>	\$2,239,000
Incorporation of Phase Change Materials into Building Construction Components	130,000
Determination of the Effects of Dopants on Solid-State Phase Change Materials	40,000
Corrosion-Resistant Coatings for High-Temperature, High-Sulfur Activity Applications	129,000
Ceramics Research	1,000,000
Metals and Alloys	200,000
Organometallic Compounds	500,000
Polymers	100,000
Composite High Temperature Thermal Storage Media	140,000
Formation of Encapsulated Metallic Eutectic Thermal Storage Alloy	0
<u>Materials Properties, Behavior, Characterization or Testing</u>	\$1,345,800
Development of Ice Self-Release Mechanisms	30,000
Development of a Complex Compound Chill Storage System	225,000
Evaluation of Heats of Mixing Systems for Thermal Energy Storage	50,000
Dendritic Zinc Deposition in Flow Batteries	70,000
Fast Ion Conduction in Lithium Glasses	100,000
Polymeric Electrolytes for Ambient-Temperature Lithium Batteries	50,000
Exploratory Cell Research and Study of Fundamental Processes in Solid State Electrochemical Cells	95,000
Corrosion, Passivity, and Breakdown of Alloys Used in High-Energy-Density Batteries	80,000
Materials for Fuel Cells	150,000
Electrocatalysts for Oxygen Reduction and Generation	177,000
Materials Durability in the Zinc/Bromine System	145,000

OFFICE OF ENERGY STORAGE AND DISTRIBUTION (Continued)

FY 1988

Materials Properties, Behavior, Characterization or Testing (continued)

Use of Micro Particles as Heat Exchangers and Catalysts	32,800
Evaluation of Heats of Mixing Systems for Thermal Energy Storage	41,000
Development of Solid/Vapor Ammoniated Complexes as Thermal Energy Storage Materials	100,000

Materials Structure and Composition \$ 316,000

New Lithium-Based Battery Materials	202,000
Spectroscopic Studies of the Passive Films on Alkali and Alkaline Earth Metals in Nonaqueous Solvents	67,000
Raman Spectroscopy of Electrode Surface in Ambient-Temperature Lithium Secondary Battery	47,000

Device or Component Fabrication, Behavior or Testing \$ 550,500

Glass Electrolytes and Advanced Cell Concepts	150,000
Proton Exchange Membrane Electrode Optimization	50,000
Electrode Fabrication and Fuel Cell Evaluation	10,000
β -Alumina Electrolyte Development	0
Advanced Membrane Development for the Zinc/Bromine System	280,000
Improved Chromium Platings for Sodium/Sulfur Cell Containers	20,000
TES Media Evaluation	40,500

Electric Energy Systems \$3,175,000Materials Properties, Behavior, Characterization or Testing \$2,535,000

Microfilamentary Superconducting Composite	100,000
Practical Superconductor Development for Electric Power Applications	500,000
Practical Conductor Development for Electric Power Systems	350,000
Films Processing Methods and Device Technology Development	400,000

OFFICE OF ENERGY STORAGE AND DISTRIBUTION (Continued)FY 1988

<u>Materials Properties, Behavior, Characterization or Testing (continued)</u>	
Thin Film Superconductors for Electric Power Systems	200,000
High Temperature Superconductor Materials and Power Device Development	280,000
Fabrication Development of High Temperature Superconductor for Electric Utility Applications	300,000
Development of Practical Conductors Utilizing High-Temperature Oxides	300,000
Evaluation of Polymers for Electric Insulation	105,000
<u>Materials Structure and Composition</u>	\$ 40,000
Fast-Response Zinc Oxide Varistor Material Development	40,000
<u>Device or Component Fabrication, Behavior or Testing</u>	\$ 600,000
Fabrication of High-T _c , High-J _c Superconductors by Dynamic Compaction of Oriented High-T _c Powders and Processing Superconducting Materials Under High-O ₂ Pressure	300,000
Interfacial Aging Phenomena in Power Cable Insulation Systems	100,000
Conducting Polymer Research for Electric Power Equipment Applications	200,000

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 knowledge and scientific advances into new options for the use of renewable energy, for electric energy delivery and control systems and for energy conversions. The Office manages programs in energy storage and electric energy systems 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 oil and gas fuels by nuclear and renewable energy sources, and will increase the reliability and efficiency of the energy economy. The goal is to provide reliable, inexpensive devices to correct the timing and location mismatch between energy sources and energy users that is presently corrected by the energy storage inherent in fossil fuels. The research is divided into three subprograms: Electrochemical Energy Storage, Battery Development, and Thermal Energy Storage.

Materials Preparation, Synthesis, Deposition, Growth or Forming

137. Incorporation of Phase Change Materials into Building Construction Components - DOE Contact E. Reimers, (202) 586-4563; ORNL Contact J. Tomlinson, (615) 574-0768; University of Dayton Research Institute Contact I. Salyer, (513) 229-2113
 - Develop low-cost, effective phase change materials that freeze and melt in a temperature range suited for thermal storage in building interiors.
 - Develop wallboard systems containing these phase change materials
138. Determination of the Effects of Dopants on Solid State Phase Change Materials - DOE Contact E. Reimers, (202) 586-4563; ORNL Contact J. Tomlinson, (615) 574-0768; The University of Nevada-Reno Contact D. Chandra, (702) 784-4960
 - Develop temperature-adjusted organic solid state phase change materials with solid-solid transitions near room temperature.

139. 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, and develop corrosion-resistant coatings for high-temperature batteries.
140. Ceramics Research - DOE Contact A. Landgrebe, (202) 586-1483; LBL Contact E. Cairns, (415) 486-5028; SNL Contact R. Clark, (505) 844-6332
- Develop superconducting ionic materials.
 - Investigate materials for electrochemical corrosion prevention in batteries.
141. Metals and Alloys - DOE Contact A. Landgrebe, (202) 586-1483; LBL Contact E. Cairns, (415) 486-5028
- Evaluate aluminum alloys for use as negative electrodes in aluminum-air batteries.
 - Assess platinum alloys prepared for use as electrocatalysts in fuel cells and aluminum/air batteries.
142. Organometallic Compounds - DOE Contact A. Landgrebe, (202) 586-1483; ELTECH Systems Corporation Contact R. W. Fenn, (216) 357-4075
- Develop macrocyclic compounds of transition metals for use as electrocatalysts in fuel cells.
143. Polymers - DOE Contact A. Landgrebe, (202) 586-1483; LBL Contact E. Cairns, (415) 486-5028
- Design electronically and ionically conducting polymers for use as electrodes and electrolytes in batteries and fuel cells.
144. Composite High Temperature Thermal Storage Media - DOE Contact Eberhart Reimers, (202) 586-4563; ORNL Contact John Tomlinson, (615) 574-0768; IGT Contact Randy Petri, (312) 567-3985
- Development of composite sensible/latent storage media for use in packed bed, direct-contact systems for storage temperatures up to 1000°C.

145. Formation of Encapsulated Metallic Eutectic Thermal Storage Alloy - DOE Contact Eberhart Reimers, (202) 586-4563; Ohio State University Contact Prof. Robert Rapp, (614) 422-2491

- Develop a method of achieving an impermeable coating on pellets of metallic eutectic with high melting temperatures for latent heat thermal energy storage.

Materials Properties, Behavior, Characterization or Testing

146. Development of Ice Self-Release Mechanisms - DOE Contact E. Reimers, (202) 586-4563; ORNL Contact J. Tomlinson, (615) 574-0768; The University of Missouri - Columbia/Kansas City Contact W. Stewart, (816) 276-1283.

- Define physical and chemical mechanisms involved in self-release of ice from submerged evaporators
- Determine suitability of ice self-release for improved cool storage systems

147. Development of a Complex Compound Chill Storage System - DOE Contact E. Reimers, (202) 586-4563; ORNL Contact J. Tomlinson, (615) 574-0768; Rocky Research, Inc. Contact U. Rockenfeller, (702) 293-0851

- Evaluate enhanced heat and mass transfer techniques applicable to sorption systems based on ammonia
- Develop a cost-effective chill storage system based on ammoniated salts in the temperature range -60°C to 0°C

148. Evaluation of Heats of Mixing Systems for Thermal Energy Storage -DOE Contact E. Reimers, (202) 586-4563; ORNL Contact J. Tomlinson, (615) 574-0768; NY Polytechnic Institute Contact L. Stiel, (718) 643-5141

- Identify and determine the heats of mixing of promising liquid-liquid and liquid-solid chemical systems for energy storage.

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

- Investigate the protrusion growth rate in acidic zinc electrode position by means of rotating concentric cylinder electrode cell.

150. Fast Ion Conduction in Lithium Glasses - DOE Contact A. Landgrebe, (202) 586-1483; MIT Contact H. Tuller, (617) 253-6890
- Identify and characterize highly conducting and stable glasses for use as solid electrolytes in lithium/sulfur and sodium/sulfur cells, and understand how glass composition and structure correlate with fast alkali ion transport and chemical durability.
151. Polymeric Electrolytes for Ambient-Temperature Lithium Batteries - DOE Contact A. Landgrebe, (202) 586-1483; University of Pennsylvania Contact G. Farrington, (215) 898-6642
- Characterize electrode/polymer interfaces, and explore the feasibility of new polymers for use as electrodes and electrolytes in ambient-temperature rechargeable lithium batteries.
152. 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.
153. 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)358-7732
- Investigate the corrosion resistance of commercial cell container materials in water-containing organic electrolytes by electrochemical and ellipsometric techniques.
154. Materials for Fuel Cells - DOE Contact A. Landgrebe, (202) 586-1483; BNL Contact J. McBreen, (516) 282-4513
- Investigate oxygen reduction in new acidic electrolytes, and evaluate new fuel cell electrocatalysts.

155. Electrocatalysts for Oxygen Reduction and Generation - DOE Contact A. Landgrebe, (202) 584-1483; Case Western Reserve University Contact E. Yeager, (216) 386-3626
- Develop more effective electrocatalysts for O₂ reduction and generation, combining high catalytic activity with long-term stability in concentrated electrolytes.
156. Materials Durability in the Zinc/Bromine System - DOE Contract J. Quinn, (202) 586-1491; SNL Contact C. Arnold, (505) 844-8728
- Determine the extent and nature of the degradation of the construction materials used in zinc/bromine batteries.
157. Use of Micro Particles as Heat Exchangers and Catalysts - DOE Contact Eberhart Reimers, (202) 586-4563; LBL Contact Arlon Hunt, (415) 586-5370
- Measurement of dissociated fraction for SO₃ → SO₂ + 1/2 O₂ when concentrated sunlight is absorbed by a gas/particle mixture.
158. Evaluation of Heats of Mixing Systems for Thermal Energy Storage - DOE Contact Eberhart Reimers, (202) 586-4563; ORNL Contact John Tomlinson, (615) 574-0768; NY Polytechnic Institute Contact Leonard Stiel, (718) 643-5141
- Evaluation of heats of mixing in multi-component systems (liquid-liquid, liquid-solid) for thermal energy storage.
159. Development of Solid/Vapor Ammoniated Complexes as Thermal Energy Storage Materials - DOE Contact Eberhart Reimers, (202) 586-4563; ORNL Contact John Tomlinson, (615) 574-0768, Rocky Research Contact Uwe Rockenfeller, (702) 293-0851
- Laboratory study of technical issues with solid/vapor complexing compound systems.

Materials Structure and Composition

160. New Lithium-Based Battery Materials - DOE Contact A. Landgrebe, (202) 586-1483; Stanford University Contact R. Huggins, (415) 723-4110
- Evaluate the structural, thermodynamic, and kinetic parameters related to the use of materials as electrolytes and electrode components in high-performance, lithium-based battery systems and develop new materials.

161. 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.

162. 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 nonaqueous solutions by *in situ* Raman spectroscopy.

Device or Component Fabrication, Behavior or Testing

163. Glass Electrolytes and Advanced Cell Concepts - DOE Contact A. Landgrebe, (202) 586-1483; ANL Contact I. D. Bloom, (312) 972-4516

- Develop a high-conductivity glass electrolyte with low resistivity and the chemical stability to withstand the hostile Na/S cell environment.

164. Proton Exchange Membrane Electrode Optimization - DOE Contact A. Landgrebe, (202) 586-1483; LANL Contact J. Huff, (505) 667-6832

- Conduct basic research in electrochemistry and electrocatalysis to explore and improve the potential of a fuel cell system for use in transportation applications.

165. Electrode Fabrication and Fuel Cell Evaluation - DOE Contact A. Landgrebe, (202) 586-1483; LANL Contact J. Huff, (505) 667-6832

- Attain high power densities in fuel cells.

166. β -Alumina Electrolyte Development - DOE Contact J. Quinn, (202) 586-1491; Ceramtec Inc., Contact J. Rasmussen, (801) 486-5071

- Develop and evaluate low-cost β -alumina electrolytes for the sodium/sulfur battery system that demonstrate high fracture strength, high electrical conductivity, long life, and high performance.

167. Advanced Membrane Development for the Zinc/Bromine System - DOE Contact J. Quinn, (202) 586-1491; SNL Contact C. Arnold, (505) 844-8728
- Identify pretreatment techniques to improve the performance of the separator material currently used in the zinc/bromine battery, and identify new ion-exchange membrane materials that intrinsically have improved stability, permeability, and conductivity.
168. Improved Chromium Platings for Sodium/Sulfur Cell Containers - DOE Contact J. Quinn, (202) 596-1491; SNL Contact W. D. Bonivert, (415) 294-2987
- Improve the techniques employed to electroplate high-quality chromium coatings onto carbon steel cathode containers used in the sodium-sulfur battery.
169. TES Media Evaluation - DOE Contact E. Reimers, (202) 486-4563; PNL Contact J. Bates, (509) 375-2539
- Evaluate the ceramic/molten carbonate salt matrix thermal energy storage (TES) media in a typical industrial environment.

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 to promote 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, Electric Systems, and Materials Research.

Materials Properties, Behavior, Characterization or Testing

170. Microfilamentary Superconducting Composite - DOE Contact R. Eaton, (202) 586-1506; Ames Laboratory Contact D.K. Finnemore, (515) 294-4037
- Make stabilized microfilamentary superconducting wires from high- T_c copper oxide materials suitable for magnets that operate at 35 degrees K.
 - Conduct diagnostic studies to demonstrate sample quality.

171. Practical Superconductor Development for Electric Power Applications - DOE Contact R. Eaton, (202) 586-1506; Argonne National Laboratory Contact R. W. Weeks, (312) 972-4931
- Improve critical current density and other properties of high temperature superconducting (HTS) conductors in the fabrication of structurally reliable conductors for commercially viable electric power device applications.
172. Practical Conductor Development for Electric Power Systems - DOE Contact R. Eaton, (202) 586-1506; Brookhaven National Laboratory Contact A. Goland, (516) 282-3819
- Investigate methods for fabricating composite conductors containing high- T_c oxides.
 - Characterize the composite conductors fabricated by various methods by measurements of T_c , AC losses and J_c , as well as the effect of mechanical strain on the superconducting properties.
173. Films Processing Methods and Device Technology Development - DOE Contact R. Eaton, (202) 586-1506; Lawrence Berkeley Laboratory Contact N. Phillips, (415) 486-6062
- Explore methods for producing thin films of high- T_c superconductors that could be the basis for practical conductors (e.g., tapes).
 - Conduct AC electrical characterization of superconducting films.
174. Thin Film Superconductors for Electric Power Systems - DOE Contact R. Eaton, (202) 586-1506; SERI Contact R. McConnell, (303) 231-1019
- Characterize properties of fabricated thin film high temperature superconductors with sufficient current-carrying capability and stability in configuration suitable for use in electric power system devices.
175. High Temperature Superconductor Materials and Power Device Development - DOE Contact R. Eaton, (202) 586-1506; SNL Contact D. Scheuler, (505) 844-4041
- Develop high temperature ceramic conductors with improved superconductivity properties suited for use in electric energy systems.

176. 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 density capability of 10^4 A/cm² in a field of 2 Tesla at a temperature above 50K.
177. Development of Practical Conductors Utilizing High-Temperature Oxides - DOE Contract R. Eaton, (202) 586-1506; ORNL Contact D. Kroeger, (615) 574-5177
- Resolve problems associated with grain boundaries in polycrystalline high-T_c oxide superconductors to produce practical high current-carrying conductors.
178. Evaluation of Polymers for Electric Insulation - DOE Contact R. Eaton, (202) 586-1506; ORNL Contact H. McCoy, (615) 574-5115
- Characterize material properties of polymers suitable for use as dielectric materials.

Materials Structure and Composition

179. Fast-Response Zinc Oxide Varistor Material Development - DOE Contact R. Eaton, (202) 586-1506; ORNL Contact F. A. Modine, (615) 574-6287
- Investigate the electrical properties of ZnO varistors as a function of microstructure.

Device or Component Fabrication, Behavior or Testing

180. Fabrication of High-T_c and High-J_c Superconductors by Dynamic Compaction of Oriented High-T_c Powders and Processing Superconducting Materials Under High-O₂ Pressure - DOE Contact R. Eaton, (202) 586-1506; LLNL Contact W. Nellis, (415) 423-6665
- Develop technology to fabricate filamentary superconducting wire and cable with high critical parameters by dynamic compaction.
 - Develop processing techniques at elevated temperatures and oxygen pressure to make fully dense superconducting phases.

181. 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 effect of semiconducting compounds on the aging of extruded power cable insulation.
182. Conducting Polymer Research for Electric Power Equipment Applications - ORNL Contact S. J. Dale, (615) 574-4826, Westinghouse Contact E. Schoch, (412) 256-1960
- Investigate technical and economical feasibility of using conducting polymers as a replacement for carbon black-loaded materials in power equipment.

OFFICE OF SOLAR HEAT TECHNOLOGIES

	<u>FY 1988</u>
<u>Office of Solar Heat Technologies - Grand Total</u>	\$4,020,000
<u>Solar Buildings Technology Division</u>	\$2,080,000
<u>Materials Preparation, Synthesis, Deposition, Growth or Forming</u>	\$ 823,000
Thermochromic Materials Research for Optical Switching Films	8,000
Electrochromic Films and Deposition Processes	175,000
Electrochromic Glazings (Nickel-based)	170,000
Solid State Electrochromic "Smart" Windows (Tungsten-based)	130,000
Electrochromic Materials for Controlled Radiant Energy in Buildings (Tungsten-based)	230,000
Holographic Diffractive Structures for Enhanced Daylighting	110,000
<u>Materials Properties, Behavior, Characterization or Testing</u>	\$1,257,000
Advanced Phase-Change Materials and Systems for Solar- Passive Heating and Cooling of Residential Buildings	0
Thermal Energy Storage in "Plastic Crystals"	45,000
Desiccant Materials/Dehumidifier Geometries Research	150,000
Advanced Desiccant Materials Research	150,000
Open-Cycle Absorption Solar Cooling	110,000
Solar Cooling Research Facility	575,000
Evaluation of Photochromic Plastics	53,000
Daylighting Enhancement	80,000
Research and Development of a Static Optical System to Reduce Apparent Motion of the Sun	41,000
Advanced Evacuated Tubular Concentrator Research	53,000
<u>Solar Thermal Technology Division</u>	\$1,940,000
<u>Materials Preparation, Synthesis, Deposition Growth or Forming</u>	\$1,240,000
Silver/Polymer Reflector Research	1,240,000

OFFICE OF SOLAR HEAT TECHNOLOGIES (Continued)

	<u>FY 1988</u>
<u>Materials Properties, Behavior, Characterization or Testing</u>	\$ 700,000
Sol-Gel Protective Films for Metal Solar Mirrors	200,000
High Flux Effects on Materials	350,000
Surface Transformations of Metals	50,000
Materials for Applications in Regenerative Thermal Electrochemical (RTEC) Technology	50,000
Transport and Optical Properties of Molten Salt Blackeners	50,000

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

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 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

183. Thermochromic Materials Research for Optical Switching Films - DOE Contact M. M. Jenior, (202) 586-2998; Honeywell Contact G. V. Jorgensen, (612) 378-4655
- Development of a thermochromatic material that can be used on opaque wall surfaces to control insolation through building envelopes by passively switching between a heat-transmitting state and a heat-reflecting state at specific design temperatures.
184. Electrochromic Films and Deposition Processes - DOE Contact M. M. Jenior, (202) 586-2998; SERI Contact D. Blake, (303) 231-1202
- Optimization of the plasma-enhanced chemical vapor deposition (PE-CVD) process for producing electrochromic tungsten and molybdenum oxide films.
185. Electrochromic Glazings (Nickel-based) - DOE Contact M. M. Jenior, (202) 586-2998; LBL Contact Steven Selkowitz, (415) 486-5064
- 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.
186. Solid State Electrochromic "Smart" Windows (Tungsten-based) - DOE Contact M. M. Jenior, (202) 586-2998, 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 radiation through windows by the application of a small DC electric current.
 - Fabricate an all solid-state structure without cycle limitations.
187. Electrochromic Materials for Controlled Radiant Energy in Buildings (Tungsten-based) - DOE Contact M. M. Jenior, (202) 586-2998; Tufts University Contact R. B. Goldner, (617) 628-5000
- Development and modeling of all-solid optical switching devices for glazings and electrochromic based on films.

188. Holographic Diffractive Structures for Enhanced Daylighting - DOE Contact M. M. Jenior, (202) 586-2998; 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

189. Advanced Phase-Change Materials and Systems for Solar-Passive Heating and Cooling of Residential Buildings¹ - DOE Contact Robert Hassett, (202) 586-8163; University of Dayton Contact I. O. Salyer, (513) 229-2113

- Develop cost-effective methods for incorporating phase-change materials (PCMs) into construction materials (concrete, plasterboard, etc.)

190. Thermal Energy Storage in "Plastic Crystals"² - DOE Contact Robert Hassett, (202) 586-8163; University of Nevada-Reno Contact D. Chandra, (702) 784-4960

- Gain fundamental understanding of the nature of crystal structure changes in the lattice of solid-solid phase change materials (SSPCMs) and their effects on thermal properties of SSPCMs so that their transition temperatures can be lowered to near room temperature.

191. Desiccant Materials/Dehumidifier Geometries Research - DOE Contact J. Goldsmith, (202) 586-8779; SERI Contact A. Pesaran, (303) 231-7636

- Generate data bases on heat and mass transfer performance of promising dehumidifier geometry/material combinations and validate fundamental models that can be used as modules for overall systems-analysis computer programs.

¹Contract was stopped in May 1988 as the research was to be continued under a subcontract to the Oak Ridge Laboratory.

²Contract was terminated and all subsequent development efforts transferred to the Oak Ridge Laboratory.

192. Advanced Desiccant Materials Research - DOE Contact J. Goldsmith, (202) 586-8779; SERI Contact A. Czanderna, (303) 231-1240
- 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 is used for regenerating the water vapor sorption activity of the desiccant.
193. Open-Cycle Absorption Solar Cooling - DOE Contact John Goldsmith, (202) 586-8779; 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 concentration as a function of temperature.
 - Develop equations for calculating the thermophysical properties of various solutions.
194. 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.
195. Evaluation of Photochromic Plastics - DOE Contact M. M. Jenior, (202) 586-2998; American Optical Corporation Contact N. Chu, (617) 765-9711
- Evaluate photochromic plastic materials for their potential application to architectural glazing in buildings designed to use or control solar energy.

196. Daylighting Enhancement - DOE Contact M. M. Jenior, (202) 586-2998; LBL Contact Steven Selkowitz, (415) 486-5064
- Identify, develop, and characterize light guide materials and systems for collecting and transmitting sunlight within buildings to reduce electric lighting requirements.
197. Research and Development of a Static Optical System to Reduce Apparent Motion of the Sun - DOE Contact M. M. Jenior, (202) 586-2998; Lighting Sciences, Inc., Contact I. Lewin, (602) 991-9260
- Design a lens system with high transmittance as well as desired directional control for maximum efficiency.
198. Advanced Evacuated Tubular Concentrator Research - DOE Contact John Goldsmith (202) 586-8779; 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.

Solar Thermal Technology Division

Solar Thermal Technology is developing central receiver systems and parabolic dish systems to concentrate the sun’s energy. This concentrated energy can then be used for industrial process heat, generating electricity, or producing fuels and chemicals. The combination of concentrated direct solar flux (to 14,000 suns) and high temperature (to 5000°F) can cause unique and beneficial material transformations of metals, alloys, ceramics, and fibers. In addition, solar induced degradation of materials such as silver polymer films and metals for use in solar thermal receiver systems is being studied.

Materials Preparation, Synthesis, Deposition, Growth or Forming

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

200. 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, for applications in the next generation solar concentrators.
201. High Flux Effects on Materials - DOE Contact Frank Wilkins, (202) 586-1684; SERI Contact Daniel O'Neill, (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.
202. 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 metal powders alloyed to metal substrates using high solar flux.
203. Materials for Applications in Regenerative Thermal Electrochemical (RTEC) Technology - DOE Contact Frank Wilkins, (202) 586-1684; SERI Contact L. Marty Murphy, (303) 231-1050
- Identify and characterize materials needed for containment of corrosive chemicals used in electrochemical applications; the materials used for containment will be exposed to moderate intensity flux and reasonably high temperatures.

204. Transport and Optical Properties of Molten Salt Darkeners - DOE Contact Sigmund Gronich, (202) 586-1623; SERI Contact Daniel M. Blake, (303) 231-1222
- Determine the radiant transport and optical properties of cobalt oxide powders for possible use as darkeners for molten nitrate salts. Flowing molten nitrate salts are used as a radiant energy absorber in the Direct Absorption Receiver (DAR).

OFFICE OF SOLAR ELECTRIC TECHNOLOGIES

	<u>FY 1988</u>
<u>Office of Solar Electric Technologies - Grand Total</u>	\$20,900,000
<u>Photovoltaic Energy Technology Division</u>	\$20,900,000
<u>Materials Preparation, Synthesis, Deposition, Growth or Forming</u>	\$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
<u>Materials Properties, Behavior, Characterization or Testing</u>	\$ 2,900,000
Materials and Device Characterization	2,900,000
<u>Device or Component Fabrication, Behavior or Testing</u>	\$ 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

205. Amorphous Silicon for Solar Cells - DOE Contact Morton B. Prince, (202) 586-1725; SERI Contact William Wallace, (303) 231-1380
- Plasma enhanced chemical vapor deposition (CVD), thermal CVD, and sputtering techniques with goal of developing 12 percent efficient cells of area of 1000 cm².
206. 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 CuInSe₂ and CdTe.
 - Large area, (1000 cm²) control of interlayer diffusion, lattice matching and stoichiometry for long-term enhancement of 15 percent efficient large area solar cells.

207. 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 King, (505) 844-8220

- 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 cm² flat plate cells.

Materials Properties, Behavior, Characterization or Testing

208. 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

209. High-Efficiency Crystal Silicon Solar Cells - DOE Contact Morton B. Prince, (202) 586-1725; SERI Contact John Benner, (303) 231-1396; SNLA Contact David King, (505) 844-8220

- 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

	<u>FY 1988</u>
<u>Office of Renewable Energy Technologies - Grand Total</u>	\$1,451,000
<u>Geothermal Technology Division (GTD)</u>	\$ 645,000
<u>Materials Preparation, Synthesis, Deposition, Growth or Forming</u>	\$ 350,000
High Temperature Elastomers for Dynamic Sealing Applications	5,000
Geothermal Waste Utilization and Disposal	10,000
Materials for Non-Metallic Heat Exchangers	110,000
Biochemical Concentration and Removal of Toxic Components from Geothermal Wastes	225,000
<u>Materials Properties, Behavior, Characterization or Testing</u>	\$ 295,000
Advanced High Temperature Geothermal Well Cements	185,000
Corrosion in Binary Geothermal Systems	10,000
Advanced High Temperature Chemical Systems for Lost Circulation Control	100,000
<u>Biofuels and Municipal Waste Technology (BMWT) Division</u>	\$ 806,000
<u>Materials Preparation, Synthesis, Deposition, Growth or Forming</u>	\$ 280,000
Medium Temperature Solid Electrolytes: Proton Conductors	155,000
Hydrogen Production with Photoactive Semiconductor Catalysts	125,000
<u>Materials Properties, Behavior, Characterization or Testing</u>	\$ 526,000
High Temperature Steam Electrolysis	50,000
Cold Storage of Hydrogen on Activated Carbon	76,000
Hydrogen Production via Photoelectrolysis	60,000
Novel Methods for Solar Hydrogen Production	340,000

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

210. High Temperature Elastomers for Dynamic Sealing Applications - DOE Contact R. LaSala, (202) 896-4198; BNL Contact L. E. Kukacka, (516) 282-3065
 - Chemical modification of previously developed and tested Y-267 EPDM 260°C static seal material for use in dynamic sealing applications.
 - Optimization of EPDM formulations for use in critical high cost applications such as in drill pipe protectors, rotating head seals and blow-out preventors.
211. Geothermal Waste Utilization and Disposal - DOE Contact G. J. Cooper, (202) 896-1146; BNL Contact L. E. Kukacka, (516) 282-3065
 - Studies of methods for stabilizing toxic geothermal residues in composites so that they can be used for general construction purposes.
212. Materials for Non-Metallic Heat Exchangers - DOE Contact R. LaSala, (202) 896-4198; BNL Contact L. E. Kukacka, (516) 282-3065
 - Development of corrosion resistant metallic and silicon carbide-filled composites that have thermal conductivities in the range of stainless steels.
213. 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

214. 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, high temperature well cements under placement and downhole environmental conditions.
 - Mechanisms of cement deterioration in high CO₂-containing geothermal brines.
215. Corrosion in Binary Geothermal Systems - DOE Contact R. LaSala, (202) 896-4198; BNL Contact D. van Rooyen, (516) 282-4050
- Quantitative corrosion data from laboratory and plant tests for metals presently used in binary plants and other more potentially resistive metals.
216. 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

217. Medium Temperature Solid Electrolytes: Proton Conductors - DOE Contact M. Gurevich, (202) 586-6104; BNL Contact C. Linkous, (516) 282-7949; Stanford Contact R. Huggins, (415) 723-4110
- Investigation of candidate electrolytes capable of operating in 300-600°C temperature regime.
218. 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

219. High Temperature Steam Electrolysis - DOE Contact M. Gurevich, (202) 586-6104; Westinghouse R&D Center Contact W. Feduska, (412) 256-1951
- Characterization of life and stability of solid oxide electrolyte cells operated in the high temperature electrolysis mode at 1000°C for hydrogen production.
220. 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.
221. 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.

222. 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

	<u>FY 1988</u>
<u>Office of Energy Research - Grand Total</u>	\$210,331,763
<u>Office of Basic Energy Sciences</u>	\$177,486,000
<u>Division of Materials Sciences</u>	\$172,500,000
<u>Division of Engineering and Geosciences</u>	\$ 4,986,000
<u>Materials Properties, Behavior, Characterization or Testing</u>	\$ 4,371,000
Bounds on Dynamic Plastic Deformation	125,000
Diffusion, Fluid Flow, and Sound Propagation in Disordered Media	68,000
In-Flight Measurement of the Temperature of Small, High Velocity Particles	133,000
Experimental Measurement of the Plasma/Particle Interaction	319,000
Integrated Sensor/Model Development for Automated Welding	450,000
Nondestructive Characterization of Fracture Dynamics and Crack Growth	183,000
Plasma Reduction of Metallic Oxide Particles	71,000
High-Temperature Gas-Particle Reactions	125,000
Mathematical Modeling of Transport Phenomena in Plasma Systems	95,000
In-Process Control of Residual Stresses and Distortion in Automatic Welding	41,000
Multivariable Control of the Gas-Metal Arc Welding Process	156,000
Metal Transfer in Gas Metal Arc Welding	127,000
Modeling and Analysis of Surface Cracks	192,000
Thermal Plasma Processing of Materials	361,000
Transport Properties of Disordered Porous Media from the Microstructure	94,000

OFFICE OF ENERGY RESEARCH (Continued)

FY 1988

Division of Engineering and Geosciences (continued)Materials Properties, Behavior, Characterization
or Testing (continued)

Inelastic Deformation and Damage at High Temperature	125,000
Energy Changes in Transforming Solids	165,000
Nondestructive Testing	250,000
Effective Elastic Properties of Cracked Solids	55,000
Laser Diagnostics of Plasma Assisted Chemical Vapor Deposition (PACVD) Processes	185,000
Elastic-Plastic Fracture Analysis Emphasis on Surface Flaws	439,000
Continuous Damage Theory	54,000
New Ultrasonic Imaging and Measurement Techniques for NDE	250,000
Effects of Crack Geometry and Near-Crack Materials Behavior on Scattering of Ultrasonic Waves for QNDE Applications	68,000
Diffusion and Ion Transport in Multicomponent Electrolyte Solutions	140,000
Reactive Flow Modeling	100,000

Division of Advanced Energy Projects \$ 615,000

Aerodynamic Focusing of Particles and Heavy Molecules	67,000
Superconductive Electric Motor	394,000
Gas Jet Deposition of Metallic, Semiconducting and Insulating Films	154,000

Office of Health and Environmental Research \$ 364,000Division of Physical and Technological Research \$ 364,000

<u>Materials Properties, Behavior, Characterization or Testing</u>	\$ 364,000
Semiconductor Radiation Detector Technology	364,000

OFFICE OF ENERGY RESEARCH (Continued)

	<u>FY 1988</u>
<u>Office of Fusion Energy</u>	\$11,377,410
<u>Materials Properties, Behavior, Characterization or Testing</u>	\$11,317,410
Irradiation Damage in Ceramics for Fusion Applications	400,000
Neutron-Interactive Materials	2,600,000
Neutron-Interactive Materials (U.S./Japan)	1,300,000
Development of Vanadium-Base Alloys for Fusion Reactor Applications	325,000
Corrosion/Compatibility of Fusion Reactor Structural Materials	250,000
Solid Breeder Materials	290,000
Tritium Oxidation Kinetics	340,000
FLIBE (Fluorine-Lithium-Beryllium Salt)	77,000
Statistical Theory of Radiation Effects	105,000
Welding of Low Activation and Fusion First Wall Materials	90,000
Neutron Interactive Materials Program	1,555,000
BEATRIX-II	1,150,000
Neutron Interactive Materials Calculations	290,000
Damage Analysis and Fundamental Studies for Fusion Reactor Materials	200,410
Plasma-Materials Interactions	990,000
Aqueous Corrosion Studied in Support of the ITER Project	300,000
Key Issues of Fusion Nuclear Technology Development	0
Thermal Convection Loop Experiments and Analysis of Mass Transport in Lithium/Fe-12Cr-1MoVW Systems	200,000
Solid Breeder Materials Program	395,000
High Heat Flux Irradiations	60,000
Materials Studies for Magnetic Fusion Energy Applications at Low Temperatures	400,000
<u>Instrumentation and Facilities</u>	\$ 60,000
Beam Plasma Neutron Source	60,000

OFFICE OF ENERGY RESEARCH (Continued)

	<u>FY 1988</u>
<u>Small Business Innovation Research Program</u>	\$21,104,353*
<u>Materials Preparation, Synthesis, Deposition, Growth or Forming</u>	\$ 9,736,324*
<u>Phase I Projects:</u>	
Extrusion of High Temperature Superconducting Materials	48,884
Optimized Plastic Scintillating Optical Fibers with Improved Radiation Resistance for Use at the Superconducting Super Collider	50,000
The Fabrication and Processing of High Temperature Superconducting Materials	50,000
A Ceramic Membrane for Gas Separations	49,989
Radiation-Modified Pyroelectric Conversion Materials	49,990
Improvement of the Oxidation Resistance of Alumina-Forming Alloys by Nitriding	50,000
A Novel Thin Film Diamond Stripper Foil for Tandem Ion Accelerators	49,778
The Development of Multifilamentary Superconducting Composites	49,375
Fabrication of High Temperature Superconductor Filaments from Metal-Containing Polymeric Precursors	49,028
A Novel Oxygen-Plasma Spray System for the Processing of High Temperature Superconductors	49,314
An Oriented High Temperature Superconductor Fabricated by a Novel Technique for Use in Power Applications at Liquid Nitrogen Temperature	49,121
The Development of High Strength Superconducting Wire for High Magnetic Field Applications	49,893
Enhancement of Critical Current Density in High Temperature Superconducting Ceramic Wire Through Hot-Extrusion Induced Texture	50,000

*Includes 41 new Phase I and 29 new Phase II awards made in FY 1988 and second year incremental funding for 11 Phase II projects initiated in FY 1987. Totals reflect the fact that Phase II funding levels are spread over a two-year period.

OFFICE OF ENERGY RESEARCH (Continued)

FY 1988

Small Business Innovation Research Program (continued)Materials Preparation, Synthesis, Deposition, Growth or Forming (continued)Phase I Projects: (continued)

The Synthesis of New Metastable Ultrahard Materials	49,992
High-Temperature Advanced Structural Ceramics	49,367
A New and Novel Technique for the Sputter Deposition of High Temperature Superconducting Thin Films and Coatings	49,944
The Preparation of Thin Film Superconductors by Chemical Vapor Deposition of Volatile Metal Chelates	49,970
Enhancement of Transport Current Density in $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$ Superconductors Using Dual-Temperature Extrusion Processing	50,000
Enhancement of Transport Current Density in $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$ Superconductors Using Low Temperature Densification	49,993
Enhancement of Transport Current Density in $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$ Fibers Using Laser Zone Refinement	49,999
Hot Deformation of Niobium Nitride Composites	49,970
Increased Tin Content in a Ductile Matrix for Niobium Tin Conductors	49,989
Improvement of the Ductility of Fine Filamentary Superconductors for the Superconducting Super Collider and Other Applications	49,979
Plasma-Enhanced Thermal Reaction Coatings of NbN for Conductor Applications	49,999
Low Cost High Resistivity Float-Zone Silicon Diodes	48,500

Phase II Projects: (First 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	478,743

OFFICE OF ENERGY RESEARCH (Continued)

FY 1988

Small Business Innovation Research Program (continued)Materials Preparation, Synthesis, Deposition, Growth or Forming (continued)Phase II Projects: (continued)

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 VLS SiC Whiskers	499,933
High Performance, Distributed-Tin Nb ₃ Sn Superconductor Wire	356,837
Advanced Insulating Coatings for Plasma Confinement Systems	499,466
Electrically Conductive Polymers by Ion Implantation	499,280
Process Development for Producing Nb ₃ Sn Multifilament Superconductors of High Current Density	491,155
The Development of a Process for Making Multifilamentary NbN	486,943
A Graphite Fiber Reinforced Copper Composite for Fusion Reactor Applications	500,000

Phase II Projects: (Second Year)

The Development of Nb ₃ Sn Superconductor with Micron-Size Filaments, High-Current Densities, and Low Magnetization	456,278
Neutron Stable Carbon-Carbon Composites	444,935
The Improvement of Copper/Epoxy Composites for Fusion Energy Magnet Applications	499,918
An Internal-External Bronze Process for the Manufacture of Large Filament Nb ₃ Sn	499,981

OFFICE OF ENERGY RESEARCH (Continued)

FY 1988

Small Business Innovation Research Program (continued)Materials Properties, Behavior, Characterization or Testing

\$ 2,098,460**

Phase I Projects:Noncontact, High-Resolution, Thermal Wave Detection
of Superconductive Transitions in High Critical
Temperature Materials

50,000

Closed-Loop Figuring of Mirrors

48,530

Phase II Projects: (First Year)

High Thermal Conductivity Sintered AlN

499,961

High-Speed, High-Resolution Ultrasonic HDT/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

Phase II Projects: (Second Year)Investigation of Fatigue Failure Initiation and
Propagation in Wind-Turbine-Grade Wood/Epoxy
Laminate Containing Several Veneer Joint Styles

499,980

**Totals reflect the fact that Phase II funding levels are spread over a two year period.

OFFICE OF ENERGY RESEARCH (Continued)

FY 1988

Small Business Innovation Research Program (continued)Device or Component Fabrication, Behavior or Testing \$ 9,269,569*Phase I Projects:

Infrared Detectors Using High Critical Temperature Granular Josephson Junctions	49,877
Diamond Coatings and Windows for Millimeter Microwave Tubes and Transmission Lines	50,000
Large Area Hydrogenated Amorphous Silicon Thin Film Particle Detectors	49,977
Fiber Driven Acoustic Cavity Sensors	49,998
Diamond-like Films for Microwave Transmission Window Applications	49,132
Ultra High Resistivity Silicon Crystals for Radiation Detectors	49,832
High Temperature Fiber Optic Sensors	49,529
A Laser Surface Profilometer for Steep Aspheric Surfaces	49,875
A Non-Contracting Dimensional Profiler	49,773
The Development of a Method for Greatly Increasing the Count-Rate Capability and Endurance for Position-Sensitive Detector Systems	50,000
Magnetic Control of Critical Currents in Superconducting Quantum Interference Devices Operating at 77K	49,851
Large-Area Photodetector Arrays	49,551
Ion-Implanted Semiconducting Polymeric Devices	49,995
A Search for a Rapid Oxygen Sensor Using High-Temperature, Complex Eutectic Thin Films	49,334

Phase II Projects: (First Year)

Research and Development of Multisegment Ceramic Ring Cryogenic Seals	489,634
Gate Valves for Fusion Application - Radial-Directed, Fluid-Pressure-Loaded, All-Metal-Sealed Double Gates	500,000
Continuous Casting of Metallic Nuclear Fuel Rods	491,018
Electromagnetic Bearings for Cryogenic Applications	499,893

OFFICE OF ENERGY RESEARCH (Continued)

FY 1988

Small Business Innovation Research Program (continued)

Device or Component Fabrication, Behavior or Testing (continued)

Phase II Projects: (First Year) (continued)

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 - The Membrane Liquid Trap	497,500
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
Heat Pipe Technology for AVLIS Processes	494,119

Phase II Projects: (Second Year)

An All-Metal, Demountable Cryogenic Seal	480,332
The Development of a New Direct Energy Conversion Device: The Thermotunnel Converter	499,981
An Optimized NbTi Superconducting Strand and Cable for Accelerator Magnet Applications	455,062
A Real Time, Non-Contact Optical Surface Motion Monitor	472,831
Surface Figure Measurements of X-Ray Optics	328,347
The Development of an Improved Composite Conductor with Electrically Uncoupled Fine NbTi Filaments and High Current Density	500,000

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 1988 for the Division of Materials Sciences were \$172,500,000. This was allocated to 554 projects. Many projects cross the traditional categories and, for example, involve property-structure relationships. Nevertheless, the approximate funding distribution for FY 1988 was:

	<u>\$ (Millions)</u>
Materials Preparation, Synthesis, Deposition, Growth or Forming	21.0
Materials Structure and Composition	27.5
Materials Properties, Behavior, Characterization or Testing	80.8
Device or Component Fabrication, Behavior or Testing	--
Facilities	43.2

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 1988 (DOE/ER-0389 dated September 1988). 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; Collaborative Research Centers (descriptive information); cross-cutting indices: investigators, materials, techniques, phenomena, environment. Limited copies may be obtained by calling (301) 353-3427.

Division of Engineering and Geosciences

Materials Properties, Behavior, Characterization or Testing

223. 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 details numerical analysis.
224. 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.
225. 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 electrostatically 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.

226. Experimental Measurement of the Plasma/Particle Interaction - DOE Contact Oscar P. Manley, (301) 353-5822; Idaho National Engineering Laboratory Contacts M. E. McIlwain, (208) 526-8818, C. B. Shaw, 208-526-8818, S. C. Snyder, (208) 526-1507, 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.
227. 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.
228. Nondestructive Characterization of Fracture Dynamics and Crack Growth - DOE Contact Oscar P. Manley, (301) 353-5822; Idaho National Engineering Laboratory Contacts J. A. Johnson, (208) 526-9021, B. A. Barna, (208) 526-6124, R. A. Allemeir, (208) 526-9588
- 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.
229. Plasma Reduction of Metallic Oxide Particles - DOE Contact Oscar P. Manley, (301) 353-5822; MIT Contacts J. F. Elliott, (617) 253-3305 and J. Szekely, (617) 253-3305
- Characterize the reduction to metal of oxide particles into the tail flame of an arc plasma.

230. High-Temperature Gas-Particle Reactions - DOE Contact Oscar P. Manley, (301) 353-5822; MIT Contacts J. F. Elliott, (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.
231. 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.
232. In-Process Control of Residual Stresses and Distortion in Automatic Welding - DOE Contact Oscar P. Manley, (301) 353-5822; MIT Contact Koichi Masubuchi, (617) 253-6820
- Develop technology of in-process control of residual stress and distortion in automatic welding.
233. 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.
234. 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.
235. 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.

236. 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.
237. 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.
238. 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.
239. 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.
240. 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.
241. 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.

242. 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.
243. 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.
244. Continuous Damage Theory - DOE Contact Oscar P. Manley, (301) 353-5822; University of Illinois Contact D. Krajcinovic, (312) 996-7000
- 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 viscous 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.
245. 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 of 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).
246. Effects of Crack Geometry and Near-Crack Materials Behavior on Scattering of Ultrasonic Waves for ONDE 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.
247. Diffusion and Ion Transport in Multicomponent Electrolyte Solutions - DOE Contact G. Kolstad, (301) 353-5822/FTS 233-5822; LLNL Contact D. G. Miller, (415) 422-8074/FTS 532-8074
- Our purpose is to characterize the diffusion properties of the ternary electrolyte mixture $\text{NaCl-MgCl}_2\text{-H}_2\text{O}$ over a large range of composition at 25°C. These data, plus other transport properties obtained at other labs, will provide an accurate data base for testing statistical mechanical theories and semi-empirical estimation models in the concentrated electrolyte solutions of real world interest.
248. Reactive Flow Modeling - DOE Contact G. Kolstad, (301) 353-5822/FTS 233-5822; LLNL Contact Craig Tarver, (415) 423-3259/FTS 543-3259
- The objective of this project is to develop reliable and physically realistic one-, two- and three-dimensional hydrodynamic computer code models of shock initiation and detonation of heterogeneous solid explosives. These models are then used to predict the vulnerability of these explosives to various hazard scenarios and the energy delivered by reacting explosives.

Division of Advanced Energy Projects

249. Aerodynamic Focusing of Particles and Heavy Molecules - DOE Contact Ryszard Gajewski, (301) 353-5995; Yale University Contact Juan Fernandez de la Mora, (203) 432-4347
- Acceleration of a gas-particle mixture through a converging nozzle to concentrate a dense beam of small uncharged particles into a narrow focus and study the dynamics of the focusing process.
 - Accompanying theoretical studies using Brownian dynamics simulations.
250. Superconductive Electric Motor - DOE Contact Ryszard Gajewski, (301) 353-5995; Los Alamos National Laboratory Contact David S. Phillips, (505) 667-5128
- Evaluate concept of an electric motor utilizing high temperature superconducting ceramic elements.
251. Gas Jet Deposition of Metallic, Semiconducting and Insulating Films - DOE Contact Ryszard Gajewski, (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.

Office of Health and Environmental Research

The Office of Health and Environmental Research supports a broad multi-disciplinary 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.

Division of Physical and Technological Research

The Physical and Technological Research Division conducts physical, chemical, and instrumentation research related to the health and environmental aspects of energy technology development. Included are support of physical and chemical characterization studies, atmospheric sciences research, research on measurement and dosimetry techniques, and fundamental radiation biophysics.

Materials Properties, Behavior, Characterization or Testing

252. Semiconductor Radiation Detector Technology - DOE Contact G. Goldstein, (301) 353-5348; LBL Contact F. S. Goulding, (415) 486-6432

- Study of semiconductor materials, primarily germanium and silicon, for use as radiation detectors. Research includes crystal growth and purification, measurement of materials properties, and signal processing.

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.

Materials Properties, Behavior, Characterization or Testing

253. Irradiation Damage in Ceramics for Fusion Applications - DOE Contact T. C. Reuther, (301) 353-4963; LANL Contact F. W. Clinard, Jr., (505) 667-5102
- Irradiation testing of refractory ceramics and ceramic insulators to determine performance and lifetime in a fusion environment.
254. Neutron-Interactive Materials - DOE Contact T. C. Reuther, (301) 353-4963; ORNL Contact E. E. Bloom, (615) 574-5053
- Effects of neutron irradiation on the physical and mechanical properties of structural materials for fusion first wall and blanket applications.
 - Development of austenitic steels, ferritic steels, and vanadium alloys with rapid radioactive decay characteristics.
 - Corrosion behavior of structural alloys in liquid metal and aqueous environments.
 - Effects of neutron and heavy ion damage on the physical and mechanical properties of ceramic materials.
255. Neutron-Interactive Materials (U.S./Japan) - DOE Contact T. C. Reuther, (301) 353-4963; ORNL Contact E. E. Bloom, (615) 574-5053
- Effects of neutron irradiation on the physical and mechanical properties of austenitic stainless steels irradiation under fusion-relevant conditions.
256. Development of Vanadium-Base Alloys for Fusion Reactor Applications - DOE Contact T. C. Reuther, (301) 353-4963; ANL Contact D. L. Smith, (312) 972-5180
- Baseline mechanical properties of vanadium-base alloys.
 - Effects of nonmetallic element impurities on properties.
 - Effects of neutron irradiation on properties.

257. Corrosion/Compatibility of Fusion Reactor Structural Materials - DOE Contact T. C. Reuther, (301) 353-4963; ANL Contact D. L. Smith, (312) 972-5180
- Liquid metal corrosion of fusion reactor structural materials.
 - Aqueous stress corrosion of fusion reactor structural materials.
258. Solid Breeder Materials - DOE Contact S. Berk, (301) 353-4171; ANL Contact C. Johnson, (312) 972-7533
- Determine H₂O/H₂ adsorption/desorption isotherms for LiAlO₂.
 - Compare tritium release model with in-reactor experiments.
259. Tritium Oxidation Kinetics - DOE Contact S. Berk, (301) 353-4171; ANL Contact R. F. Mattas, (312) 972-8673
- Measure rate of oxidation of tritium in a stainless steel system.
260. FLIBE (Fluorine-Lithium-Beryllium Salt) - DOE Contact S. Berk, (301) 353-4171; ANL Contact R. F. Mattas, (312) 972-8673
- Testing to determine potential of MoF₆ additives to FLIBE for inhibiting corrosion and for controlling tritium solubility.
261. Statistical Theory of Radiation Effects - DOE Contact T. C. Reuther, (301) 353-4963; UCLA Contact N. M. Ghoniem, (213) 825-4866
- To provide a fundamental understanding of the underlying physical phenomena which govern the interaction of radiation with structural and non-structural materials in a fusion environment. This environment is quite complex and is impossible to simulate experimentally at the present time.
262. Welding of Low Activation and Fusion First Wall Materials - DOE Contact T. C. Reuther, (301) 353-4963; Auburn University Contact B. A. Chin, (205) 826-4575
- Investigate the weldability of low activation ferritic alloys and problems which occur during the welding of He containing previously irradiated materials.

263. Neutron Interactive Materials Program - DOE Contact T. C. Reuther, (301) 353-4963/FTS 233-4963; PNL Contact R. H. Jones, (509) 376-4276/FTS 444-4276
- Conduct a broad program of fundamental studies, theory and alloy development, particularly low activation materials for fusion energy applications.
264. BEATRIX-II - DOE Contact T. C. Reuther, (301) 353-4963/FTS 233-4963; PNL Contact G. W. Hollenberg, (509) 376-5515/FTS 444-5515
- Conduct *in situ* tritium breeding and gas release and recovery experiments in the FFTF/MOTA in collaboration with International Energy Agency (IEA) partners.
265. Neutron Interactive Materials Calculations - DOE Contact T. C. Reuther, (301) 353-4963; LLNL Contact M. Guinan, (415) 422-5776
- Development of an optimized molecular dynamics code for the characterization of fusion neutron damage.
266. Damage Analysis and Fundamental Studies for Fusion Reactor Materials - DOE Contact T. C. Reuther, (301) 353-4963; University of California Santa Barbara Contact G. R. Odette, (805) 961-3525
- Modeling of microstructural evolution in neutron irradiated steels.
 - Development and application of small specimen mechanical test techniques.
 - Analysis of failure and fracture criteria in structural steels.
267. Plasma-Materials Interactions - DOE Contact M. M. Cohen, (301) 353-4253; Sandia Contact K. L. Wilson, (415) 294-2497
- Interactions of hydrogenic plasmas with materials are assessed for magnetic fusion energy first wall applications.
 - Selection and development of improved materials for plasma-interactive components.

268. Aqueous Corrosion Studied in Support of the ITER Project - DOE Contact S. Berk, (301) 353-4171; RPI Contact D. J. Duquette, (518) 276-6459
- Testing of structural materials, shielding materials, and neutron multiplication materials for corrosion resistance in aqueous lithium salt solutions.
269. Key Issues of Fusion Nuclear Technology Development - DOE Contact S. E. Berk, (301) 353-4171; UCLA Contact M. A. Abdou, (213) 206-0501
- Identify key technical issues for the development of nuclear components in fusion reactors.
 - Develop strategies for resolution of key technical issues through experimental and analytical research programs.
270. Thermal Convection Loop Experiments and Analysis of Mass Transport in Lithium/Fe-12Cr-1MoVW Systems - DOE Contact S. E. Berk, (301) 353-4171; UCLA Contact M. A. Abdou, (213) 206-0501
- Experimental investigation of mass transport phenomena for corrosion in lithium-ferritic steel systems.
 - Development of models to interpret experimental results and extrapolate to prototypical fusion conditions.
271. Solid Breeder Materials Program - DOE Contact S. E. Berk, (301) 353-4171/FTS 233-4171; PNL Contact G. W. Hollenberg, (509) 376-5515/FTS 444-5515
- Irradiation of ceramic lithium bearing compounds to determine performance under thermal and neutronic environments characteristic of localized fusion blanket conditions.
272. High Heat Flux Irradiations - DOE Contact M. M. Cohen, (301) 353-4253/FTS 233-4253; PNL Contact O. D. Slagle, (509) 376-3424/FTS 444-3424
- Conduct irradiation testing of high heat flux materials, specifically including various carbon-carbon composite materials, and the FFTF/MOTA.
273. Materials Studies for Magnetic Fusion Energy Applications at Low Temperatures - DOE Contact D. Beard, (301) 353-4958; NIST Contact R. P. Reed, (303) 497-3870
- Development of high strength, fracture tough structural alloys for superconducting magnets at 4°K.

- Development of testing standards for low-temperature mechanical property measurements.
- Publication of evaluated low-temperature mechanical and physical data at low temperatures in handbook, "Materials for Superconducting Magnet Systems."

Instrumentation and Facilities

274. Beam Plasma Neutron Source - DOE Contact T. C. Reuther, (301) 353-4963; LLNL Contact F. H. Coengsen, (415) 422-1166

- Design a 14 MeV neutron source for use in development of fusion reactor materials.

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, 1988 (DOE/ER-0378), Abstracts of Phase II Awards, 1988 (DOE/ER-0379), and Abstracts of Phase II Awards, 1987 (DOE/ER-0337).

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:

Extrusion of High Temperature Superconducting Materials - DOE Contact Walter Polansky, (301) 353-5995; Atek Metals Center, Inc., Contact James C. Hunt, (513) 984-5544

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

The Fabrication and Processing of High Temperature Superconducting Materials - DOE Contact Walter Polansky, (301) 353-5995; Cape Cod Research Contact Gregory D'Andrea, (617) 759-5911

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

Improvement of the Oxidation Resistance of Alumina-Forming Alloys by Nitriding - DOE Contact James Carr, (301) 353-6519; Coates Engineering Services Contact D. J. Coates, (415) 494-0780

A Novel Thin Film Diamond Stripper Foil for Tandem Ion Accelerators - DOE Contact Stanley Whetstone, (301) 353-3613; Diamond Materials Institute, Inc., Contact Richard Koba, (814) 231-6200

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

Fabrication of High Temperature Superconductor Filaments from Metal-Containing Polymeric Precursors - DOE Contact Walter Polansky, (301) 353-5995; Fibertek, Inc., Contact German de la Fuente, (703) 471-7671

A Novel Oxygen-Plasma Spray System for the Processing of High Temperature Superconductors - DOE Contact Walter Polansky, (301) 353-5995; Flame-Spray Industries, Inc., Contact Daniel R. Marantz, (516) 944-3511

An Oriented High Temperature Superconductor Fabricated by a Novel Technique for Use in Power Applications at Liquid Nitrogen Temperature - DOE Contact Walter Polansky, (301) 353-5995; Intermagnetics General Corporation Contact Leszek R. Motowidlo, (203) 753-5215

The Development of High Strength Superconducting Wire for High Magnetic Field Applications - DOE Contact Donald Beard, (301) 353-4958; Intermagnetics General Corporation Contact Leszek R. Motowidlo, (203) 753-5215

Enhancement of Critical Current Density in High Temperature Superconducting Ceramic Wire Through Hot-Extrusion Induced Texture - DOE Contact Walter Polansky, (301) 353-5995; Jupiter Technologies, Inc., Contact Prakash C. Panda, (607) 257-4514

The Synthesis of New Metastable Ultrahard Materials - DOE Contact Richard Kelley, (301) 353-3426; KMS Fusion, Inc., Contact Thomas P. O'Holleran, (313) 769-8500

High Temperature Advanced Structural Ceramics - DOE Contact Richard Kelley, (301) 353-3426; Materials and Electrochemical Research Corporation Contact C. F. Chen, (602) 746-9442

A New and Novel Technique for the Sputter Deposition of High Temperature Superconducting Thin Films and Coatings - DOE Contact Walter Polansky, (301) 353-5995; Plasma and Materials Technologies, Inc., Contact Gregor Campbell, (818) 841-4094

The Preparation of Thin Film Superconductors by Chemical Vapor Deposition of Volatile Metal Chelates - DOE Contact Walter Polansky, (301) 353-5995; Sievers Research, Inc., Contact Richard Hutte, (303) 444-2009

Enhancement of Transport Current Density in $YB_2Cu_3O_{7-x}$ Superconductors Using Dual-Temperature Extrusion Processing - DOE Contact Walter Polansky, (301) 353-5995; Supercon, Inc., Contact Donald W. Capone, (508) 842-0174

Enhancement of Transport Current Density in $YB_2Cu_3O_{7-x}$ Superconductors Using Low-Temperature Densification - DOE Contact Walter Polansky, (301) 353-5995; Supercon, Inc., Contact Donald W. Capone, (508) 842-0174

Enhancement of Transport Current Density in $YB_2Cu_3O_{7-x}$ Fibers Using Laser Zone Refinement - DOE Contact Earle Fowler, (301) 353-4801; Supercon, Inc., Contact Donald W. Capone, (508) 842-0174

Hot Deformation of Niobium Nitride Composites - DOE Contact Earle Fowler, (301) 353-4801; Supercon, Inc., Donald W. Capone, (508) 842-0174

Increased Tin Content in a Ductile Matrix for Niobium Tin Conductors - DOE Contact Earle Fowler, (301) 353-4801; Supercon, Inc., Donald W. Capone, (508) 842-0174

Improvement of the Ductility of Fine Filamentary Superconductors for the Superconducting Super Collider and Other Applications - DOE Contact Robert Diebold, (301) 353-5490; Supercon, Inc., Contact T. Scott Krelick, (508) 842-0174

Plasma-Enhanced Thermal Reaction Coatings of NbN for Conductor Applications - DOE Contact Donald Beard, (301) 353-4958; Supercon, Inc., Contact Donald W. Capone, (508) 842-0174

Low Cost High Resistivity Float-Zone Silicon Diodes - DOE Contact Robert Diebold, (301) 353-5490; Universal Energy Systems, Inc., Contact John A. Baker, (513) 426-6900

Phase II Projects: (First 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 HbSn 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 Nb₃Sn 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

Phase II Projects: (Second Year)

The Development of Nb₃Sn Superconducting with Micron-Size Filaments, High-Current Densities, and Low Magnetization - DOE Contact Donald Beard, (301) 353-4958; Intermagnetics General Corporation Contact Gennady Ozeryansky, (203) 753-5215

Neutron Stable Carbon-Carbon Composites - DOE Contact Marvin Cohen, (301) 353-4253; Nuclear and Aerospace Materials Corporation Contact Glen B. Engle, (619) 487-0325

The Improvement of Copper/Epoxy Composites for Fusion Energy Magnet Applications - DOE Contact Theodore Reuther, (301) 353-4963; PDA Engineering Contact Ronald E. Allred, (714) 540-8900

An Internal-External Bronze Process for the Manufacture of Large Filament Nb₃Sn - DOE Contact Donald Beard, (301) 353-4958; Supercon, Inc., Contact Donald W. Capone, (508) 842-0174

Materials Properties, Behavior, Characterization or Testing

Phase I Projects:

Noncontract, High-Resolution, Thermal Wave Detection of Superconductive Transitions in High Critical Temperature Materials - DOE Contact Richard Kelley, (301) 353-3426; Therma-Wave, Inc., Contact Allan Rosenwaig, (415) 490-3663

Closed-Loop Figuring of Mirrors - DOE Contact Richard Kelley, (301) 353-3426; Universal Energy Systems, Inc., Contact Erik S. Buck, (513) 426-6900

Phase II Projects: (First 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. Oravec, (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

Phase II Projects: (Second Year)

Investigation of Fatigue Failure Initiation and Propagation in Wind-Turbine-Grade Wood/Epoxy Laminate Containing Several Veneer Joint Styles - DOE Contact Jeffrey Rumbaugh, (202) 586-1696; Gougeon Brothers, Inc., Contact William D. Bertelsen, (517) 684-7286

Device or Component Fabrication, Behavior or Testing

Phase I Projects:

Infrared Detectors Using High Critical Temperature Granular Josephson Junctions - DOE Contact Walter Polansky, (301) 353-5995; Advanced Fuel Research, Inc., Contact David G. Hamblen, (203) 528-9806

Diamond Coatings and Windows for Millimeter Microwave Tubes and Transmission Lines - DOE Contact T. V. George, (301) 353-4957; Applied Science and Technology, Inc., Contact Richard S. Post, (617) 876-5545

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

Fiber Driven Acoustic Cavity Sensors - DOE Contact Eugene Eckhart, (202) 586-8668; Innovative Sciences, Inc., Contact Bruce W. Maxfield, (415) 568-1720

Diamond-like Films for Microwave Transmission Window Applications - DOE Contact T. V. George, (301) 353-4957; Interscience, Inc., Contact James T. Woo, (518) 283-7500

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

High Temperature Fiber Optic Sensors - DOE Contact Curtis Nakaishi, (304) 291-4275; LaserGenics Corporation Contact Richard G. Schlecht, (408) 433-0161

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; Opra, Inc., Contact Michael Hercher, (617) 535-7670

The Development of a 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

Magnetic Control of Critical Currents in Superconducting Quantum Interference Devices Operating at 77K - DOE Contact Walter Polansky, (301) 353-5995; Physical Dynamics, Inc., Walter N. Podney, (619) 587-1050

Large-Area Photodetector Arrays - DOE Contact Robert Diebold, (301) 353-5490; Plasma Physics Corporation Contact John H. Coleman, (516) 676-8468

Ion-Implanted Semiconductors Polymeric Devices - DOE Contact Robert Diebold, (301) 353-5490; Spire Corporation Contact Ih-Huang Loh, (617) 275-6000

A Search for a Rapid Oxygen Sensor Using High-Temperature, Complex Eutectic Thin Films - DOE Contact Matthew McMonigle, (202) 586-2082; Syn Crys, Inc., Contact G. Wayne Clark, (615) 482-3411

Phase II Projects: (First 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) 353-4801; 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 Douglas 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

Phase II Projects: (Second Year)

An All-Metal, Demountable, Cryogenic Seal - DOE Contact Earle Fowler, (301) 353-4801; Creare, Inc., Contact Herbert Sixsmith, (603) 643-3800

The Development of a New Direct Energy Conversion Device: The Thermotunnel Converter - DOE Contact William Barnett, (301) 353-3097; Energetics, Inc., Contact Thomas S. Bustard, (301) 992-4000

An Optimized NbTi Superconducting Strand and Cable for Accelerator Magnet Applications - DOE Contact Earle Fowler, (301) 353-4801; Intermagnetics General Corporation Contact Kanithi Hamachalam, (203) 753-5215

A Real Time, Non-Contact Optical Surface Motion Monitor - DOE Contact Stanley Sobczynski, (202) 586-1878; Opra, Inc., Contact Geert Wytjes, (617) 535-7670

Surface Figure Measurements of X-Ray Optics - DOE Contact Richard Kelley, (301) 353-3426; Photographic Sciences Corporation Contact Thomas C. Bristow, (716) 265-1600

The Development of an Improved Composite Conductor with Electrically Uncoupled Fine NbTi Filaments and High Current Density - DOE Contact Earle Fowler, (301) 353-4801; Supercon, Inc., Contact T. Scott Krelick, (508) 842-0174

OFFICE OF NUCLEAR ENERGY

	<u>FY 1988</u>
<u>Office of Nuclear Energy - Grand Total</u>	\$125,718,000
<u>Office of Remedial Action and Waste Technology</u>	\$2,285,000
<u>Division of Waste Treatment Projects</u>	\$2,285,000
<u>Materials Preparation, Synthesis, Deposition, Growth or Forming</u>	\$ 800,000
Technical Support to West Valley Demonstration Project	800,000
<u>Materials Properties, Behavior, Characterization or Testing</u>	\$ 1,485,000
Materials Characterization Center Testing of West Valley Formulation Glass	480,000
Development of Test Methods and Testing of West Valley Reference Formulation Glass	750,000
Process and Product Quality Optimization for the West Valley Waste Form	255,000
<u>Office of Uranium Enrichment</u>	\$17,462,000
<u>Gaseous Diffusion</u>	
<u>Device or Component Fabrication, Behavior or Testing</u>	\$ 5,730,000
Gaseous Diffusion: Barrier Quality	2,755,000
Gaseous Diffusion: Materials and Chemistry Support	2,975,000
<u>Atomic Vapor Laser Isotope Separation (AVLIS)</u>	\$11,732,000
AVLIS: Separator Materials	8,267,000
AVLIS: Uranium Processing	3,465,000

OFFICE OF NUCLEAR ENERGY (Continued)

	<u>FY 1988</u>
<u>Office of Civilian Reactor Development</u>	\$36,771,000
<u>Office of Advanced Reactor Programs</u>	\$ 5,646,000
<u>Division of High Temperature Gas-Cooled Reactors</u>	\$ 5,646,000
<u>Materials Preparation, Synthesis, Deposition, Growth or Forming</u>	\$ 960,000
Fuel Process Development	960,000
<u>Materials Properties, Behavior, Characterization or Testing</u>	\$ 4,686,000
Fuel Materials Development	635,000
Fuel Development and Testing	2,120,000
Graphite Development	155,000
Graphite Development and Testing	736,000
Metals Technology Development	35,000
Structural Materials Development	715,000
Advanced Gas Reactor Materials Development	290,000
<u>Office of Technology Support Programs (LMRs)</u>	\$31,125,000
<u>Fuels and Core Materials</u>	\$25,025,000
<u>Materials Properties, Behavior, Characterization or Testing</u>	\$25,025,000
Fuel Performance Demonstration	5,300,000
Pyroprocess Development	4,625,000
Fuel Safety Experiments and Analysis	4,000,000
Core Design Studies	1,800,000
Fuel Cycle Studies	3,800,000
LMR Technology R&D	5,500,000

OFFICE OF NUCLEAR ENERGY (Continued)

	<u>FY 1988</u>
<u>Structural Materials and Design Methodology</u>	\$ 6,100,000
<u>Materials Properties, Behavior, Characterization or Testing</u>	\$ 6,100,000
Structural Design/Life Assurance Technology	500,000
Modified 9 Cr-1 Mo Steel Design Properties	390,000
Nondestructive Testing Technology for Heat Exchangers	130,000
Nuclear Systems Materials Handbook	30,000
MOTA Fabrication and Operation	1,278,000
Absorber Development	193,000
FFTF Metal Fuel Testing	1,025,000
Core Demonstration Experiment (CDE)	2,393,000
International Collaboration	161,000
<u>Office of Space and Defense Power Systems</u>	\$2,200,000
<u>Materials Preparation, Synthesis, Deposition, Growth or Forming</u>	\$1,530,000
Development of Improved Thermoelectric Materials for Space Nuclear Power Systems	200,000
Development of an Improved Process for the Manufacture of DOP-26 Iridium Alloy Blanks	730,000
Carbon Bonded Carbon Fiber Insulation Manufacturing Process Development and Product Characterization	600,000
<u>Device or Component Fabrication, Behavior or Testing</u>	\$ 170,000
Nondestructive Testing Methods Development and Application to Thermoelectric Materials and Devices	170,000

OFFICE OF NUCLEAR ENERGY (Continued)

	<u>FY 1988</u>
<u>Materials Properties, Behavior, Characterization or Testing</u>	\$ 500,000
Characterization of State-of-the-Art Improved Silicon-Germanium Thermoelectric Device/Materials and Silicon-Germanium Materials Development	500,000
<u>Office of Naval Reactors</u>	\$67,000,000*

*Approximate

OFFICE OF NUCLEAR ENERGY

The Office of Nuclear Energy conducts research projects in the Office of Advanced Reactor Programs, 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

275. 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 removal of cesium from alkaline supernate solutions at West Valley by ion exchange with zeolite.
- 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.

Materials Properties, Behavior, Characterization or Testing

276. 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 a glass having the expected composition of West Valley borosilicate glass incorporating actual West Valley high-level waste.

- Evaluate, using various MCC test methods, simulated West Valley glass and samples of glass having the expected composition of West Valley borosilicate glass incorporating actual West Valley high-level waste.
- Provide assistance to West Valley related to enhancing the quality of their analytical data.

277. 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 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.

278. 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.

Office of Uranium Enrichment

The Department of Energy is authorized by the Atomic Energy Act, 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 assure our national and energy security in an economical, reliable, safe, secure, and environmentally acceptable manner that will also assure an appropriate 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 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.

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 about 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.

One major element in the initiative to recapture the enrichment market was the selection of the Atomic Vapor Laser Isotope Separation (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 AVLIS into the enrichment enterprise is being carefully evaluated.

The 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, 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 AVLIS. This office monitors foreign enrichment technology and is the focal point for 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 a net fiscal year appropriation of \$0. Total obligations for all uranium enrichment activities in FY 1988 were \$934 million.

Materials R&D activities within the Office of Uranium Enrichment are varied and, for the most part, classified Restricted Data. In FY 1988, approximately \$17,462,000 million was used in these endeavors and \$21,100,000 is planned for FY 1989. 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

279. 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.

280. 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.

Atomic Vapor Laser Isotope Separation (AVLIS)

281. AVLIS: Separator Materials

- Selection and testing of candidate structural and component materials and coatings for the AVLIS separator system.
- Fabrication of components and subsystems for AVLIS process integrated enrichment tests.

282. AVLIS: Uranium Processing

- Design, fabrication and operation of uranium electrolysis cells for AVLIS feed. Bath chemistry, solubility and construction materials studies.
- Design and operation of prototype AVLIS product purification equipment. Flowsheet development and demonstration of schemes for converting purified product into commercial nuclear fuel oxides.

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

283. Fuel Process Development - DOE Contact J. E. Fox, (301) 353-3985; GA Technologies Contact O. M. Stansfield, (619) 455-2895

- 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

284. Fuel Materials Development - DOE Contact J. E. Fox, (301) 353-3985; GA Technologies Contact O. M. Stansfield, (619) 455-2895

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

285. 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.
286. 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.
287. 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.
288. Metals Technology Development - DOE Contact J. E. Fox, (301) 353-3985; GA Technologies Contact W. R. Johnson, (619) 455-2905
- Characterize and qualify the metallic materials selected for application in the near-term steam cycle/cogeneration HTGR system.
 - Develop base technology required for selection of alloys for advanced HTGR systems.

289. 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.
290. 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

291. 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 (modified type 316) to at least 150,000 MWD/T burnup.
292. Pyroprocess Development - DOE Contact David L. Hoof, (301) 353-2964/FTS 233-2964; ANL Contact Leslie Burris, (312) 972-4383/FTS 972-4383
 - 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.
293. Fuel Safety Experiments and Analysis - DOE Contact John Lewellen, (301) 353-3684/FTS 233-3684; 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.
294. 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 FFTF and develop optimized metal fuel core designs for advanced LMR systems.

295. Fuel Cycle Studies - DOE Contact David L. Hoof, (301) 353-2964/FTS 233-2964; 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.
296. LMR Technology R&D - DOE Contacts John Lewellen, (301) 353-3684/FTS 233-3684 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

297. 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
- Conduct tests to provide structural design methods, rules, and criteria to qualify modified 9 Cr-1 Mo for LMR service. Develop flaw assessment procedures, creep-fatigue failure criterion based on ductility exhaustion and simplified creep-fatigue methods for 9 Cr-1 Mo.
298. 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.

299. Nondestructive Testing Technology for Heat Exchangers - DOE Contact David L. Hoof, (301) 353-2964/FTS 233-2964; ORNL Contact Robert W. McClung, (615) 574-4466/FTS 624-4466
- Develop 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.
300. 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
- Develop 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.
301. MOTA Fabrication and Operation - DOE Contact Andrew Van Echo, (301) 353-3930/FTS 233-3930; WHC Contact Roger W. Powell, (509) 376-4529/FTS 444-4529
- 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.
302. Absorber Development - DOE Contact C. Chester Bigelow, (301) 353-4299/FTS 233-4299, Andrew Van Echo, (301) 353-3930/FTS 233-3930; WHC Contact Robert D. Leggett, (509) 376-2505/FTS 444-2505
- 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.
303. FFTF Metal Fuel Testing - DOE Contact Andrew Van Echo, (301) 353-3930/FTS 233-3930; WHC Contact Robert D. Leggett, (509) 376-2505/FTS 444-2505
- Conduct metal fuel (MFF-2) irradiation testing in FFTF, transient testing in TREAT with HT-9 clad to support conversion of the FFTF from an oxide-fuel core to a binary U-Zr fuel core.

304. Core Demonstration Experiment (CDE) - DOE Contact Jacob Glatter, (301) 353-3921/FTS 233-3921; WHC Contact Robert D. Leggett, (509) 376-2505/FTS 444-2505
- 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.
305. International Collaboration - DOE Contact Robert Neuhold, (301) 353-3424/FTS 233-3424; WHC Contact Robert D. Leggett, (509) 376-2505/FTS 444-2505
- 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

306. 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.

307. 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.
308. 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

309. 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

310. 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 \$67 million in FY 1988 including approximately \$37 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

	<u>FY 1988</u>
<u>Office of Civilian Radioactive Waste Management - Grand Total</u>	\$12,833,000
<u>Office of Systems Integration and Regulations</u>	\$ 711,000
<u>Materials Properties, Behavior, Characterization or Testing</u>	\$ 711,000
Development of Criteria for Nuclear Spent Fuel Storage in Air	650,000
Development of Zircaloy Deformation and Creep Rupture Models for Predicting Cladding Behavior During Interim Dry Storage	49,000
PWR and BWR Spent Fuel Assembly Crud Composition, Characterization, and Effects on Operations	12,000
<u>Office of Civilian Radioactive Waste Management/ Yucca Mountain Project (OCRWM/YMP)</u>	\$11,767,000
<u>Materials Properties, Behavior, Characterization or Testing</u>	\$ 9,264,000
Waste Package Environment	935,000
Waste Form Testing	2,951,000
Metal Barrier Testing	2,162,000
Other Engineered Barrier Waste Package Components	64,000
Integrated Testing	1,281,000
Waste Package: Performance Assessment	682,000
Research on Geochemical Modeling of Radionuclide Interaction with a Fractured Rock Matrix	1,189,000
<u>Device or Component Fabrication, Behavior or Testing</u>	\$ 2,503,000
Waste Package: Design, Fabrication and Prototype Testing	908,000
Waste Package Environmental Field Tests	1,595,000

**OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT
(Continued)**

	<u>FY 1988</u>
<u>Sandia National Laboratories: Brittle Fracture Technology Program</u>	\$ 355,000
<u>Materials Structure and Composition</u>	\$ 50,000
Microstructure Investigations of Nodular Cast Iron	25,000
Composition Investigation of Nodular Cast Iron	25,000
<u>Materials Properties, Characterization, Behavior or Testing</u>	\$ 285,000
Generate Material Property Database for Nodular Cast Iron	100,000
Mosaik Brittle Fracture Test Program	100,000
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	5,000
<u>Instrumentation and Facilities</u>	\$ 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

The objectives of the Commercial Spent Fuel Management (CSFM) Program are to encourage and expedite the implementation of existing and new spent nuclear fuel storage technologies; to accelerate the availability of dry storage and rod consolidation technologies through licensed cooperative demonstrations at reactor sites and unlicensed testing at Federal facilities; and to provide the planning for a Federal capability to store up to 1900 MT of spent fuel for those utilities that the NRC determines cannot reasonably provide increased at-reactor storage when needed.

Materials Properties, Behavior, Characterization or Testing

311. Development of Criteria for Nuclear Spent Fuel Storage in Air - DOE Contact C. R. Head, (202) 586-9606; PNL Contact E. R. Gilbert, (509) 375-2533
- Testing spent fuel and unclad UO_2 in air to determine the temperature dependence and fuel type dependence of degradation by oxidation.
 - Develop methodology to derive storage criteria to prevent degradation of spent fuel in air by oxidation.
312. Development of Zircaloy Deformation and Creep Rupture Models for Predicting Cladding Behavior During Interim Dry Storage - DOE Contact C. R. Head, (202) 586-9606; PNL Contact E. R. Gilbert, (509) 375-2533
- Analysis of existing data on deformation and creep rupture for nonirradiated Zircaloy.
 - Development of theoretical models for deformation and creep rupture for spent fuel under dry storage conditions.
 - Comparison of models with FRG deformation and creep rupture data on spent fuel and irradiated Zircaloy cladding.
 - Prediction of spent fuel cladding behavior under dry storage conditions.
 - Documentation of models and transfer to computer.

313. PWR and BWR Spent Fuel Assembly Crud Composition, Characterization, and Effects on Operations - DOE Contact C. R. Head, (202) 586-9606; PNL Contact W. J. Bailey, (509) 375-2615

- Literature was reviewed and a formal report published on spent fuel rod crud, its composition and characteristics, and the impact on storage, handling, and shipping operations.
- Tests with PWR and BWR assemblies were performed to compare spent fuel rod crud and to determine the uniformity of deposition, thickness, and difficulty in removal of the crud. Two informal reports were prepared.

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 1988.)

Materials Properties, Characterization or Testing

314. 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.

315. 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.

316. 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 barriers and its surrounding environment.
 - Six austenitic phase alloys and copper/copper based alloys are being evaluated as candidate materials.
317. 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.
318. 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.
319. 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.
320. 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

321. 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.
322. 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

323. Microstructure Investigations of Nodular Cast Iron - DOE Contact F. Falci, (301) 353-3595; SNL Contact K. B. Sorenson, (505) 844-5360
- Investigation of the effect of microstructure on material properties.
 - Study of the effect of graphite nodule size and spacing on fracture toughness.
324. Composition Investigation of Nodular Cast Iron - DOE Contact F. Falci, (301) 353-3595; SNL Contact K. B. Sorenson, (505) 844-5360
- 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

325. Generate Material Property Database for Nodular Cast Iron - DOE Contact F. Falci, (301) 353-3595; SNL Contact K. B. Sorenson, (505) 844-5360

- Generate a database for nodular cast iron which includes material properties pertinent to fracture mechanics.

326. Mosaik Brittle Fracture Test Program - DOE Contact F. Falci, (301) 353-3595; SNL Contact K. B. Sorenson, (505) 844-5360

- Perform a series of drop tests using a ductile cast iron cask to demonstrate a proof of principle for the fracture mechanics design approach.

327. Investigate Thickness Effects on Impact and Toughness Properties of Ferritic Steel - DOE Contact F. Falci, (301) 353-3595; SNL Contact K. B. Sorenson, (505) 844-5360

- Generate a database of nilductility (NDT) transition temperature, Charpy and fracture toughness measurements as a function of thickness.

328. 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) 844-5360

- Investigate the feasibility of using depleted uranium (DU) as a structural component in cask body construction.

Instrumentation and Facilities

329. Evaluate Current NDE Methods for Applicability to Thick Section Nodular Cast Iron - DOE Contact F. Falci, (301) 353-3595; SNL Contact K. B. Sorenson, (505) 844-5360

- Evaluate state-of-the-art NDE methods for specific application to thick-walled nodular cast iron.

OFFICE OF DEFENSE PROGRAMS

	<u>FY 1988</u>
<u>Office of Defense Programs - Grand Total</u>	\$50,995,250
<u>Office of Waste Research and Development</u>	\$ 9,750
<u>Materials Properties, Behavior, Characterization or Testing</u>	\$ 9,750
Waste Form Qualification	4,550
Immobilization/Volume Reduction/In-place Stabilization	5,200
<u>Office of Weapons Research, Development, and Testing</u>	\$50,985,500
<u>Weapons Research Division</u>	\$50,985,500
<u>Sandia National Laboratories - Albuquerque</u>	\$20,954,500
<u>Solid State Sciences Directorate, 1100</u>	\$ 8,800,000
<u>Ion Implantation and Microsensors Research</u>	
<u>Department, 1110</u>	\$ 1,920,000
<u>Materials Properties, Behavior, Characterization</u>	
<u>or Testing</u>	\$ 1,920,000
Ion Implantation Studies for Friction and Wear	500,000
Silicon-Based Radiation Hardened Microelectronics	670,000
New Concepts in Microsensors	750,000
<u>Laser and Chemical Physics Research Department, 1120</u>	\$ 1,500,000
<u>Materials Properties, Behavior, Characterization</u>	
<u>or Testing</u>	\$ 1,500,000
Plasma Etching	400,000
Plasma-Enhanced Chemical Vapor Deposition	200,000

OFFICE OF DEFENSE PROGRAMS (Continued)**FY 1988**

<u>Laser and Chemical Physics Research Department, 1120 (continued)</u>	
<u>Materials Properties, Behavior, Characterization or Testing (continued)</u>	\$ 1,500,000
Laser-Controlled Etching and Deposition of Materials	200,000
Surface Chemistry of Organometallics for Compound Semiconductor Epitaxy	300,000
Metallorganic Chemical Vapor Deposition	400,000
<u>Condensed Matter and Surface Science Department, 1130</u>	\$ 1,300,000
<u>Materials Properties, Behavior, Characterization or Testing</u>	\$ 1,300,000
Shock Physics and Chemistry	500,000
Electronic and Structural Properties	400,000
Surface Science	400,000
<u>Compound Semiconductor and Device Research Department, 1140</u>	\$ 2,000,000
<u>Materials Preparation, Synthesis, Deposition, Growth or Forming</u>	\$ 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)

	<u>FY 1988</u>
<u>Solid State Research Department, 1150</u>	\$ 2,080,000
<u>Materials Properties, Behavior, Characterization or Testing</u>	\$ 2,080,000
Superconductivity	540,000
Semiconductors	540,000
Surface Science	500,000
Disordered Materials	500,000
<u>Organic and Electronic Materials Department, 1810</u>	\$ 1,744,500
<u>Chemistry of Organic Materials Division, 1811</u>	\$ 450,000
<u>Materials Preparation, Synthesis, Deposition, Growth or Forming</u>	\$ 350,000
Dyed Antireflective Photoresist Material	100,000
Sulfonated Aromatic Polysulfones	100,000
Carbon Foams	150,000
<u>Materials Properties, Behavior, Characterization or Testing</u>	\$ 100,000
Radiation Hardened Dielectrics	100,000
<u>Physical Chemistry and Mechanical Properties of Polymers Division, 1812</u>	\$ 585,000
<u>Materials Preparation, Synthesis, Deposition, Growth or Forming</u>	\$ 300,000
Polysilanes, Photoresists, Photoconductors, and Non-Charring Dielectrics	150,000
Mechanistic Studies of Polysilane Synthesis	20,000
Chemistry of Plasma Etching and Deposition Processes	130,000

OFFICE OF DEFENSE PROGRAMS (Continued)

FY 1988

Physical Chemistry and Mechanical Properties of Polymers
Division, 1812 (continued)Materials Structure and Composition \$ 285,000

Materials Structure, Dynamics, and Property	
Studies by Multinuclear Pulsed NMR Spectroscopy	75,000
Studies of Adhesion at the Molecular Level by Surface Science Techniques	210,000

Physical Properties of Polymers Division, 1813 \$ 409,500Materials 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 \$ 94,500

Mechanical Properties of Encapsulants	21,000
Deformation of Kevlar Fabrics	73,500

Electronic Property Materials Division, 1815 \$ 300,000Materials 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

OFFICE OF DEFENSE PROGRAMS (Continued)

	<u>FY 1988</u>
<u>Materials Characterization Department, 1820</u>	\$ 990,000
<u>Analytical Chemistry Division, 1821</u>	\$ 250,000
<u>Instrumentation and Facilities</u>	\$ 250,000
Development of Automated Methods for Chemical Analysis	250,000
<u>Electron Optics and X-Ray Analysis Division, 1822</u>	\$ 240,000
<u>Materials Preparation, Synthesis, Deposition, Growth or Forming</u>	\$ 40,000
Thermomechanical Treatment of U Alloys	40,000
<u>Instrumentation and Facilities</u>	\$ 200,000
Advanced Methods for Electron Optical, X-Ray, and Image Analysis	200,000
<u>Surface Chemistry and Analysis Division, 1823</u>	\$ 500,000
<u>Instrumentation and Facilities</u>	\$ 500,000
Advanced Methods for Surface and Optical Analysis	500,000
<u>Metallurgy Department, 1830</u>	\$ 3,250,000
<u>Physical Metallurgy Division, 1831</u>	\$ 130,000
<u>Materials Preparation, Synthesis, Deposition, Growth or Forming</u>	\$ 130,000
Analytical Electron Microscopy of Engineering Alloys	130,000

OFFICE OF DEFENSE PROGRAMS (Continued)

	<u>FY 1988</u>
<u>Mechanical Metallurgy Division, 1832</u>	\$ 2,010,000
<u>Materials Properties, Behavior, Characterization or Testing</u>	\$ 2,010,000
Toughness of Ductile Alloys	330,000
Friction and Wear of Modified Surfaces	230,000
Alloy Deformation Response and Constitutive Modeling	300,000
Corrosion	1,150,000
<u>Process Metallurgy Division, 1833</u>	\$ 700,000
<u>Materials Preparation, Synthesis, Deposition, Growth or Forming</u>	\$ 60,000
Vacuum Arc Remelting	60,000
<u>Device or Component Fabrication, Behavior or Testing</u>	\$ 640,000
Aluminum Laser Welding	40,000
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
<u>Surface and Interface Technology Division, 1834</u>	\$ 410,000
<u>Materials Preparation, Synthesis, Deposition, Growth or Forming</u>	\$ 80,000
Development of Hard, Wear-Resistant Coatings for Mechanical Applications	80,000
<u>Materials Properties, Behavior, Characterization or Testing</u>	\$ 40,000
Modification of Mechanical Properties by Ion Implantation	40,000

OFFICE OF DEFENSE PROGRAMS (Continued)

	<u>FY 1988</u>
<u>Surface and Interface Technology Division, 1834 (continued)</u>	
<u>Device or Component Fabrication, Behavior or Testing</u>	\$ 150,000
Process Control Ultrasonic Cleaning of Delicate Parts	70,000
Plasma Oxidation and Reduction Studies	80,000
<u>Instrumentation and Facilities</u>	\$ 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
<u>Chemistry and Ceramics Department, 1840</u>	\$ 6,170,000
<u>Ceramics Development Division, 1845</u>	\$ 6,170,000
<u>Materials Preparation, Synthesis, Deposition, Growth or Forming</u>	\$ 5,250,000
Ceramic Processing	2,600,000
Electrophoretically-Deposited Coatings	150,000
Glass and Glass-Ceramic Development	2,500,000
<u>Materials Properties, Behavior, Characterization or Testing</u>	\$ 920,000
Fracture of Ceramics	680,000
Optical Diagnostics for Materials Processing	240,000
<u>Sandia National Laboratories - Livermore</u>	\$ 3,880,000
<u>Materials Preparation, Synthesis, Deposition, Growth or Forming</u>	\$ 1,100,000
Powder Metallurgy	200,000
Advanced Electrodeposition Studies	100,000
Metal Forming	200,000

OFFICE OF DEFENSE PROGRAMS (Continued)

FY 1988

Sandia National Laboratories - Livermore (continued)Materials Preparation, Synthesis, Deposition, Growth
or Forming (continued)

Advanced Organic Materials	200,000
Particulate Technology	50,000
Tritium Getter Technology	50,000
Molded Desiccant Foam	100,000
Plasma Processing	200,000

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	30,000
Tritium-Metal Interaction	350,000
Measurement of Multilayer Thin Film Structures	50,000
Helium in Metal Tritides	200,000
Analysis of Defects and Interfaces in Metals	300,000

Instrumentation and Facilities

\$ 600,000

New Spectroscopy	50,000
Tritium Facility Upgrade for Materials Characterization and Testing	500,000
New Analytical Techniques	50,000

Lawrence Livermore National Laboratory

\$ 9,577,000

Materials Preparation, Synthesis, Deposition, Growth
or Forming

\$ 3,224,000

Ion Beam Modification of Materials	110,000
Inorganic Aerogels	600,000

OFFICE OF DEFENSE PROGRAMS (Continued)

FY 1988

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)	241,000
Organic Aerogels	200,000
New Ionomer Synthesis	9,000
Polymer Foam Development	1,600,000
Atomic Engineering	64,000

Materials Structure and Composition \$ 1,549,000

Theory of the Structure and Dynamics of Molecular Fluids	300,000
Site-Specific Chemistry Using Synchrotron Radiation	180,000
Capillary Structures (in Foams)	100,000
Plutonium Pyrochemical Research	160,000
Low Density Material Aggregate Networks	186,000
Electronic Structure in Superconducting Oxides	23,000
Theory of Superconducting Oxides	450,000
A New, First-Principles Method for the Calculation of the Electronic Structure of Surfaces and Grain Boundaries	150,000

Materials Properties, Behavior, Characterization or
Testing \$ 3,628,000

Nuclear Spin Polarization	770,000
Measurement of Tritium Permeation Through Resistant Materials at Low Temperatures	90,000
Catalytic Properties of Actinide Compounds	185,000
Pretransformation Behavior in Alloys	175,000

OFFICE OF DEFENSE PROGRAMS (Continued)

FY 1988

Lawrence Livermore National Laboratory (continued)Materials Properties, Behavior, Characterization or Testing (continued)

Interfacial Bonding in Multilayer X-ray Mirrors	25,000
$\Delta N=O$ Spectroscopy Using Multilayer Gratings	162,000
Multilayer X-ray Optics Development	220,000
Thin Film Studies	160,000
In Situ Reversed Deformation Experiments	20,000
Dislocation Microstructure of Aluminum and Silver	
Deformed to Large Steady-State Creep Strains	90,000
Delayed Failure of Silver-Aided Diffusion Bonds	190,000
Constitutive and Failure Behavior of Metals at	
High Rates of Tensile Strain	225,000
High Strain Rate Mechanical Testing	129,000
Theoretical and Experimental Studies of Solid	
Combustion Reactions	190,000
Fracture Behavior of Refractory Metals and Alloys	
in Liquid Actinides	100,000
Integrated Engineering Applications Software	
(IDEAS) Project	107,000
High Temperature Metal Alloy Radiant Property	
Measurements in Conjunction with Advanced	
Surface Spectroscopy	48,000
Modeling and Experimental Measurement of Residual	
Stress	160,000
A Study of Residual Stress for Epoxy-Resin	
Composites	185,000
Failure Characterization of Composite Materials	117,000
Polymer Adhesion Science and Mechanics	35,000
Surface Modification to Reduce Abrasion and Friction	100,000
Numerical Modeling of Crack Growth	145,000

OFFICE OF DEFENSE PROGRAMS (Continued)

FY 1988

Lawrence Livermore National Laboratory (continued)

<u>Device or Component Fabrication, Behavior or Testing</u>	\$ 991,000
IC Protective Coatings	700,000
Characterization of Solid-State Microstructures in High Explosives by Synchrotron X-ray Tomography	50,000
Optical Diagnostics of High Explosives Reaction Chemistry	200,000
Application of Laser Gaging Technology to Mechanical Testing	41,000
<u>Instrumentation and Facilities</u>	\$ 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) ¹
Decontamination and Waste Treatment Facility (DWTF)	(6,600,000) ¹
<u>Los Alamos National Laboratory</u>	\$17,---,000
<u>Materials Preparation, Synthesis, Deposition, Growth or Forming</u>	\$ 8,390,000
Actinide Alloy Development	1,350,000
Plutonium Oxide Reduction	150,000
Replacement Noble-Metal Alloys	75,000
Whisker Reinforced Structural Ceramics	200,000
Ion-Beam Implantation	200,000
Electroplating Low Atomic Number Materials	120,000

¹Line-item construction projects: not included in subtotal or total.

OFFICE OF DEFENSE PROGRAMS (Continued)

FY 1988

Los Alamos National Laboratory (continued)Materials Preparation, Synthesis, Deposition, Growth
or Forming (continued)

Three New Conducting Polymers	50,000
New Highly Conductive Doped Polyacetylene	150,000
Liquid Crystal Polymer Development	200,000
Surface Property Modified Plastic Components	50,000
Low-Density, Microcellular Plastic Foams	400,000
Target Coatings	600,000
Physical Vapor Deposition and Surface Analysis	700,000
Fluidized Bed Coatings	200,000
Electrodeposition of Metallic Glasses	25,000
Polymers and Adhesives	800,000
Tritiated Materials	485,000
Salt Fabrication	530,000
Slip Casting of Ceramics	100,000
Whisker Growth Technology	120,000
New Hot Pressing Technology	300,000
Glass and Ceramic Coatings	10,000
Cold Pressing, Cold Isostatic Pressing and Sintering	10,000
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	150,000
High Temperature Superconductors for Electric Utility Applications	275,000
Synthesis of Porous Glass Structures	20,000

Materials Structure or Composition \$ 1,662,000

Actinide Surface Properties	700,000
Neutron Diffraction of Pu and Pu Alloys	237,000
Surface, Material and Analytical Studies	175,000
Modeling of Interfaces in Ordered Intermetallic Alloys	550,000

OFFICE OF DEFENSE PROGRAMS (Continued)

FY 1988

Los Alamos National Laboratory (continued)

<u>Materials Properties, Behavior, Characterization or Testing</u>	\$ 3,942,000
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
Dielectric Loss Measurements in Ceramics	400,000
Nondestructive Evaluation	500,000
Powder Characterization	45,000
Shock Deformation in Actinide Materials	200,000
Dynamic Mechanical Properties of Weapons Materials	225,000
Dynamic Testing of Materials for Hyper-Velocity Projectiles	80,000
Mechanical Properties	300,000
Radiation Damage in High-Temperature Superconductors	305,000
Insulators for Space Reactor Application	92,000
Structural Ceramics	345,000
<u>Device or Component Fabrication, Behavior or Testing</u>	\$ 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 Waste Research and Development

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 Plant 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 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) is being prepared to support selection of a disposal strategy for Hanford high-level, transuranic and tank wastes. The Preferred Alternative recommends proceeding with disposal of double-shell tank waste, retrievably-stored transuranic waste and encapsulated cesium and strontium. Further development and evaluation is recommended 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, 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

330. Waste Form Qualification - DOE Contact Ken Chacey, (301) 353-4970 and Marv Furman (509) 376-7062; Westinghouse Hanford Company Contact Seve Schaus, (509) 376-8365

- Fundamental data for immobilizing defense waste (e.g., borosilicate glass, crystalline ceramics).

331. Immobilization/Volume Reduction/In-place Stabilization - DOE Contact Ken Chacey, (301) 353-4970 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 Implantation and Microsensors 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, microsensors, ion-solid microanalysis/channeling, defects and hydrogen in solids, and laser and electron beam annealing. 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 modification and analysis of these near-surface and interfacial regions. Fundamental understanding of physical and chemical principles, materials properties and microfabrication technologies are combined to develop new approaches to sensing such parameters as radiation, hydrogen and other gases, pressure, magnetic fields, liquid viscosity, optical signals and corrosion. A major aspect of the work is thus to develop an underlying understanding and control of defects, hydrogen-materials interactions alloying processes, sensing functions, 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

332. Ion Implantation Studies for Friction and Wear - 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.
333. 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.

334. 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

- 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 propagation, and optical properties of solids.

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

335. 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.

336. 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.
337. 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.
338. 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 ($\text{Ga}(\text{CH}_3)_3$, $\text{Al}(\text{CH}_3)_3$, 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.
339. 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(CH₃)₃, Al(CH₃)₃, etc.), and Group V hydrides (AsH₃, PH₃, etc.) or alkyls (As(CH₃)₃, P(C₂H₅)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.

Condensed Matter and Surface Science Department, 1130

The mission of Department 1130 is to provide fundamental understanding and strong technology bases in two main areas: (1) shock wave physics and chemistry; and (2) electronic and structural properties; (3) surface science of materials. Current areas of emphasis include shock-induced solid state chemistry, shock initiation of heterogeneous explosives, shock-activated thermal battery, PVF₂ stress gauge, phase transitions in ferroelectrics, high T_c superconductors, defects in semiconductors, modification and control of surface properties, the early stages of oxidation and corrosion, and adhesion of metals to polymers.

Materials Properties, Behavior, Characterization or Testing

340. Shock Physics and Chemistry - DOE Contact A. E. Evans, (301) 353-3098, 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.

341. Electronic and Structural Properties - DOE Contact A. E. Evans, (301) 353-3098; Sandia Contact B. Morosin, (505) 844-8169
- The magnetic properties and crystal structures of high T_c superconductors are being investigated in order to gain new insights into the mechanisms responsible for the superconductivity and to guide the development of new superconductors.
 - Radiation-induced defects and their deep electronic levels in silicon and compound semiconductors are being studied to understand the physics and the role of these defects in device degradation.
342. Surface Science - DOE Contact A. E. Evans, (301) 353-3098; Sandia Contact T. A. Michalski, (505) 844-5829
- 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 oxidation and corrosion of metals and semiconductors, the nature of the adhesion of polymers to metals and how to improve it, and the mechanisms by which gaseous species are dissociated at the surface and transported to the insulator-semiconductor interface in MIS gas sensors.
 - Novel chemical vapor deposition techniques are being developed to produce more uniform and reliable multicomponent pyrotechnics.

Compound Semiconductor and Device Research Department, 1140

Study and application of semiconductor strained-layer superlattices and hetero-junction 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. 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

343. 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/InAs and InGaAs/GaAs strained layer superlattice (SLS) and strained quantum well (SQW) structures for electronic and optoelectronic applications.
344. 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 μ m wavelength region.
345. Strained Layer Superlattices for IR Detectors - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; Sandia Contact P. S. Percy, (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 μ m range. These IR materials are being grown by both MBE and MOCVD techniques. Detection to 12 μ m has been demonstrated.
346. 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 Schottky barrier and Ohmic contact formation, passivation layer development, and development of new metallurgical techniques for deposition of reactive alloys.
347. 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. Patterning and contacting technology for the films is also being developed.

Solid State Research Department, 1150

The mission of Department 1150 is to provide a basic understanding of solid materials with an emphasis on electronic properties. The department provides supporting experimental and theoretical research both on materials of current interest as well as on systems of importance in emerging technologies. Current studies include hydrogen and helium in metals, high temperature superconductivity, high temperature devices, surface science, high performance semiconductors, and fundamental studies of organic and polymeric materials.

Materials Properties, Behavior, Characterization or Testing

348. Superconductivity - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; Sandia Contact J. E. Schirber, (505) 844-8134

- Transport 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.

349. 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 studies of electronic properties of boron carbide at high temperatures.
- Defects in semiconductors.
- Physics of light-hole devices based on strained layer superlattices.

350. 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.

351. Disordered Materials - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; Sandia Contact D. W. Schaefer, (505) 844-7937

- Application of polymeric synthesis routes to ceramic materials.
- Gas phase materials processing.
- Gelation in foam precursors and sol-gel glasses.
- Fundamentals of film formation.

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

352. Dyed Antireflective Photoresist Material - DOE Contact A. E. Evans, (301) 353-3098; Sandia Contact C. Renschler, (505) 844-8151

- A new antireflective photoresist material has been developed and placed into production which allows dramatic improvement in line resolution for microelectronic applications.

353. 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.

354. 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

355. 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.

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. The Division carries out aging studies, compatibility

studies, and coordinates these activities with designers and quality assurance staff. To support these programs, the division carries out in-depth studies on radiation chemistry, photochemistry, surface chemistry, and spectroscopy on polymeric systems.

Materials Preparation, Synthesis, Deposition, Growth or Forming

356. Polysilanes, Photoresists, Photoconductors, and Non-Charring Dielectrics - DOE Contact A. E. Evans, (301) 353-3098; Sandia Contacts J. M. Zeigler, (505) 844-0324 and P. Walsh, (505) 844-3504

- Alkyl-substituted polysilanes and related materials are currently being developed as improved self-developing photoresists for use in advanced photopatterning processes which do not use hazardous solvents as developers.
- Transient spectroscopy techniques are being used to investigate the photochemical scission processes in polysilanes which are important in photoresist applications.
- Different polysilane structures are under investigation as high temperature, non-charring dielectrics.
- The electronic properties of polysilanes are being studied to evaluate their potential as electrooptic materials.

357. Mechanistic Studies of Polysilane Synthesis - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; SNLA Contacts J. M. Zeigler, (505) 844-0324, P. Walsh, (505) 844-3504 and R. G. Kepler, (505) 844-7520

- Polysilanes applications: photoresists, charge transport materials, non-linear optical materials.
- Mechanistic studies provide means to prepare nearly monodisperse polysilanes.
- Critical for understanding properties and applications of polysilanes.

358. Chemistry of Plasma Etching and Deposition Processes - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; Sandia Contacts J. M. Zeigler, (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

359. Materials Structure, Dynamics, and Property Studies by Multinuclear Pulsed NMR Spectroscopy - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; Sandia Contacts J. M. Zeigler, (505) 844-0324 and R. H. Assink, (505) 844-6372
- Use of ^{13}C and ^1H 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.
360. Studies of Adhesion at the Molecular Level by Surface Science Techniques - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; Sandia Contacts J. M. Zeigler, (505) 844-0324 and J. A. Kelber, (505) 844-5436
- Study of mechanism of polymer-polymer and polymer-metal adhesion using ESD, PSD, XPS, and Auger spectroscopies.
 - Relevant to problem of epoxy adhesion to oxidized Co and Al substrates, which are employed in a wide variety of microelectronic and aerospace applications.
 - Results to date indicate atmospheric moisture a contributor.

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

361. Microporous Foam Development - DOE Contact A. E. Evans, (301) 353-3098; Sandia Contact J. H. Aubert, (505) 844-3305

- We are developing new polymer and carbon foams which have both low density and 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 made in this way can be carbonized. These foams have many potential applications.

362. Development of Removable Encapsulants - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; Sandia Contacts 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

363. Mechanical Properties of Encapsulants - DOE Contact A. E. Evans, (301) 353-3098; Sandia Contact D. Adolf, (505) 844-4773

- The crucial thermophysical properties for determining the level of thermally generated stresses in polymeric encapsulants are the coefficient of thermal expansion, the bulk modulus, and either the shear or tensile modulus. We have measured these properties as a function of temperature for the common encapsulants used in our weapons facilities. Previously, the bulk modulus had been estimated from room temperature tensile modulus measurements and estimates of Poisson's ratio. We have directly measured the bulk modulus using a tri-axial testing facility and see significant differences from the historical values. In addition, the frequency dependence of the shear modulus was measured allowing modelling of the viscoelastic behavior of these materials.

364. Deformation of Kevlar Fabrics - DOE Contact A. E. Evans, (301) 353-3098; Sandia Contacts R. H. Ericksen, (505) 844-8333 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.

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 inhomogeneous materials, contacts to electronic materials, dielectrics, and special materials and processes.

Materials Properties, Behavior, Characterization or Testing

365. Nonlinear Optical Materials - DOE Contact A. E. Evans, (301) 353-3098; SNL Contacts R. G. Kepler, (505) 844-7520 and M. L. Sinclair, (505) 844-5506

- Specially synthesized organic molecules are being characterized for nonlinear hyperpolarizabilities.

366. Hydrogen Effects in Silicon - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; Sandia Contacts R. G. Kepler, (505) 844-7520 and R. A. Anderson, (505) 844-7676

- Measurements made of hydrogen diffusion through metal contacts into boron-doped silicon.
- Hydrogen bonds to boron and passivates it as an acceptor.
- Affects formation of Schottky barriers.

367. Rapid Thermal Processing of Gate Oxides - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; Sandia Contact R. G. Kepler, (505) 844-7520 and W. K. Schubert, (505) 846-6548

- Characterization of 20 nm layers of SiO₂.
- 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

368. 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

369. Thermomechanical Treatment of U Alloys - DOE Contact A. E. Evans, (301) 353-3098; Sandia Contact K. H. Eckelmeyer, (505) 844-7775

- Strengthening mechanisms are being investigated in U-Ti and U-b 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.

Instrumentation and Facilities

370. 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. Current projects include the development of quantitative imaging techniques for the electron microprobe and of particulate screening techniques for analytical electron microscope.

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

371. Advanced Methods for Surface and Optical Analysis - DOE Contact A. E. Evans, (301) 353-3098; Sandia Contact J. A. Borders, (505) 844-8855

- 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.

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 Preparation, Synthesis, Deposition, Growth or Forming

372. Analytical Electron Microscopy of Engineering Alloys - DOE Contact A. E. Evans, (301) 353-3098; Sandia Contact A. D. Romig, (505) 844-8358

- The capability to establish quantitatively the chemical concentrations with high resolution in the transmission electron microscope has progressed remarkably recently. The focus here has been to develop techniques which allow complex engineering alloys to be examined by this method by microscope modifications and the use of Monte Carlo simulations. Uranium alloys, stainless steels, and refractory alloys are currently under study.

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

373. Toughness of Ductile Alloys - DOE Contact A. E. Evans, (301) 353-3098; Sandia Contacts R. J. Salzbrenner, (505) 844-5041 and J. A. VanDenAvyle, (505) 844-1016

- Elastic-plastic fracture toughness (J_p) 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.

374. Friction and Wear of Modified Surfaces - DOE Contact A. E. Evans, (301) 353-3098; Sandia Contacts R. J. Bourcier, (505) 844-6638 and A. D. Romig, (505) 844-8358

- Novel techniques such as laser glazing and ion implantation have been applied to surfaces requiring good wear resistance. The metallurgy of the near-surface regions produced by these (or more traditional) techniques is poorly understood and the mechanisms for enhanced wear resistance are not known. This is

being addressed using finite-element computer modeling of modified materials and microstructural examination.

375. Alloy Deformation Response and Constitutive Modeling - DOE Contact A. E. Evans, (301) 353-3098; Sandia Contacts W. B. Jones, (505) 844-4026 and R. J. Bourcier, (505) 844-6638

- Computational prowess has grown to the extent that more complex models of alloy deformation behavior can now be used in finite element codes. The development of microstructurally-based constitutive models is being sought through the use of both uniaxial and biaxial mechanical testing at ambient and elevated temperatures. Stainless steels have been chosen as the focus of this effort.

376. Corrosion - DOE Contact A. E. Evans, (301) 353-3098; Sandia Contact R. B. Diegle, (505) 846-3450

- Determination of how certain glassy alloys derive resistance to corrosion and why they require less alloyed chromium than conventional stainless steels.

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

377. 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. Variable melt rates have been related to oxide films on the surface of the melt.

Device or Component Fabrication, Behavior or Testing

378. Aluminum Laser Welding - DOE Contact A. E. Evans, (301) 353-3098; Sandia Contact J. L. Jellison, (505) 844-6397
- The role of the laser plume in defocusing the laser beam is being studied. Also, the effect of alloying elements, such as magnesium, on laser energy absorption is being characterized.
379. Welding of Nickel-Based Alloys - DOE Contact A. E. Evans, (301) 353-3098; Sandia Contacts M. J. Cieslak, (505) 846-7500 and G. A. Knorovsky, (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. The roles of C, S, and Nb in Inconel 625 hot-cracking are under study.
380. 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. Significantly narrower welds have been produced in thin aluminum sheet than can be achieved with gas tungsten arc welding.
381. Laser Welding - DOE Contact A. E. Evans, (301) 353-3098; 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 convection, 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.
382. Development of Materials for Magnetic Fusion Reactors - DOE Contact A. E. Evans, (301) 353-3098; 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 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

383. 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.

- As a continuation and conclusion to an earlier study, amorphous NiCrFeSiB and NiCrSiB alloy coatings with varying amounts of Ni and Cr were deposited using a dual beam ion system. 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

384. Modification of Mechanical Properties by Ion Implantation - DOE Contact A. E. Evans, (301) 353-3098; Sandia Contact L. E. Pope, (505) 844-5041

- 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.

Device or Component Fabrication, Behavior or Testing

385. 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.
386. Plasma Oxidation and Reduction Studies - DOE Contact A. E. Evans, (301) 353-3098/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

387. 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.
388. 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
- Titanium nitride films have proven useful as tribological coatings for increased hardness and wear resistance in a variety of applications. 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.

389. In Situ Friction, Wear, and Electrical Contact Resistance Systems - DOE Contact A. E. Evans, (301) 353-3098; Sandia Contacts L. E. Pope, (505) 844-5041 and D. E. Peebles, (505) 844-1647

- 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. Surface analytical measurements are made in wear tracks without exposure to ambient environments, because exposure can mask compositional measurements. The correlation between surface composition and measured experimental parameters is determined.

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.

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.

Materials Preparation, Synthesis, Deposition, Growth or Forming

390. Ceramic Processing - DOE Contact A. E. Evans, (301) 353-3098; Sandia Contact B. C. Bunker, (505) 844-8940

- High purity homogeneous PZT powders have been prepared by sol-gel chemistry and other solution techniques. Materials prepared include ZrO_2 , PZT, ZnO, Al_2O_3 , and titanate catalyst supports.

391. Electrophoretically-Deposited Coatings - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; Sandia Contacts A. K. Hays, (505) 844-9996 and D. J. Sharp, (505) 844-8604
- Electrophoresis as a technique has been used for some time to apply organic and ceramic coatings to large, irregularly-shaped objects. 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.
392. Glass and Glass-Ceramic Development - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; Sandia Contacts F. P. Gerstle, Jr., (505) 844-4304 and D. H. Doughty, (505) 844-1933
- A family of glass ceramics is being developed to match the thermal expansion of a number of metal systems.
 - Objective is to develop tougher glass ceramics for electrical insulator applications.

Materials Properties, Behavior, Characterization or Testing

393. Fracture of Ceramics - DOE Contact A. E. Evans, (301) 353-3098; Sandia Contact F. P. Gerstle, Jr., (505) 844-4304
- Basic research to better understand fracture processes and to develop tougher ceramics based on this understanding.
394. Optical Diagnostics for Materials Processing - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; Sandia Contacts A. K. Kays, (505) 844-9996 and H. C. Peebles, (505) 846-3454
- Optical diagnostics being developed to map the temperature, composition, and velocity profiles as a function of time of species present in the atmosphere during standard ceramic and metallurgical processes (e.g., welding, vacuum arc remelting, and plasma spraying).

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395. Powder Metallurgy - DOE Contact A. E. Evans, (301) 353-3098; Sandia Contacts J. A. Brooks, 415-422-2051, J. E. Smugeresky, (415) 422-2910 and J. W. Zindel, (415) 294-3614

- Inert gas atomization, spark erosion, 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.

396. Advanced Electrodeposition Studies - DOE Contact A. E. Evans, (301) 353-3098; Sandia Contacts H. R. Johnson, (415) 422-2822 and W. D. Bonivert, (415) 294-2987

- Engineering applications, electroanalytical development, and fundamental investigations are being pursued in the area of electrodeposition and electroforming.

397. Metal Forming - DOE Contact A. E. Evans, (301) 353-3098; Sandia Contacts J. Lipkin, (415) 422-2417, T. C. Lowe, 415-422-3187 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.

398. Advanced Organic Materials - DOE Contact A. E. Evans, (301) 353-3098; Sandia Contacts D. L. Lindner, (415) 422-3306, J. G. Curro, (505) 844-3963, W. R. Even, (415) 422-3217 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.

399. 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.
400. 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 getting large amounts of tritium gas even in the presence of contained amounts of oxygen and water without releasing radioactive species as it ages.
401. 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.
402. 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

403. 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) 422-2209, S. H. Goods, (415) 422-3274 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.

404. Joining Science and Technology - DOE Contact A. E. Evans, (301) 353-3098; Sandia Contacts J. A. Brooks, (415) 422-2051, K. W. Mahin, (415) 294-3582 and J. E. Costa, (415) 294-2352
- 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 brazing, solid state welding, and adhesives are being developed for advanced structural materials.
405. Composites: Characterization and Joining - DOE Contact A. E. Evans, (301) 353-3098; Sandia Contacts J. B. Woodard, (415) 422-3115; B. C. Odegard, (415) 294-2789; J. R. Springarn, (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.
406. Compatibility, Corrosion, and Cleaning of Materials - DOE Contact, A. E. Evans, (301) 353-3098; Sandia Contacts H. R. Johnson, (415) 422-2822, D. L. Lindner, (415) 294-3306 and D. K. Ottesen, (415) 294-2787
- We have developed special techniques using FTIR to examine the effects of corrosion and cleaning techniques on materials.
407. 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.
408. Measurement of Multilayer Thin Film Structures - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; Sandia Contacts B. B. 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.

409. Helium in Metal Tritides - DOE Contact A. E. Evans, (301) 353-3098; Sandia Contacts W. A. Swansiger, FTS 234-2496, S. E. Guthrie, FTS 422-2360 and D. F. Cowgill, (505) 844-7480
- Helium evolution in metal tritides is being studied by NMR, gas sampling and dilatometry techniques.
410. 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

411. 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.
412. 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.
413. 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.

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Materials Preparation, Synthesis, Deposition, Growth or Forming

414. Ion Beam Modification of Materials - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; LLNL Contact R. G. Musket, (415) 422-0483
- Investigations of surfaces modified by ion beams enhance our understanding of (a) the fundamental processes occurring during ion implantation and (b) the response of modified materials to various environments.
415. 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.
416. 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.
417. 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.
418. 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.

419. 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.
420. New Ionomer Synthesis - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; LLNL Contact M. O. Riley, (415) 422-6865/FTS 532-3045
- This project was directed towards the synthesis of new transition metal and rare earth-containing EAA ionomers for application as spectral filters; additionally, we prepared highly loaded metal ion containing ionomers.
421. Polymer 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.
422. 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

423. 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.

424. 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.
425. 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.
426. 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.
427. Low Density Material Aggregate Networks - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; LLNL Contact Lucy M. Hair, (415) 423-7823/FTS 543-7823
- The focus of this project was the development of a general copolymerization and crosslinking scheme using epoxy-amine chemistry to make "aggregate network" LDM (low-density-materials) gel precursors to serve as models for existing submicron LDM gel precursors, e.g., silica aerogel and resorcinol-formaldehyde.
428. 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
- This is an experimental and theoretical investigation of electronic structure in superconducting oxides and related materials using calculations based on a cluster model and positron annihilation spectroscopy including high resolution angular correlation spectroscopy.

429. 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.

430. A New, First-Principles Method for the Calculation of the Electronic Structure of Surfaces and Grain Boundaries - 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

431. 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.

432. 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

- Using a very sensitive method developed in this laboratory, we measure tritium permeation through resistant metals at 10-170°C to enhance our understanding of the low-temperature permeation process.

433. Catalytic Properties of Actinide Compounds - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; LLNL Contact C. A. Colmenares, (415) 422-6352

- Our objective is to study the electronic structure and the surface and catalytic properties of actinide compounds. We are particularly interested in the role that valence electrons, particularly 5f electrons, play in the reactivity of solid actinide compounds with gases and vapors.

434. 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.
435. 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/B₄C multilayer X-ray mirrors.
436. $\Delta N=O$ 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 $\Delta N=O$ transitions in helium-like ions.
437. 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
- Multilayer synthesis technology for the fabrication of small period structures (~1.0 nm) has been the focus of this research and development effort. This will allow extension of optics based on multilayer structures to significantly higher energies.
438. Thin Film Studies - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; LLNL Contact Troy W. Barbee, Jr., (415) 423-7796
- Development of multilayer based X-ray optics instrumentation has been the objective of this program. Specific optics studied include Cassegrain telescopes, diffraction gratings and double multilayer monochromator systems.

439. 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).
440. 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 dislocation feature associated with the rate-controlling process for plastic deformation in aluminum at elevated temperature, (b) the source for large-strain softening of aluminum at elevated temperature, and (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.
441. 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.
442. 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
- The electromagnetically launched expanding ring has been developed as a means of studying the constitutive and fragmentation behavior of metals at tensile strain-rates of approximately 10^4S^{-1} .
443. High Strain Rate Mechanical Testing - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; LLNL Contact D. H. Lassila, (415) 423-9537/FTS 543-9537
- An upgrade project was undertaken to provide capabilities for the mechanical testing of materials at high strain rates in tension using the split Hopkinson bar technique.

444. 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.
445. 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.
446. Integrated Engineering Applications Software (IDEAS) Project - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; LLNL Contact N. Nguyen, (415) 422-7458/FTS 532-7458
- The objective of this project is to automate mechanical testing as well as to provide engineers and technicians in the section a tool to aid them in their everyday engineering functions.
447. High Temperature Metal Alloy Radiant Property Measurements in Conjunction with Advanced Surface Spectroscopy - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; LLNL Contact M. A. Havstad, (415) 423-2598/FTS 543-2598
- The principal objective of this work is to advance fundamental understanding of the radiant properties of metals by application of spectroscopic tools never before applied to radiant property measurements.
448. 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.

449. A Study of Residual Stress for Epoxy-Resin Composites - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; LLNL Contact W. W. Feng, (415) 422-8701/FTS 532-8701
- We have developed a mathematical model of the residual stress caused when epoxy-resin composites are cured and have designed an experiment to verify the accuracy of the analytical results. These results are used to study the residual stress and, hence, improve the integrity of composite structures.
450. 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.
451. Polymer Adhesion Science and Mechanics - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; LLNL Contact S. J. DeTeresa, FTS 532-6466
- Our objective is to understand the relationships between strengths surface energies and the thermodynamic work of adhesion of polymer adhesive bonds.
452. 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).
453. 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.

Device or Component, Fabrication, Behavior or Testing

454. 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.

455. 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 objects in high explosive single crystals, and to examine their respective influences on hot-spot generation and propagation.

456. 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.

457. Application of Laser Gaging Technology to Mechanical Testing - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; LLNL Contact D. R. Lesuer, (415) 422-9633/FTS 532-9633

- The objective of this development project was to evaluate the applications and limitations of a non-contacting laser gaging apparatus to testing in hostile environments.

Instrumentation and Facilities

458. 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).

459. 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.
460. 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.
461. 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 management of laboratory generated wastes.

Los Alamos National Laboratory

Materials Preparation, Synthesis, Deposition, Growth or Forming

462. 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, thermo-mechanical working, sputtering, and stability studies.
 - Measurements of resistivity, thermal expansion and bend ductility to evaluate fabrication processes and alloy stability.

463. Plutonium Oxide Reduction - DOE Contact G. Bennett (301) 353-3197/ FTS 233-3197; LANL Contact D. Peterson, (505) 667-5181/FTS 843-5181
- Determination of thermodynamics of interactions used in direct-oxide reduction of plutonium.
464. Replacement Noble-Metal Alloys - DOE Contact G. Bennett, (301) 353-3197/ FTS 233-3197; LANL Contact T. George, (505) 667-4931/FTS 843-4931
- Development of new noble-metal-based alloys to provide improved containment for plutonium oxide in space power systems.
465. Whisker Reinforced Structural Ceramics - DOE Contact E. E. Hoffman, (615) 576-0735/FTS 626-0735; LANL (Contract No. W-7405-ENG-36) Contact P. D. Shalek, (505) 667-6863/FTS 843-6863
- Development of ceramic composites utilizing oriented VLS silicon carbide whiskers.
466. 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.
467. 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.
468. Three New Conducting Polymers - DOE Contact A. E. Evans, (301) 353-3098/ FTS 233-3098; LANL Contact D. V. Duchane, (505) 667-3238/FTS 843-3238
- Synthesis of one polyphenylguinoxaline and two polypyrrones showing unique electrically conductive properties when treated with appropriate doping agents.

469. New Highly Conductive Doped Polyacetylene - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; LANL Contact D. V. Duchane, (505) 667-3238/FTS 843-3238
- Use of new cesium electride to induce a high level of electrical conductivity and to improve the stability in polyacetylene films.
470. Liquid Crystal Polymer Development - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; LANL Contact R. May, (505) 667-3238/FTS 843-3238
- Synthesis of a liquid crystal polymer with strength in three dimensions.
471. Surface Property Modified Plastic Components - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; LANL Contact D. V. Duchane, (505) 667-3238/FTS 843-3238
- 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.
472. Low-Density, Microcellular Plastic Foams - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; LANL Contact D. V. Duchane, (505) 667-3238/FTS 843-3238
- Manufacture of microstructural polyolefin foams with densities between 0.01 g/cc and 0.2 g/cc by a nonconventional foaming process.
473. Target Coatings - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3912; LANL Contact D. V. Duchane, (505) 667-3238/FTS 843-3238
- Development of single and multilayer metallic and nonmetallic thin film coatings, smooth and uniform in thickness.
474. Physical Vapor Deposition and Surface Analysis - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; LANL Contact D. V. Duchane, (505) 667-3238/FTS 843-3238
- Physical vapor deposition and sputtering to produce materials for structural applications, corrosion resistance, optical properties, and thin film transducers.

475. Fluidized Bed Coatings - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-098; LANL Contact D. W. Carroll, (505) 667-2145/FTS 843-2145
- Development of techniques for low temperature deposition of tungsten, molybdenum, rhenium, and nickel on hollow substrates of spherical and cylindrical shapes.
 - Fabrication of ultra-thin, free-standing shapes.
476. Electrodeposition 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.
 - Applications: hard coatings, corrosion-resistant coatings, weapons physics, inertial confinement fusion.
477. Polymers and Adhesives - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; LANL Contact W. A. May, Jr., (505) 667-6362/FTS 843-6362
- Development of fabrication processes, and evaluation and testing of commercial plastic materials for weapons programs.
 - Development of highly filled polymers, reinforced composites, cushioning materials, and high-explosives compatible adhesives.
 - Applications of commercial and developmental plastics fabrication techniques to specific weapons-related materials and components for the purpose of improving efficiency and economy of weapons design.
478. 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.

479. 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 hot isostatic pressing to near net shape to improve part shape versatility, density, and surface quality.
 - Conduct of component integrity studies involving radiation induced growth and outgassing.
480. Slip Casting of Ceramics - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; LANL Contact H. Casey, (505) 667-4365/FTS 843-4365
- Slip casting of many ceramics including alumina, magnesia, and thoria.
 - Use of colloidal chemistry and powder characterization theory along with materials engineering.
481. 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.
482. 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.
483. 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.

484. Cold Pressing, Cold Isostatic Pressing and Sintering - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; LANL Contact H. Casey, (505) 667-4365/FTS 843-4365
- Use of cold pressing and cold isostatic pressing to consolidate ceramic and metal powders in support of laboratory programs.
485. 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.
486. 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.
487. 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 (2 μ m grain size) in biaxial forming.
488. Microwave Sintering/Processing - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; LANL Contact J. Katz, (505) 667-1424/FTS 843-1424
- Investigating techniques of bonding and sintering ceramics such as Al₂O₃ and glass.
 - Use of very high frequency microwaves which suscept directly to the area in which the heat is needed.
 - Investigation of the control of the heating and its effect on microstructure.

489. Predictions of Super Strong Polymers - DOE Contact S. M. Wolf, (202) 586-5377/FTS 896-5377; LANL 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.
490. High Energy Storage Material - DOE Contact C. B. Hillard, (301) 353-3687; LANL Contact D. V. Duchane, (505) 667-6887
- Development of vinyl fluoride/tetrafluoroethylene copolymer with improved dielectric properties for energy storage.
491. High Temperature Superconductors for Electric Utility Applications - DOE Contact A. E. Evans, (301) 353-3098; LANL Contact G. Maestas, (505) 667-1372/FTS 843-1372
- Preparation of superconducting ceramics into useful "generic conductor" configurations requires substantial improvements in critical current density along with provisions for both electrical and mechanical stabilization of the conductor. These combined goals are approached by classical powder synthesis and consolidation and by direct melting routes.
492. Synthesis of Porous Glass Structures - - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; LANL C. P. Scherer, (505) 665-3202
- Synthesis of high surface area, porous glass fibers from silicon alkoxide gel.

Materials Structure or Composition

493. 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.

494. Neutron Diffraction of Pu and Pu Alloys - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; LANL Contact S. E. Bronisz, (505) 667-4665/FTS 843-4665
- Neutron diffraction studies of plutonium and its alloys conducted at the Los Alamos WNR pulsed neutron source.
 - Time-of-flight technique used to measure diffraction at elevated temperatures and pressures.
495. 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.
496. Modeling of Interfaces in Ordered Intermetallic Alloys - DOE Contact S. M. Wolf, (202) 586-5377; LANL Contact P. J. Hay, (505) 667-3663
- Development of models for interfacial cohesion in Ni-Al alloys.
 - Role of solute atoms in brittle fracture.

Materials Properties, Behavior, Characterization or Testing

497. 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.

498. 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.
499. 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.
500. Plutonium Shock Deformation - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; LANL Contact R. Gray, (505) 667-5452/FTS 843-5452
- Plutonium alloys subjected to shock deformation, recovered and examined to determine effects of shock on microstructures and mechanical properties.
501. Dielectric Loss Measurement in Ceramics - DOE Contact Marvin Cohen, (301) 353-4253; LANL Contact H. M. Frost, (505) 667-1290/FTS 843-1290
- Loss tangent measurements in ceramics at very high frequencies to evaluate effects of neutron damage for magnetic fusion energy applications.
 - Evaluation of microwave sintering properties of ceramics for fabrication purposes.
502. Nondestructive Evaluation - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; LANL Contact A. Wilson, (505) 667-6404/FTS 843-6404
- Development of nondestructive evaluation techniques that produce quantitative estimates of material properties.
 - Application of multivariate analysis to welding processes. Use of tomographic techniques to extend radiographic inspections.
503. Powder Characterization - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; LANL Contact G. J. Vogt, (505) 667-5432
- Characterization of particle size, surface area, morphology, pore size and zeta potential.

- Powders of thoria, silicon nitride, magnesia, alumina, tungsten, tungsten carbide, and copper.
504. Shock Deformation in Actinide Materials - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; LANL Contact M. Stevens, (505) 667-4414
- Characterization of shock effects in uranium, plutonium and plutonium alloys through use of soft recovery techniques.
505. 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.
506. 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) 667-5442
- Microstructural characterization of soft-shocked materials.
 - Dynamic and quasi-static mechanical testing.
507. Mechanical Properties - DOE Contact F. V. Nolfi, (301) 353-3428; LANL Contact M. G. Stout, (505) 667-4665
- Multiaxial testing of metal and alloys.
 - Prediction of texture development and its effects.
508. Radiation Damage in High-Temperature Superconductors - DOE Contact R. J. Gottschall, (301) 353-3428/FTS 233-3428; LANL Contact F. W. Clinard, Jr., (505) 667-5102/FTS 843-5102
- 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.

509. Insulators for Space Reactor Applications - DOE Contact S. Samuelson, (415) 273-4233/FTS 536-4253; LANL Contact F. W. Clinard, Jr., (505) 667-5102/FTS 843-5102

- Insulators for thermionic convertors (used to generate electricity in fission reactors) face a severe environment, including high temperature, a DC electric field, and an intense neutron flux. In this program candidate materials are exposed to that environment, and degradation effects monitored by measurements made during and after testing.

510. Structural Ceramics - DOE Contact R. J. Gottschall, (301) 353-3428; LANL Contact D. S. Phillips, (505) 667-5128

- Mechanistic studies of crack propagation in whisker composites.

Device or Component Fabrication, Behavior or Testing

511. 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.

512. 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.
- Targets filled with deuterium tritium gas.

513. 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 helices, cones, spheres, closed-end vessels of glass, kevlar, carbon, tungsten, and alumina fibers.

514. Polymeric Laser Rods - DOE Contact A. E. Evans, (301) 353-3098/FTS 233-3098; LANL Contact H. K. McDowell, (505) 667-4686/FTS 843-4686
- Development of polymeric-host dye-laser rods.
 - In situ polymerization of dye/monomer mixture.
 - Inexpensive "disposal" laser rods.
515. 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.
516. 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 Varstraint testing established as techniques to investigate crack susceptibility of gas-tungsten-arc welds.
517. 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

	<u>FY 1988</u>
<u>Office of Fossil Energy - Grand Total</u>	\$7,028,000
<u>Office of Technical Coordination</u>	\$6,902,000
<u>AR&TD Fossil Energy Materials Program</u>	\$6,902,000
<u>Materials Preparation, Synthesis, Deposition, Growth or Forming</u>	\$1,949,000
Fundamental Study of Aluminizing and Chromizing Processes	50,000
Fabrication Development of Nickel-Iron Aluminides	172,000
Development of Iron Aluminides	144,000
Development and Evaluation of Advanced Austenitic Alloys	268,000
Evaluation of the Fabricability of Candidate Advanced Austenitic Alloys	100,000
Consolidation of Rapidly Solidified Aluminide Metal Powders	150,000
Investigation of Electrospark Deposited Coatings for Protection of Materials in Sulfidizing Atmospheres	50,000
Short Fiber Reinforced Structural Ceramics	225,000
Fabrication of Fiber-Reinforced Composites by Chemical Vapor Infiltration (CVI)	181,000
Characterization of Fiber-CVD Matrix Interfacial Bonds	120,000
Microwave Sintering of Ceramics	144,000
Development of Advanced Fiber Reinforced Ceramics	100,000
Modeling of Fibrous Preforms for CVD Infiltration	45,000
Improved Ceramic Composites Through Controlled Fiber-Matrix Interaction	200,000
<u>Materials Structure and Composition</u>	\$ 300,000
Analytical Characterization of Coal Surfaces and Interfaces	300,000
<u>Materials Properties, Behavior, Characterization or Testing</u>	\$2,986,000
Transfer Model Predicting Thermomechanical Behavior of Refractory Linings to Industry	40,000
Transformation, Metallurgical Response and Behavior of the Weld Fusion and Heat Affected Zone in Cr-Mo Steels for Fossil Energy Applications	0

OFFICE OF FOSSIL ENERGY (Continued)

FY 1988

Materials Properties, Behavior, Characterization or Testing (continued)

Mechanical Properties and Microstructural Stability of Advanced Austenitic Alloys	85,000
Analysis of Hydrogen Attack on Pressure Vessel Steels	0
Development of a Design Methodology for High-Temperature Cyclic Application of Materials Which Experience Cyclic Softening	0
Investigation of the Weldability of Ductile Aluminides	50,000
Corrosion Studies of Iron Aluminides	22,000
Fireside Corrosion Tests of Candidate Advanced Austenitic Alloys, Coatings, and Claddings	60,000
Microstructural Studies of Advanced Austenitic Steels	36,000
Joining Techniques for Advanced Austenitic Alloys	43,000
Corrosion and Mechanical Properties of Alloys in FBC and Mixed-Gas Environments	320,000
Investigation of Corrosion-Resistant Oxide Scales on Iron-Based Alloys in Mixed-Gas Environments	177,000
Investigation of Corrosion Mechanisms of Coal Combustion Products on Alloys and Coatings	0
Investigation of the Effects of Microalloy Constituents, Surface Treatment, and Oxidation Conditions on Development and Breakdown of Protective Oxide Scales	270,000
Investigation of the Effects of Microalloy Constituents, Surface Treatment, and Oxidation Conditions on Development and Breakdown of Protective Oxide Scales	250,000
Investigation of the Effects of Microalloy Constituents, Surface Treatment, and Oxidation Conditions on Development and Breakdown of Protective Oxide Scales	211,000
A Study of Erosive Particle Rebound Parameters	40,000
Studies of Materials Erosion in Coal Conversion and Utilization Systems	250,000
In-Situ Scanning Electron Microscopy Studies of Erosion and Erosion-Corrosion	177,000
Solid Particle Erosion in Turbulent Flows Past Tube Banks	40,000
Study of Particle Rebound Characteristics and Material Erosion at High Temperatures	0

OFFICE OF FOSSIL ENERGY (Continued)

FY 1988

Materials Properties, Behavior, Characterization or Testing (continued)

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	150,000
Nondestructive Evaluation of Advanced Ceramic Composite Materials	150,000
Structural Reliability and Damage Tolerance of Ceramic Composites	150,000
Mechanical Properties of Ceramic Fiber-Ceramic Matrix Composites	50,000
Ceramic Catalyst Materials	100,000
<u>Device or Component Fabrication, Behavior or Testing</u>	\$1,274,000
Materials and Components in Fossil Energy Applications (Newsletter)	115,000
Assessment of the Causes of Failure of Ceramic Filters for Hot-Gas Cleanup in Fossil Energy Systems and Determination of Materials Research and Development Needs	0
Assessment of Potential Applications of Ceramic Composites in Gas Turbines	0
Mechanisms of Galling and Abrasive Wear	75,000
Fabrication of Commercial-Scale Fiber-Reinforced Hot-Gas Filters by Chemical Vapor Deposition	100,000
Development of Ceramic Membranes for Gas Separation	150,000
Investigation of the Mechanical Properties of CVD Infiltrated Ceramic Composite Tubular Components	85,000
Thermomechanical Modeling of Refractory Brick Linings for Slagging Gasifiers	62,000
Evaluation of Candidate Materials for Solid Oxide Fuel Cells	150,000
Gas Separations Using Inorganic Membranes	200,000
Ceramic Fiber-Ceramic Matrix Hot Gas Filters	200,000
Identification of Materials for Hot-Gas Filter Tubesheets	137,000

OFFICE OF FOSSIL ENERGY (Continued)

	<u>FY 1988</u>
<u>Instrumentation and Facilities</u>	\$ 393,000
Management of the AR&TD Fossil Energy Materials Program	350,000
Coal Conversion and Utilization Plant Support Services	43,000
<u>Office of Coal Technology</u>	\$ 126,000
<u>Division of Coal Conversion</u>	\$ 101,000
<u>Instrumentation and Facilities</u>	\$ 101,000
Materials Technical Support for the Great Plains Coal Gasification Plant	101,000
<u>Division of Clean Coal Technology</u>	\$ 25,000
<u>Instrumentation and Facilities</u>	\$ 25,000
Materials Technical Support for the Clean Coal Program	25,000

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

AR&TD Fossil Energy 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

518. 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.
519. Fabrication Development of Nickel-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 V. K. Sikka, (615) 574-5112/FTS 624-5112
- The purpose of this task is to develop the fabrication technology for nickel-iron aluminides in sufficiently large heat sizes to provide assurance that the alloys can be fabricated by standard industrial processes.
520. 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.

521. 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.
522. Evaluation of the Fabricability of Candidate 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.
523. 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.
524. 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.

525. Short Fiber Reinforced Structural Ceramics - 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 investigate the utility of whisker reinforcement technology for producing structural ceramic composites of improved strength and fracture toughness.
526. 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 and R. A. Lowden, (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.
527. 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.
528. 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 primary purpose of this program is to conduct coordinated research and development on ceramic materials with major emphasis on the microwave processing of new ceramics at ORNL.
529. 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.

530. 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.

531. Improved Ceramic Composites Through Controlled Fiber-Matrix Interaction - 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 purpose of this work is to understand and control the fiber-matrix interface to improve the performance of ceramic matrix composites in fossil energy systems.

Materials Structure and Composition

532. 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

533. 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 D. A. Patterson, (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.

534. Transformation, Metallurgical Response and Behavior of the Weld Fusion and Heat Affected Zone in Cr-Mo Steels for Fossil Energy Applications - 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) 974-5310
- The objective of this research was to develop fundamental information on the metallurgical behavior of the heat affected zone of welds in chromium-molybdenum alloys.
535. 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.
536. Analysis of Hydrogen Attack on Pressure Vessel Steels - DOE Contacts J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; University of California at Santa Barbara Contact G. R. Odette, (805) 961-3525
- Physical models were developed that describe the initiation and development of methane damage in carbon steel, C-Mn-Si steels, 2 1/4 Cr-1 Mo steel, and weldments.
537. Development of a Design Methodology for High-Temperature Cyclic Application of Materials Which Experience Cyclic Softening - DOE Contacts J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; University of Illinois Contact D. L. Marriott, (217) 333-7237
- The objective of this project is to develop a design methodology for high-temperature cyclic conditions, taking into account the effects of strain softening.
538. 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.

539. 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 .
540. 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.
541. 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.
542. 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.
543. 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.

544. Investigation of Corrosion-Resistant Oxide Scales on Iron-Based Alloys in Mixed-Gas Environments - 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 .
545. Investigation of Corrosion Mechanisms of Coal Combustion Products on Alloys and Coatings - DOE Contacts J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; University of Pittsburgh Contact G. H. Meier, (412) 624-5316
- The objective of this research project was to investigate the formation and breakdown of protective oxide scales in mixed oxidant gases.
546. 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.
547. 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.

548. 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.
549. 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.
550. 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.
551. 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.

552. 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.
553. 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.
554. 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.
555. 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.
556. 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.

557. 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.

558. 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).

559. 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

560. 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.

561. Assessment of the Causes of Failure of Ceramic Filters for Hot-Gas Cleanup in Fossil Energy Systems and Determination of Materials Research and Development Needs - DOE Contacts J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; Acurex Corporation Contact J. W. Sawyer, (415) 961-5700

- The purpose of this project was to determine the principal causes of failure of ceramic filters used for removal of fine particulates from high-temperature,

high-pressure gas streams in coal conversion and utilization systems such as fluidized-bed combustors, direct coal-fired gas turbines, and coal gasification systems.

562. 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.
563. 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.
564. 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.
565. 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.

566. 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.
567. Thermomechanical Modeling of Refractory Brick Linings for Slagging Gasifiers - 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.
568. Evaluation of Candidate Materials for Solid Oxide Fuel Cells - 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 to find and develop highly electronically conducting oxides for use as cathodes in solid oxide fuel cells (SOFC).
569. Gas Separations Using Inorganic Membranes - DOE Contacts J. S. Halow, FTS 923-4109 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.
570. Ceramic Fiber-Ceramic Matrix Hot Gas Filters - DOE Contacts N. Holcombe, FTS 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.

571. Identification of Materials for Hot-Gas Filter Tubesheets - DOE Contacts J. W. Byam, FTS 923-4533 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

572. Management of the AR&TD Fossil Energy 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 AR&TD Fossil Energy Materials Program in accordance with procedures described in the Program Management Plan approved by DOE.

573. 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.

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

574. 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 is to provide materials technical support services to the Great Plains Coal Gasification Project.

Division of Clean Coal Technology

Instrumentation and Facilities

575. 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 (ECUT)

The mission of the ECUT Program 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 Program is in two projects, the Materials Project and the Tribology Project. The DOE contacts are Stanley M. Wolf (202/586-1514, FTS 896-1514) for the Materials Project and David Mello (202/586-9345, FTS 896-9345) for the Tribology Project. The Oak Ridge National Laboratory (ORNL) technical manager of the Materials Project is Peter Angelini (615/574-6094, FTS 624-6094). The Tribology Project is managed by Argonne National Laboratory (ANL), technical manager is Fred Nichols (312/972-8292, FTS 972-8292). 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 Project is in the areas of ductile ordered alloys, ceramic-ceramic and ceramic-metal attachments, surface modifications of ceramics, recovery and reuse of plastic scrap, building insulation, ceramic coatings, ceramic composites, and materials structures theory. Materials research in the Tribology Project is in the areas of friction and wear of ceramics, lubricants, and tribological surface modifications and coatings.

Materials Preparation, Synthesis, Deposition, Growth, or Forming

1. Solid Lubricants Deposited From the Gas Phase

FY 1988
\$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.

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

2. Engineered Tribological Surfaces

FY 1988
\$750,000

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 Al₂O₃ and B₂O₃ 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. Modeling of Hard Coatings for Tribological Systems Operating Under Extreme Conditions

FY 1988
\$ 0

DOE Contact: D. Mello, (202) 586-9345

George Washington University (Contract No. DE-AC02-84CE90225) Contact:
Bruce Kramer, (202) 676-8237

A specific model of the wear behavior of hard wear coatings has been developed that includes the effects of chemical dissolution and mechanical abrasion on the wear rate. Inputs to the model include the free energy of formation of the potential coating material, the excess free energies of solution of the constituent elements of the coating in the workpiece, the hardness of the coating and the cutting temperature. An algorithm

was written and used to search the available literature database and estimate the wear performance of candidate materials. Coatings were prepared and tested to experimentally evaluate the predictions of the theory and calibrate the wear model. Relative wear rate predictions of the model were not confirmed due to softening and deformation of the steel substrate under the coating during cutting, however TiN, TiC, ZrN, ZrC, HfN and HfC coatings on T-15 tool steel produced wear lifetimes 3 to 10 times larger than that of uncoated tool steel. This project is being concluded in FY 1988.

Keywords: Coatings, Friction, Wear, Metals, Machining

4. Abrasion and Impact Resistant Coatings FY 1988
\$ 0

DOE Contact: D. Mello, (202) 586-9345

LLNL (Contract No. W-7405-ENG-48) Contact: William Steele, (415) 423-2949

This project is developing innovative wear resistant coatings constructed by anchoring a high density mat of very fine, hard filaments or "hairs" into the surface of a bulk matrix, at near vertical angles. These filaments form an intertwined, compliant mat which effectively resists impacts. Tests were conducted in a sandblaster with controlled air flow, and controlled sand size and flow. Initial tests conducted on carbon fibers imbedded in an epoxy matrix, established that a dense mat of 2 to 5 micron carbon fibers can provide complete protection. Unprotected epoxy specimens were completely destroyed. An initial test of a polyvinyl chloride pipe lined with an 8 mm carbon fiber coating in a simulated industrial oil shale retort flow line resulted in failure of the coating due to shearing by fly ash and silica particles. Large pressure drops also occurred. This project was concluded in early FY 1988.

Keywords: Coatings, Wear, Friction, Fibers, Metals, Polymers

5. Coordination of ECUT Plastics Recycling and Reuse Efforts FY 1988
\$ 0

DOE Contact: Stanley M. Wolf, (202) 586-1514

Plastics Institute of America (ORNL Subcontract 19X-09100C) Contact: Mike Curry or Al Spaak, (201) 420-5552

The PIA is coordinating efforts to assess the potential of transfer technologies for recycling or reusing post-consumer plastic scrap via various approaches. Previous work concentrated on techniques involving bonding and/or separations of mixed plastic scrap. The results of these efforts were published in FY 1987. In FY 1986 and FY 1987 the PIA held large national workshops intended to promote interest in plastics recycling as business opportunities for the private sector. Work will be solicited by an open competition in FY 1988 in the area of recovery and reuse of plastic scrap by means of

techniques in which the scrap plastics are decomposed in some way to products such as uncrosslinked polymers, chemical feedstocks, free monomer, or fuels.

Keywords: Polymers, Recycle

6. Surface Roughness Wear Model for Ceramics

FY 1988

\$78,000

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 which predicts wear and load-bearing area, and aids in surface finish selection for ceramic bearings. The program entered the validation phase in FY 1988 based on testing support from ORNL and ANL. The computer software development work has led to the ability to estimate frictional flash temperatures. Support of further modeling work, proposed to be extended to surface-modified materials, is dependent on the results of the validation underway in FY 1988.

Keywords: Friction, Wear, Surface Topology, Surface Microstructure, Ceramics, Modeling

7. Assessment of the Economic Potential of Plastics Reuse

FY 1988

\$10,000

DOE Contact: Stanley M. Wolf, (202) 586-1514

ORNL (Contract No. DE-AC05-84OR21400) Contact: Randall Curlee, (615) 576-4864

The objective of this work is to assess the general economic potential of plastics reuse. The work focuses on projections of particular types of plastic waste in different waste streams and on the various economic and institutional incentives and barriers that impact the market acceptance of different recycle technologies.

Keywords: Plastics, Recycle, Economic Analysis

8. Laser Surface Modifications of Ceramics

FY 1988
\$125,000

DOE Contact: Stanley M. Wolf, (202) 586-1514
North Carolina State University (ORNL Subcontract 19X-43377C) Contact:
Jagdish Narayan, (919) 737-7874

The objective of this effort is to investigate the nature and implications of surface modifications induced by driving or diffusing certain metal ions into ceramic surfaces by irradiation with a pulsed laser. Thin layers of either Cr, Fe, or Ni are deposited onto flat surfaces of either alpha- or beta-SiC, Si₃N₄, or Al₂O₃ and then irradiated by pulsed lasers. Fracture strength and toughness, friction and wear behavior, fatigue resistance, and microstructural and compositional variations are determined and related to the wavelength of the laser radiation, the pulse duration, and the energy density. This project will also examine high temperature superconducting films on various substrates.

Keywords: Structural Ceramics, Coatings and Films, Laser Annealing

9. Plasma-Assisted Sintering of Ceramics

FY 1988
\$94,000

DOE Contact: Stanley M. Wolf, (202) 586-1514
Northwestern (ORNL Subcontract 19X-55900C) Contact: D. Lynn Johnson,
(312) 492-3537

The objective of this effort is to investigate sintering of ceramic materials in furnaces filled with low pressure gas plasmas. Previous work (supported by DoD and NSF) has shown that some ceramics can be sintered to high densities quite rapidly by means of plasmas and microwaves by means of (1) simple heating and (2) activation of mass transport properties (e.g., grain boundary diffusion) important to sintering. In the present work, attempts are being made to decouple the two mechanisms, i.e., the specimen is heated by conventional means such as resistance heating while in a low-pressure, non-equilibrium plasma. Such a sintering system has been built and studies are in progress.

Keywords: Structural Ceramics, Consolidation of Powder, Sintering, Plasma

10. Ion Implantation of Ceramics

FY 1988
\$345,000

DOE Contact: Stanley M. Wolf, (202) 586-1514
ORNL (Contract No. DE-AC05-84OR21400) Contact: Carl McHargue, (615) 574-4344
Georgia Institute of Technology (ORNL Subcontract 19B-07802C) Contact:
Joseph Cochran, Jr., (404) 894-6104
Universal Energy Systems (ORNL Subcontract 86X-22015C) Contact: Peter Pronko,
(513) 426-6900, ext. 113

These efforts explore the effects of ion implantation on certain properties of ceramics. Properties measured include strength, strength reliability (Weibull modulus), hardness, fracture toughness, coefficient of friction, and wear rates. Work at ORNL is concentrated on implantation into TiB_2 ; at Georgia Tech, into Al_2O_3 and ZrO_2 ; and at UES, into SiC , Si_3N_4 , and $SiAlON$.

Keywords: Structural Ceramics, Ion Implantation

11. Compositionally Modified Ceramics

FY 1988
\$342,000

DOE Contact: Stanley M. Wolf, (202) 586-1514
ORNL (Contract DE-AC05-84OR21400) Contact: Rodney McKee, (615) 574-5144

The objective of this task is to synthesize layered oxides of aluminum and titanium using ultra high vacuum Molecular Beam Epitaxy techniques to control microstructure in a two-dimensional thin-film structure. Emphasis is placed on the development of unique material combinations to control mechanical and electrical properties of thin films. A new growth chamber is being designed to accommodate the synthesis of superconducting materials as well.

Keywords: Structural Ceramics, Molecular Beam Epitaxy, Layers

12. Injection Molding of Electrosterically-Stabilized Oxide Suspensions in an Aqueous Medium

FY 1988
\$25,000

DOE Contact: Stanley M. Wolf, (202) 586-1514
University of Washington (ORNL Subcontract 19X-27458C) Contact: Ilhan Aksay,
(206) 543-2625

A method of preparing highly concentrated but fluid colloidal aqueous suspensions of ceramic particles is being studied. The objective is to produce an injection-moldable aqueous slurry with little or no organic binders by adsorbing organic polyelectrolytes onto the surfaces of the powder particles in order to minimize the particle agglomeration usually encountered in aqueous-based slurries. Model experiments with submicron-size

alumina have been designed to determine the guidelines for the selection of the proper molecular weight polyelectrolytes used to stabilize the suspensions.

Keywords: Structural Ceramics, Consolidation of Powder, Modeling, Polymers

13. Assessment of the State of the Art in Machining and Surface Preparation of Ceramics

FY 1988

\$ 0

DOE Contact: Stanley M. Wolf, (202) 586-1514

ORNL (Contract No. DE-AC05-84OR21400) Contact: Dave Stinton, (615) 574-4556 and Ted Besmann, (615) 574-6852

This task is an assessment of current machining and surface preparation methods on the performance of ceramic materials developed for use in high-temperature engineering systems. These new materials, which include fiber-reinforced ceramics, high-strength aluminas, and transformation toughened zirconia, exhibit high-temperature strengths comparable to conventional ceramics but also possess improved fracture toughness. The machining and surface preparation of these materials has a significant effect on the mechanical properties and cost of the materials, but has received little attention. This assessment will be concluded in FY 1988.

Keywords: Structural Ceramics, Machining, Surface Preparation

14. Microporous Ceramics

FY 1988

\$150,000

DOE Contact: Stanley M. Wolf, (202) 586-1514

LBL (Contract DE-AC03-76SF00090) Contact: Arlon Hunt, (415) 486-5370

A process is under development to produce 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: Structural Ceramics, Fabrication, Sol-Gel, Separations

15. Chemical Vapor Deposition of Ceramic Composites

FY 1988

\$150,000

DOE Contact: Stanley M. Wolf, (202) 586-1514

ORNL (Contract No. DE-AC05-84OR21400) Contact: Ted Besmann, (615) 574-6852

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.

Keywords: Structural Ceramics, Chemical Vapor Deposition, Composites, Coatings

16. Thin-Wall Hollow Ceramic Spheres from Slurries

FY 1988
\$203,000

DOE Contact: Stanley M. Wolf, (202) 586-1514

Georgia Institute of Technology (ORNL Subcontract 86X-22043C) Contact:
A. T. Chapman, (404) 894-4815

ORNL (Contract No. DE-AC05-84OR21400) Contact: David L. McElroy, (615) 574-5976

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 $\text{Al}_2\text{O}_3\text{-Cr}_2\text{O}_3$ 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. Thermal conductivities for beds of spheres of varying diameters, densities, and compositions are under study at ORNL while Georgia Tech is examining their structural integrities.

Keywords: Structural Ceramics, Refractory Ceramics, Solidification, High Temperature Service, Insulation

17. Strain Tolerant Ceramic Fibers from Liquid Crystal Polymer Precursors

FY 1988
\$55,000

DOE Contact: Stanley M. Wolf, (202) 586-1514

The University of Tennessee (ORNL Subcontract 41B-07685C) Contact: Jack Fellers,
(615) 974-5345. Collaborating ORNL Contact: Mark Janney, (615) 574-4281,
FTS 624-4281

This is a highly speculative exploratory effort aimed at determining whether it is possible to produce ceramic fibers with strain tolerance. Liquid crystal polymers when drawn into a fiber usually fibrillate, that is, the fiber breaks down into smaller microfibrils so that, in the end, the liquid crystal fiber is actually composed of many smaller strands similar to a rope structure. The notion here is to produce a liquid crystal fiber composed of certain chemical elements in certain combinations such that, upon

heating, the polymeric liquid crystal fiber converts to a ceramic fiber which is also microfibrillated and therefore may have some torsional strain tolerance like that of a bundle of twigs or pick-up sticks.

Keywords: Structural Ceramics, Fibers, Strain-Tolerance

18. Synthesis of SiC Whisker - MoSi₂ Matrix Composites for Elevated Temperature Applications FY 1988
\$100,000

DOE Contact: Stanley M. Wolf, (202) 586-1514

LANL (Contract W-7405-Eng-36) Contact: Frank Gac, (505) 667-5452

SiC whisker-MoSi₂ matrix composites are being examined for potential elevated temperature structural applications in oxidizing environments. A composite approach will be employed to improve the mechanical properties of MoSi₂. Initial room temperature mechanical property measurements indicate a composite strength nearly twice that of the pure MoSi₂, and a composite fracture toughness 30% higher than that of the pure MoSi₂.

Keywords: Metals, Alloys, Ceramics, Composites, Whiskers

19. Assessment of Curing and Joining of Polymers FY 1988
\$15,000

DOE Contact: Stanley M. Wolf, (202) 586-1514

ORNL (Contract No. DE-AC05-84OR21400) Contact: Ron Bradley, (615) 574-6094 and Paul Phillips, (615) 974-5304

The objective of this effort is to determine the DOE ECUT Program's proper role, if any, in support of base technologies involved in the curing and joining of polymeric materials, primarily those to be used in automobiles. It is hoped that support of such technologies will assist U.S. automakers in deploying future vehicles with lighter weight—and therefore energy conserving—components made of polymeric materials. It is felt that the steps of curing and joining need to be improved in order for such components to be cost competitive and reliable. Work to date has primarily consisted of literature reviews and site visits. This project will conclude in FY 1988.

Keywords: Polymers, Curing, Joining and Welding, Lightweight Materials, Automobiles

20. Separation of Impurities from Molten Metals Using MHD Forces FY 1988
\$100,000

DOE Contact: Stanley M. Wolf, (202) 586-1514

ORNL (Contract No. DE-AC05-84OR21400) Contact: David O. Hobson, (615) 574-5109

Experimental work and computer modeling are being used to show that MHD forces can effect the redistribution and removal of particulate impurities from molten metals. Experiments have included proof-of-concept tests involving impurities in both Hg and molten aluminum. Computer modeling of the possible configurations is being used for process optimization.

Keywords: Molten Metals, Purification, Processing

21. Additives for High-Temperature Liquid Lubricants FY 1988
\$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.

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

22. IAD of Tin and Cr₂O₃ FY 1988
\$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

23. Self-Lubricating Ceramic Surfaces

FY 1988
\$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 will be 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 will be 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

24. Surface Laser Treatment of Partially Stabilized Zirconia (PSZ)

FY 1988
\$78,000

DOE Contact: D. Mello, (202) 586-9345

Illinois Institute of 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 will be compared to wear tests. This project will be critically reviewed during FY 1989 to determine whether the approach is supported by experiments and warrants further fundings.

Keywords: Surface Modification, Laser, Zirconia, Friction, Wear, Microstructure

Materials Structures and Composition

25. Mechanisms of Adherence at Ceramic Joints

FY 1988
\$150,000

DOE Contact: Stanley M. Wolf, (202) 586-1514
ORNL (Contract No. DE-AC05-84OR21400) Contact: Mike Santella, (615) 574-4805
Carnegie-Mellon University (ORNL Subcontract 19X-SA866C) Contact: Dick Fruehan,
(412) 268-2677

This task investigates the fundamental physical and chemical parameters controlling the adhesion of ceramics to ceramics and metals in order to increase the understanding of the problems and limitations inherent in such attachments if they are to be used in structural components of future heat engines and high temperature industrial heat exchangers. The ORNL work is mainly concerned with the physical parameters whereas the CMU work is mainly on the thermodynamic (chemical) parameters.

Keywords: Structural Ceramics, Joining and Welding, Adherence

26. Modeling of Boron-Effect in Ni₃Al

FY 1988
\$650,000

DOE Contact: Stanley M. Wolf, (202) 586-1514
LANL (Contract W-7405-Eng-36) Contact: Jeff Hay, (505) 667-2097
Virginia Polytechnic Institute and State University (ORNL Contract 19X-89678V)
Contact: Diana Farkas, (703) 961-4742

The ECUT Materials by Design effort is currently developing models to predict the interfacial properties of Ni₃Al and the role of solute atoms such as B in preventing brittle fracture at grain boundaries. A hierarchy of models has been implemented which encompass electronic properties, interatomic potentials, atomistic simulation, and phenomenological models of crack propagation. In addition to the main efforts at Los Alamos, there are collaborations with investigators at Virginia Polytechnic Institute and State University and others (mostly funded by the DOE Office of Basic Energy Sciences) working on experimental investigations of the B-effect-in-Ni₃Al.

Keywords: Metals, Alloys, Intermetallics, Modeling, Grain Boundary, Structure

27. Predictions of Ordered Intermetallics

FY 1988
\$275,000

DOE Contact: Stanley M. Wolf, (202) 586-1514
Imperial College of London (ORNL Subcontract 19X-55992V) Contact: David Pettifor,
1-589-5111, ext. 5756 (England)
ORNL (Contract DE-AC05-84OR21400) Contact: Don Nicholson, (615) 574-5873

The objective of this task is to develop and experimentally verify models for predicting ductile ordered intermetallic alloys which would be expected to be the most likely candidates for further development as useful structural materials. The expected results are a model, or models, which can predict the possible existence of such materials which could not otherwise be identified by more classical approaches. Initial approach is based on structure maps.

Keywords: Metals, Alloys, Modeling, Ordered, Intermetallics

28. Predictions of Super-Strong Liquid Crystal Polymers

FY 1988
\$50,000

DOE Contact: Stanley M. Wolf, (202) 586-1514
LANL (Contract W-7405-Eng-36) Contact: Flonnie Dowell, (505) 667-8765

Advanced, first-principles, microscopic, molecular statistical-physics theories will be originated and developed into mathematical models to predict (with the aid of computer-based modeling) new molecular structures most likely to form liquid crystal polymers. These candidate molecules will then be chemically synthesized and experimentally characterized.

Keywords: Modeling, Polymers, Liquid Crystals

29. Predictions of Polymer Decompositions

FY 1988
\$135,000

DOE Contact: Stanley M. Wolf, (202) 586-1514
ORNL (Contract DE-AC05-84OR21400) Contact: Bill Thiessen, (615) 574-4973

The objective of this task is to develop computer models for the likely routes and yields of polymer decompositions. The intent is to predict possible schemes for recovering value from polymers in the waste stream.

Keywords: Polymers, Decomposition, Modeling

30. Influence of Electronic Structure on Ordered Intermetallics

FY 1988
\$ 0

DOE Contact: Stanley M. Wolf, (202) 586-1514

Carnegie-Mellon University (ORNL Subcontract 19X-89672C) Contact: T. B. Massalski,
(412) 578-2708

This work seeks to identify phenomenological correlations between the electronic structure and the ordering temperature and stacking arrangement in ordered intermetallics. Available data were analyzed and apparent correlations were identified among the electron-to-atom ratio, average electron energy for valence electrons and the atomic plane stacking characteristics for two ordered pseudo-binary alloys. Electronic-level calculations were initiated to explain the correlations in terms of valence electronic energies as functions of the atomic arrangements in various stacking sequences. This project will be concluded in FY 1988.

Keywords: Metals, Alloys, Modeling, Electronic Structure, Intermetallics

31. Liquid Crystalline Polymers Assessment

FY 1988
\$ 0
(\$25,000 in FY 85)

DOE Contact: Stanley M. Wolf, (202) 586-1514

University of Tennessee Contact: Paul Phillips, (615) 974-5304

This project assesses the potential of emerging liquid crystal technologies for producing polymeric materials for structural applications. Liquid crystal polymers are curious materials which retain a degree of molecular regularity and orientation even in the melt stage. A possibility exists that such materials may be capable of forming a self-reinforcing composite in which the solid part of the melt stage acts as a reinforcement for the remainder after solidification. A unique advantage of such material would be that it could be melted and shaped like any thermoplastic. This project will conclude in FY 1988.

Keywords: Polymers, Liquid Crystals

32. Thermosetting Resins with Reversible Crosslinks

FY 1988
\$100,000

DOE Contact: Stanley M. Wolf, (202) 586-1514

Polytechnic of New York (ORNL Subcontract 19X-55935C) 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. The feasibility of the concept was demonstrated in FY 1986 for an epoxy resin using a crosslink containing a disulfide bond.

Keywords: Polymers, Thermosets, Resins, Crosslinks

33. Biobased Polymers

FY 1988
\$150,000

DOE Contact: Stanley M. Wolf, (202) 586-1514

SERI (Contract DE-AC02-83CH10093) Contact: Helena Chum, (303) 231-7249

The objective of this work is to explore the potential of producing polymers from biomass, as well as biobased materials in general, for the production of inexpensive materials at a substantial overall energy savings. The initial focus has been on the formulation of a research program for the development of biobased materials. Two main components have been identified: (1) production of known polymeric materials from biomass and (2) production of entirely new polymeric materials either from biomass or by biochemical processing. Work on both components was initiated in FY 1987.

Keywords: Polymers, Biomass

34. Assessment of DoD/NASA Thermal Insulation Technology

FY 1988
\$ 0

DOE Contact: Stanley M. Wolf, (202) 586-1514

University of Kentucky (ORNL Subcontract 19X-55951V) Contact: Alan Fine,
(606) 257-3713

This task focuses on the possibilities of technology transfer of specialized concepts from aerospace and other government programs to energy conservation applications in the civilian sector. This project will be concluded in FY 1988.

Keywords: Thermal Insulations, Aerospace

35. The Role of Inert Gas Entrapped in Rapidly Solidified Materials FY 1988
\$225,000

DOE Contact: Stanley M. Wolf, (202) 586-1514
INEL (Contract DE-AC07-76IDO1570) Contact: John Flinn, (208) 526-8127
SNLL (Contract DE-AC04-76DP00789) Contact: W. G. Wolfer, (415) 294-2307
University of Wisconsin (INEL Subcontract C87-101251) Contact: T. F. Kelly,
(608) 263-1073

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.

Keywords: Metals, Rapid Solidification, Powder Synthesis

Materials Properties, Characterization, Behavior or Testing

36. Ordered Metallic Alloys for High Temperature Applications FY 1988
\$440,000

DOE Contact: Stanley M. Wolf, (202) 586-1514
ORNL (Contract DE-AC05-84OR21400) Contact: Chain Liu, (615) 574-4459,
NC State (ORNL Subcontract 19X-43368C) Contact: Carl Koch, (919) 737-7340
Columbia (ORNL Subcontract 19X-89664C) Contact: John Tien, (212) 280-5192
University of Tennessee (ORNL Subcontract S7685-S91) Contact: Ben Oliver,
(615) 974-5326
Rensselaer Polytechnic Institute (ORNL Subcontract 19X-55958C) Contact: Norm
Stoloff, (518) 266-6436

Ordered metallic alloys based mainly on nickel and titanium aluminides and nickel and titanium silicides are being developed and assessed for a variety of high temperature applications such as advanced automotive engines, steam turbines, and industrial heat exchangers. At ORNL developmental alloys are prepared using classical metallurgical approaches and important properties are measured. ORNL is also assessing the weldability of the ductile aluminides, their potential for use in steam turbines, and leading efforts to transfer the technologies of the alloys to industry as rapidly as possible. At NC State, alloys based on mechanical alloying approaches are prepared and investigated. Directionally solidified single crystal and polycrystalline alloys are prepared and evaluated at Columbia. Single crystals of TiAl are prepared at the University of Tennessee. The fatigue and creep properties are investigated at Rensselaer.

Keywords: Metals: Non-Ferrous, High Temperature Service, Ordered Intermetallics

37. Measurements of Grain Boundary and Surface Energies of Metals and Ceramics FY 1988
\$25,000

DOE Contact: Stanley M. Wolf, (202) 586-1514
ORNL (Contract DE-AC05-84OR21400) Contact: Ron Bradley, (615) 574-6094

The objective of this effort is to make high quality experimental measurements of the energies of grain boundaries and surfaces of metals and ceramics. Current efforts are aimed at establishing a program for making such measurements in India using US Held Rupee funds (formerly called PL-480 funds).

Keywords: Metals, Alloys, Structural Ceramics, Grain Boundary, Surface, Energies

38. Effects of Laser Machining of Silicon Nitride FY 1988
\$15,000

DOE Contact: Stanley M. Wolf, (202) 586-1514
University of Southern California (ORNL Subcontract 19X-SA665C) Contact: Steve Copley, (213) 743-6223

The objective of this effort is to explain certain phenomena associated with laser machining of silicon nitride. Copley et al. at USC have observed that the fracture strengths of bend bars of silicon nitride (Norton NC 132) whose tensile faces have been laser machined are thirty to forty percent lower than the strengths of bend bars of the same silicon nitride whose tensile faces have been diamond ground but the Weibull moduli of the strength data for the laser machined bend bars are much higher than those of the diamond ground bend bars. The hope is that by elucidating the mechanism(s), ways could be found to achieve both the high strength of the diamond ground specimens and the high Weibull moduli of the laser machined specimens.

Keywords: Structural Ceramics, Machining, Surface

39. Friction and Wear Research and Development FY 1988
\$415,000

DOE Contact: D. Mello, (202) 586-9345
ORNL (Contract No. DE-AC05-84OR21400) Contact: Peter Blau, (615) 574-5377

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 $\text{Al}_2\text{O}_3\text{-SiC}$ 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.

It was observed at ORNL under the ECUT Materials Program that the unlubricated room-temperature sliding of a diamond stylus on the surface of titanium diboride resulted in the formation of an adherent film on the wear path and an unexpectedly low sliding-friction coefficient of 0.02 to 0.04. The composition of the film has been tentatively identified as a form of carbon with an entrained oxide constituent. This area of study has now been transferred to the tribology program under which the generality of the low-friction phenomenon will be systematically tested by sliding a diamond stylus on alternate substrates and by using alternate pin materials sliding on the film formed initially by a sliding diamond. Other sources of carbon for application to the substrates will also be investigated and the structure of the resultant films characterized before and after sliding.

A preliminary, one-year project at ORNL examines issues relevant to the fabrication and use of high-temperature superconducting materials for friction-and-wear applications. Such issues as shear deformation response, microindentation, scratch-testing behavior and retention of superconducting properties under sliding conditions will be addressed.

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.

This new activity at ORNL would investigate the role of particle conglomerates on the frictional behavior of sliding interfaces of high-temperature wear materials. Numerous previous studies have indicated the importance of debris particles in the sliding interface; however, very few have addressed this topic in a systematic series of experiments, particularly with regard to high-temperature wear materials. This basic-research program would synthesize wear-debris compacts using materials for high-temperature tribological service, and test their shear behavior under confined elevated-temperature sliding conditions. This program is important for understanding interfacial particle mechanics of unlubricated sliding friction at elevated temperatures.

Keywords: Ceramics, Friction, Wear

Device or Component Fabrication, Behavior or Testing

40. Development of a Wear Model for Lubricated Sliding of Ceramics FY 1988
\$114,000

DOE Contact: D. Mello, (202) 586-9345

Georgia Institute of Technology (ORNL Subcontract 780219X-15) Contact: Ward Winer,
(404) 894-3270

Will investigate 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 will include rolling-element EHD tests and pin-on-disc tests under lubricated conditions and temperatures up to 150°C. Test results will be applied to the development of an initial wear model based on ceramic-lubricant/additive interactions. This is initially a one-year effort, with continuation contingent on the achievement of sufficiently promising results.

Keywords: Ceramics, Erosion and Wear, Friction, Lubrication

41. Lubrication Research and Development FY 1988
\$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

Research conducted at NIST, sponsored in part by DOE-ECUT, achieved state-of-the-art separation technology by which it was possible to separate a base oil into several components. Subsequent testing of the subfractions revealed a remarkably better performance by the P-6 subfraction of a 600N oil. Further separation of the P-6 subfraction into compound classes was made and the classes were examined by FTIR. Two prototype model compounds, gamma lactone and myristoyl chloride, were suggested by the latter data. Testing of these model compounds showed the same unusually good

coefficient of friction and wear protection. A new batch of P-6 will be produced from other batches of 600N base oil. The new P-6 will be subjected to a wide range of chemical analytical techniques by a subcontractor, such as elemental analysis, high-resolution mass spectrometry, LC-MS or GC-MS, X-ray fluorescence and other techniques. Subsequent performance testing of selected identified compounds will be conducted at NIST. A model will be developed for the mechanisms of friction reduction with these compounds.

In order to elucidate tribochemical reactions in the contact zone, a resolved micro-Raman laser system is being developed at NIST. This technique uses an Nd-YAG laser to provide periodic pulses of monochromatic light which are focused onto the tribocontact by a specially designed optics system and recorded by a gated, intensified, diode-array detector. The detector system is governed by a device-specific controller, and data storage, retrieval and analysis are performed on-line.

Research at NIST has developed basic information on the limitations of liquid lubricants as to volatility and thermal and oxidation stability by means of thermal gravimetric analysis (TGA), differential scanning calorimetry (DSC) and thin-film micro-oxidation methods. The initial studies utilized steel, inert (gold) and Al_2O_3 substrates. The stability of some fluids was affected by the ceramic substrate. However, whether this was due to catalytic effects or an increase in reaction surface area was not resolved and is still being pursued.

The research this year is aimed at expanding the basic information on these interactions to other materials, including SiC, Si_3N_4 , and partially stabilized zirconia. Analysis methods developed earlier in the ECUT program will be coupled with surface-analysis methods to establish the role of impurities and surface properties.

The effectiveness of a lubricant at elevated temperatures is dependent on the base-fluid properties, the additive performance and the substrate. New additive chemistries that can function at the higher operating temperatures for the next generation of advanced heat engines will be investigated. Available additive friction and wear information in the 200-600°C range and higher will be reviewed to identify candidates for screening. The modified, high-temperature, 4-ball and micro-oxidation tests will be used to determine if interactive synergistic or antagonistic effects are occurring at elevated temperatures. Cooperative input from industry will also be sought.

The evaluation of oils by engine manufacturers and oil suppliers involves considerable full-scale-engine testing. The cost of these tests in manpower and energy can exceed \$10K per engine test. A simple laboratory test utilizing the DSC, developed at NIST in cooperation with Cummins Engine, appears to correlate well with oil performance in the engine. The DSC method involves comparison of the primary and secondary reaction peaks. Comparing these data to performance data obtained at

Cummins provides the same relative performance ranking in both tests. Looking at the top-ring-groove fill versus the ratio of high- and low-molecular-weight products also gives good correlation. The method is being pursued independently by Cummins Engine, Detroit Diesel Allison Division of GMC and Caterpillar. The effort underway will expand the technical basis for the test and verify the initial results with a limited number of samples. The oils from Caterpillar were also independently correlated by two laboratories using the microoxidation (MO) test on engine test samples. The DSC has an advantage over the MO test in the amount of time required to process the samples and in the amount and type of information obtained.

Keywords: Metals, Oils, Friction, Wear, Engines

42. Energy-Efficient Gear-Lubrication Model

FY 1988

\$50,000

DOE Contact: D. Mello, (202) 586-9345

Northwestern University (NIST 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 1988 and 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

43. Modeling of Solid Ceramic Joints

FY 1988

\$ 0

(\$175,000 in FY 1986)

DOE Contact: Stanley M. Wolf, (202) 586-1514

The Norton Company (ORNL Subcontract 86X-00208C) Contact: Don Patten, (617) 393-5962

Generalized finite element models are being developed by Norton to predict the stress states existing in and near solid ceramic-ceramic and ceramic-metal joints of simple geometries. Butt-on-butt joints of rectangular cross sections and cylindrical cross sections were modeled first and attempts are now being made to experimentally verify the models before proceeding to develop models for more complex geometries. The purpose of the

effort is to provide guidance concerning compatible ceramic joints and applications. This project will be concluded in FY 1988.

Keywords: Ceramics, Metals, Joining and Welding, Models

44. Electromagnetic Joining of Ceramics - Laboratory Proof of Concept FY 1988
\$25,000

DOE Contact: Stanley M. Wolf, (202) 586-1514

QuesTech, Inc. (formerly DHR, Incorporated) (ORNL Subcontract 86X-00217C), Contact:
Richard Silberglitt, (703) 760-1043

NRL (Interagency Agreement DE-AI05-86OR21655 through ORO) Contact: Dave Lewis,
(202) 767-2131

The objective of this effort is to develop methods for joining ceramic materials to one another by means of microwave-induced heating of the joint interface. A device has been made for heating the joint region while holding the sample pieces under compression and nondestructively determining by acoustic methods when the bonding is complete. All work to date has been on mullite, alumina, and silicon nitride joined to themselves.

Keywords: Structural Ceramics, Joining and Welding, Microwave Joining

45. Development of Tests for Ceramic-Ceramic and Ceramic-Metal Joints FY 1988
\$30,000

DOE Contact: Stanley M. Wolf, (202) 586-1514

ORNL (Contract No. DE-AC05-84OR21400) Contact: Artie Moorhead, (615) 574-5153

Test specimens and procedures are being developed for measurement of the strength and fracture toughness of ceramic-ceramic and ceramic-metal joints. Specimens are tested to provide experimental data that can be compared with the theoretical predictions generated by finite element models of joints.

Keywords: Structural Ceramics, Joining and Welding, Tests

46. Nondestructive Evaluation (NDE) of Ceramic Joints

FY 1988

\$80,000

DOE Contact: Stanley M. Wolf, (202) 586-1514

ORNL (Contract No. DE-AC05-84OR21400) Contact: Bob McClung, (615) 574-4466

This task is exploring the development of nondestructive evaluation (NDE) techniques for ceramic-ceramic and ceramic-metal joints. Various NDE techniques are being tried on joints with known defects in sample attachments and attempts were made to correlate the signals with performance of the attachments. Selected specimens are nondestructively evaluated using radiography and ultrasound prior to destructive testing in order to try to develop a correlation between "indications" found by NDE and the mechanical behavior of the brazements. A high-frequency ultrasound system has been assembled and used to demonstrate resolution commensurate with the thickness scale of the braze components in a typical ceramic joint and with the critical flaw size in the ceramic itself. Elastic moduli of the ceramic materials available have also been determined ultrasonically. This project will be concluded in FY 1988.

Keywords: Structural Ceramics, Joining and Welding, NDE

47. Assessment of Energy Applications of High Temperature Superconductors

FY 1988

\$135,000

DOE Contact: Stanley M. Wolf, (202) 586-1514

ORNL (Contract No. DE-AC05-84OR21400) Contact: Steinar Dale, (615) 574-4829

The purpose of this assessment is to evaluate the potential applications of high-temperature superconductors for end-use technologies and devices with improved energy productivity and utilization. As new concepts and promising technologies are identified, in-depth technical evaluations of selected applications will be made. Economic evaluations will be made on the most promising applications, based on mature technology. The assessment is being performed through the multi-laboratory efforts of Argonne National Laboratory, Lawrence Berkeley Laboratory and Idaho National Engineering Laboratory.

Keywords: Superconductors, Ceramics, Assessment

48. Advanced Laser Fluorescence Measurements of Lubricant Film Behavior in a Diesel Engine

FY 1988
\$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

49. Ring/Cylinder Modeling

FY 1988
\$ 0

DOE Contact: D. Mello, (202) 586-9345

Compu-Tec Engineering (Contract No. DE-AC02-86CE-90236) Contact:
Larry Brombolich, (314) 532-4062

The RING model developed in this project is an analytical code for the prediction of the effect of cylinder-bore distortions on oil consumption, emission, friction and wear in internal-combustion engines for both conventional and advanced designs using, for example, ceramic materials for rings and liners. A testing program was conducted to validate the code. Gaps between rings and an out-of-round ring-gauge fixture were measured, oil-consumption tests on a production eight-cylinder engine were conducted, and friction was measured using a one-cylinder experimental engine. This project is concluding in FY 1988.

Keywords: Lubrication, Wear, Friction, Engines, Modeling

50. Effect of Cycle-to-Cycle Variations on Instantaneous Friction Torque FY 1988
\$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 1988. 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 (CVV) 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.

Instrumentation and Facilities

51. Assessment of X-Ray Methods for Investigations of Ceramic Wear Surfaces

FY 1988
\$ 0

DOE Contact: Stanley M. Wolf, (202) 586-1514

Virginia Polytechnic Institute and State University (ORNL Subcontract 19-B07733C)
Contact: Charles Houska, (703) 961-5652

This is an assessment of the potential of X-ray diffraction and fluorescence techniques for nondestructive investigations of the near-surface region of ceramic wear surfaces. The limitations of standard X-ray diffraction and fluorescence equipment are defined and the possibilities afforded by the Brookhaven Synchrotron Light Source are explored. The ultimate output expected from this work is a program of research to develop and use X-ray techniques for investigating ceramic wear surfaces. This project will be concluded in FY 1988.

Keywords: Ceramics, X-ray Diffraction, Wear

52. Thin Film Thermocouples for Heat Engines

FY 1988

\$ 0

(100,000 in FY 1987)

DOE Contact: Stanley M. Wolf, (202) 586-1514

National Institute of Science and Technology: Gaithersburg (Interagency Agreement OR-21375) Contact: Ken Kreider, (301) 921-3281

The goal of the project is to demonstrate the feasibility of a materials system and fabrication technique for measuring temperature inside the combustion chamber of ceramic insulated engines using thin film thermocouples. The ceramic insulating materials under investigation include partially stabilized zirconia (PSZ) in both monolithic and plasma sprayed forms and alumina. The thermocouple systems have included type E (chromel-constantan); type N (nasil-nicrosil); and platinum-platinum 6 percent rhodium. Scanning electron microscopy and electron microprobe analysis have indicated that the sputtered films were produced with the same composition as the target alloys and continuous, strong, pore-free deposits can be sputtered 1-4 mm thick. A thin-film thermocouple was successfully tested in an engine during FY 1987. This project will be concluded early in FY 1988.

Keywords: Structural Ceramics, Engines

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.

Building Systems Division

The goal of this Division is to provide a scientific and technical basis (including model standards) for reducing the use of energy in residential and commercial buildings by 35 percent by the year 2000 from that used in 1975, while maintaining existing levels of human comfort, health and safety. The Division's primary objectives are to support research that advances the scientific and technical options for increased energy efficiency in buildings, to promote the substitution of abundant fuels for scarce fuels in buildings, and to promulgate standards for increased efficiency of energy use. To accomplish a portion of this, the Building Materials Program seeks to increase the knowledge base concerning the physical, chemical and mechanical properties of building materials that determine their thermal energy performance effectiveness, durability, safety, and health impacts; 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 of materials; and to provide technical assistance, advice and data to organizations that develop consensus standards for the performance characteristics of materials. The DOE contact is Peter Scofield, (202) 586-9193.

Materials Properties, Behavior, Characterization or Testing

53. Unguarded Thin Heater Tester

FY 1988
\$200,000

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

54. Heat Flux Transducer Calibration Design

FY 1988
\$45,000

DOE Contact: Peter Scofield, (202) 586-9193
ORNL Contact: David McElroy, (615) 574-5976

Laboratory study of calibration of imbedded heat flux transducers to allow complete design and construction of a prototype calibration apparatus for heat flux transducers, conduct preliminary tests to establish the accuracy and repeatability of experimental data, and develop and verify test procedures for the apparatus. This task is being conducted in response to a need identified by the BTESM roof research key activity and to reduce the magnitude of data errors reported by materials researchers throughout the industry.

Keywords: Calibration, Heat Flux Transducers, Roof Tester Panels

55. Variable R/Switchable Surface Analysis

FY 1988
\$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

56. Moisture Specimen Test Procedures FY 1988
\$25,000

DOE Contact: Peter Scofield, (202) 586-9193

NJIT Contact: Erv Bales, (201) 596-3010

Moisture content and transport in building materials has a major impact on measured thermal properties. A procedure to measure moisture and heat transfer does not exist. This project will use the thin heater and moisture measurement techniques to define a procedure for measuring and analyzing moisture interactions.

Keywords: Moisture, Test Procedures

57. Recommended R-Levels - ZIP Program FY 1988
\$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

58. CFC Foam Characterization

FY 1988
\$45,000

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: Insulation Sheathing, Walls, Roofs, Economic Analysis

59. Foam Insulation Research

FY 1988
\$108,000

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 of insulation foamed with low thermal conductivity refrigerants can be reduced by cutting the radiation component of the effective conductivity. The transparency of the cell walls to infrared radiation and the transmission of thin layers of insulation is being measured to evaluate the extinction coefficient versus wavelength. A multi-layer heat transfer model is used together with the measured extinction coefficient to calculate the overall thermal conductivity. The project objective is to develop a combined mass and heat transfer model which will predict that material's overall thermal resistance to aging as well as to develop new concepts which reduce overall conductivity. This work is in follow-up to work begun by the ECUT program.

Keywords: Building Insulation, Heat Transfer, Diffusion

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

60. Composite Cathode Material Development FY 1988
\$218,000

DOE Contact: M. J. McMonigle, (202) 586-2082
Great Lakes Contact: L. A. Joo, (615) 543-3111

TiB₂-Graphite samples have been tested in commercial cells to determine optimum composition and factors that affect long term life. Configuration and voltage reduction tests have been performed in a 6000 ampere test cell.

Keywords: Composites, Cathode

61. Cerox Inert Anode Material FY 1988
\$150,000

DOE Contact: M. J. McMonigle, (202) 586-2082
EL TECH Contact: Tom Gilligan, (216) 357-4066

The addition of CeO₂ 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

62. Corrosion Resistant Amorphous Metallic Films

FY 1988

\$246,000

DOE Contact: William Sonnett, (202) 586-2389

JPL Contact: Edward Cuddihy, (818) 354-3188

Final report received—to be published after patent clearance.

Keywords: Coatings and Films, Sputtering, Corrosion, Metallic Glasses

63. Investigation of Material for Inert Electrodes in Aluminum Electrodeposition Cells

FY 1988

\$ 0

DOE Contact: M. J. McMonigle, (202) 586-2082

MIT Contact: J. S. Haggarty, (617) 253-3300

Final report published September 1987 (DOE/ID/12380-18).

Keywords: Ceramics, Material Science, Aluminum, Cryolite

Materials Properties, Behavior, Characterization or Testing

64. Diagnostic Sources of Current Inefficiency in Industrial Molten Salt Electrolytic Cells by Raman Spectroscopy

FY 1988

\$ 0

DOE Contact: M. J. McMonigle, (202) 586-2082

MIT Contact: D. R. Sadoway, (617) 253-3300

Final report published July 1988 (DOE/CE/40545-25).

Keywords: Molten Salts, Cryolite, Aluminum Chloride, Magnesium Chloride

65. Expand and Control Inert Electrode Cell Operating Conditions

FY 1988

\$800,000

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. Failure mechanisms for TiB₂ based materials have been investigated. TiB₂ graphite was determined to be the most commercially viable material based on chemical stability and cost.

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

66. Microwave Sintering of β -Alumina for Use in the Sodium Heat Engine FY 1988
\$ 0

DOE Contact: J. Eustis, (202) 586-2098

ORNL Contact: W. Snyder, (615) 574-2178

This project is developing the alkali 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

67. Advanced Heat Exchanger Material Technology Development FY 1988
\$825,000

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, assessing commercially available surface coatings for ability to protect ceramic surfaces from corrosive elements, and developing advanced wet forming techniques for monolithic ceramic components.

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

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

FY 1988
\$50,000

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

69. National Laboratory Support to Assessment of Strength Limiting Flaws in Ceramic Heat Exchanger Components

FY 1988
\$65,000

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

Device or Component Fabrication, Behavior or Testing

70. Ceramic Composite Heat Exchanger for the Chemical Industry

FY 1988
\$ 0

DOE Contact: S. Richlen, (202) 586-2078
Babcock & Wilcox Contact: W. Parks, (804) 522-5260

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 design is being revised and additional material tests are being planned.

Keywords: Ceramic Composites, Structure

71. HiPHES System Design Study for Energy Production from Hazardous Wastes FY 1988
\$302,000

DOE Contact: S. Richlen, (202) 586-2078
Solar Turbines Contact: M. Ward, (619) 544-2553

This project is an initial phase of a three-phase effort to develop high pressure heat exchange systems for recovery of energy from hazardous wastes. Preliminary designs of advanced heat exchange processes based on the use of ceramic composites will be developed in this initial phase.

Keywords: Ceramic Composites, Heat Exchangers

72. HiPHES System Design Study for Energy Production from Hazardous Wastes FY 1988
\$174,000

DOE Contact: S. Richlen, (202) 586-2078
Babcock & Wilcox Contact: W. Parks, (804) 522-5260

This project is an initial phase of a three-phase effort to develop high pressure heat exchange systems for recovery of energy from hazardous wastes. Preliminary designs of advanced heat exchange processes based on the use of ceramic composites will be developed in this initial phase.

Keywords: Ceramic Composites, Heat Exchangers

73. HiPHES System Design Study for an Advanced Reformer FY 1988
\$195,000

DOE Contact: S. Richlen, (202) 586-2078
Stone & Webster Engineering Corp. Contact: J. Williams, (617) 589-7197

This project is an initial phase of a three-phase effort to develop high pressure heat exchange systems for an advanced convective reformer. Preliminary designs of advanced heat exchange processes based on the use of ceramic composites will be developed in this initial phase.

Keywords: Ceramic Composites, Heat Exchangers

74. Ceramic Components for Stationary Gas Turbines in Cogeneration Service

FY 1988
\$175,000

DOE Contact: J. Eustis, (202) 586-2098

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 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 of the following Office of Transportation Systems material projects.

Materials Preparation, Synthesis, Deposition, Growth or Forming

75. Silicon Carbide Powder Synthesis

FY 1988
\$80,000

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 is 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, which has also been completed, incorporated the following elements:

- Scale-up of the process 5-10X over the laboratory scale process.
- Perform confirmatory experiments and 3-5 experimental runs to confirm laboratory scale results and to fine-tune operating conditions.

Keywords: Silicon Carbide, Powder Synthesis, Sintering, Structural Ceramics

76. Turbomilling of SiC

FY 1988
\$130,000

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 on 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, Structural Ceramics, Whiskers, Turbomilling

77. Sintered Silicon Nitride

FY 1988
\$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 $\text{Si}_3\text{N}_4\text{-Y}_2\text{O}_3\text{-SiO}_2$ 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.

Sintered silicon nitride bodies containing yttria/silica and small additions of Mo_2C have been sintered to full density using a two-step sintering approach. 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, Structural Ceramics

78. Si_3N_4 Powder Synthesis

FY 1988
\$305,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: E. L. Long, Jr., (615) 574-5172
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 has been 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.

For the next phase of the project, the current goal is to test for unique properties of the ceramics sintered from low carbon powders before committing to a pilot plant of the 110 L scale previously designed. In view of powder quantities needed to allow tests of the ceramics, the major task is 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, Powder Synthesis, Structural Ceramics

79. Processing of Monolithics

FY 1988
\$305,000

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, is the process chosen for initial consideration.

Experimental work has been concluded on the base formulation to be used in the initial production for this program.

Keywords: Engines, NDE, Structural Ceramics, Monolithics, Processing, Weibull

80. Dispersion Toughened Si₃N₄FY 1988
\$371,000

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

The objective of this effort is to develop the technology base for fabricating a ceramic composite consisting of silicon carbide whiskers dispersed in a dense silicon nitride matrix. This is to be accomplished by slip casting as the green shape forming method, and sintering or sinter/HIP as the densification method. A goal of the program is a 2-fold increase in fracture toughness over the unreinforced silicon nitride matrix without a degradation of other properties.

SiC whiskers from different manufacturers have been evaluated, indicating that composite properties vary with whisker source as well as loading. Correlations between whisker properties, processing behavior, and mechanical properties have been identified. Techniques for evaluating whisker/matrix interfaces and whisker degradation have been established. Slips with desired rheology with up to 40% SiC whisker content have been reproducibly made. Thick section castings have been consistently processed through the drying stage without cracking or deformation.

The objective of Phase II of this program is to maximize the toughness in a high strength, high temperature SiC whisker/Si₃N₄ matrix materials 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. Selection of a SiC whisker as the reinforcement in GN-10 Si₃N₄ matrix is ongoing, and will be completed prior to the start of the process optimization and property evaluation studies.

Keywords: Silicon Carbide, Composites, Silicon Nitride, Whiskers, Structural Ceramics, Sintering, Hot Isostatic Pressing

81. Dispersion Toughened Si₃N₄FY 1988
\$550,000

DOE Contact: Robert B. Schulz, (202) 586-8051

ORNL Contact: M. A. Janney, (615) 574-4281

GTE Contact: S. T. Buljan, (617) 890-8460

Phase I had three primary objectives: (1) to develop a whisker- and particulate-reinforced silicon nitride matrix composite based on a commercial GTE material utilizing SiC and TiC particles or whiskers dispersed in the matrix, (2) to characterize the material, and (3) to develop a low-cost, near-net-shape process (injection molding) for fabricating CATE turbine blades.

Composites with 40-70 percent higher fracture toughness and 25 percent higher room temperature fracture strength over that of the base silicon nitride "monolith" were prepared using SiC whisker dispersoid. Both fracture toughness and strength improvements persisted over a wide range of temperatures. These composites also exhibited excellent oxidation resistance and improved resistance to slow crack growth and creep at elevated temperatures. In addition, a process for fabrication of complex composite ceramic parts was developed and demonstrated.

The objective of the current Phase II effort is to study the effect of sintering aids on the microstructure and properties of Si_3N_4 -SiC(W) composites and utilize the results obtained to design and synthesize an advanced composite of improved properties. It is also an objective of this effort to refine forming and consolidation processes and develop technology for prototype part fabrication.

The room temperature data base for the study of the effect of sintering aid species on the microstructure/mechanical properties of Si_3N_4 -based ceramics has been completed.

Keywords: Silicon Nitride, Structural Ceramics, Whiskers, Fracture, Creep, Molding, Composites, Dispersion Toughened, Sintering

82. Composite Development

FY 1988
\$560,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. Ray Johnson, (615) 576-6832
Norton Contact: C. A. Ebel, (508) 393-5950

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 effect fracture toughness appear to be composition related. CVD coatings have been applied to SiC whiskers and evaluation of coatings is continuing.

For the second phase of this program 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 $>10 \text{ MPa(m)}^{1/2}$ and capable of operating up to 1400°C .

Keywords: Composites, Whiskers, Silicon Carbide, Silicon Nitride, Glass Ceramics, Hot Isostatic Pressing, Chemical Vapor Deposition, Sintering

83. Advanced Composites

FY 1988
\$149,000

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($\text{Y}_3\text{Al}_5\text{O}_{12}$) and SiAlON-Cordierite($\text{Mg}_2\text{Al}_4\text{Si}_5\text{O}_{18}$) 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, Whiskers, Silicon Carbide, Sintering, SiAlON

84. Dispersion Toughened Oxide Composites

FY 1988
\$325,000

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 system will be on pressureless sintering and control of the whisker-matrix interface properties.

Keywords: Alumina, Mullite, Composites, Whiskers, Silicon Carbide, SiAlON

85. Transformation Toughened Ceramics Processing

FY 1988

\$346,000

DOE Contact: Robert B. Schulz, (202) 586-8051

ORNL Contact: D. Ray Johnson, (615) 576-6832

Norton Contact: Giulio A. Rossi, (508) 393-6600

The objective of Phase I was the production of improved zirconia toughened ceramics (ZTC) 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 ones.

The objective of Phase IIA of this program is to 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 toughened Al_2O_3), studied in Phase I. The main effort for the Y-TZP materials is 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, Transformation Toughened Zirconia Oxide, Powder, Sintering, Alumina

86. Development of Toughened Ceramics

FY 1988

\$150,000

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 the 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.

Keywords: Composites, Sintering, Alumina, Zirconia, Transformation Toughened

87. Injection Molded Composites

FY 1988
\$ 0

DOE Contact: Robert B. Schulz, (202) 586-8051

ORNL Contact: D. Ray Johnson, (615) 576-6832

ORNL Contact: M. A. Janney, (615) 574-4281

The goals of this activity were: (1) to evaluate the ability of advanced ceramic-ceramic composites to be injection molded and processed using standard wax- and/or polymer-based binder systems, and (2) to develop advanced complex-shape-forming technologies to eliminate some of the problems (long binder removal times, cracking, low green strength, etc.) associated with wax- and polymer-based binder systems.

A new complex-shape-forming technology was developed.

Keywords: Composites, Molding

88. Low Expansion Ceramics

FY 1988
\$153,000

DOE Contact: Robert B. Schulz, (202) 586-8051

ORNL Contact: D. Ray Johnson, (615) 576-6832

Virginia Polytechnic 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 β -eucryptite, silica, mullite, and zircon. At the present time, encouraging results have been obtained for the development of improved thermal shock resistant β -eucryptite compositions and zircon (NZP) compositions.

Keywords: Structural Ceramics, Aluminum Phosphate, Silica, Mullite, Zirconia, Ultra-low Expansion, β -eucryptite

89. Active Metal Brazing PSZ-Iron

FY 1988

\$210,000

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. The emphasis of this activity during FY 1988 was to investigate (1) the effects of testing temperature and zirconia surface finish on the flexure strength of zirconia-to-zirconia joints, (2) correlate zirconia braze joint microstructures with strength data to identify any factors that may limit joint strength, (3) flexure testing of silicon nitride braze joints, and (4) to develop a method of calibrating the indentation fracture technique to determine the accuracy of residual stress measurements in ceramic-to-metal joints.

Keywords: Metals, Structural Ceramics, Joining and Welding, Brazing, Cast Iron, Zirconia, Alumina

90. TiB₂ Whiskers

FY 1988

\$131,000

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 TiB₂ whiskers, TiB₂-coated alpha-SiC whiskers, consolidate SiC matrix composites, and test in air above 1200°C.

Keywords: Titanium Diboride, Whiskers

91. Advanced Processing

FY 1988

\$1,000,000

DOE Contact: Robert B. Schulz, (202) 586-8051

ORNL Contact: R. L. Beatty, (615) 574-4536

Norton Contact: S. D. Hartline, (508) 393-5828

The purpose of this task is the development of new and/or improved ceramic processing tasks and in-process inspections that will eliminate many of the sources of strength-limiting flaws in structural ceramics, e.g., organic material in the powder, powder

agglomerates, foreign inclusions, large grains. The expected result is a high-temperature ceramic with the strength and toughness required of an AGT rotor, and with a Weibull modulus of approximately 20.

Keywords: Engines, Processing, NDE, Structural Ceramics, Weibull

92. Advanced Processing

FY 1988
\$500,000

DOE Contact: Robert B. Schulz, (202) 586-8051

ORNL Contact: R. L. Beatty, (615) 574-4536

GTE Contact: Les Bowen, (617) 466-2536

The purpose of this task is the development of new and/or improved ceramic processing tasks and in-process inspections that will eliminate many of the sources of strength-limiting flaws in structural ceramics, e.g., organic material in the powder, powder agglomerates, foreign inclusions, large grains. The expected result is a high-temperature ceramic with the strength and toughness required of an AGT rotor, and with a Weibull modulus of approximately 20.

Keywords: Engines, Processing, NDE, Structural Ceramics, Weibull

Materials Properties, Behavior, Characterization or Testing

93. Ceramic Component Design Technology

FY 1988
\$100,000

DOE Contact: Saunders B. Kramer, (202) 586-8000

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 with new subroutines continues.

Keywords: Design Methodology, Engines

94. Microstructural Modeling of Cracks

FY 1988
\$69,000

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 investigate and develop models for fracture of cracks with realistic geometry under arbitrary stress states. One important feature of crack geometry missing from existing models is the roughness of the crack face.

For brittle fracture of such cracks, interference between surface irregularities (bumps) on opposing crack faces may significantly influence fracture initiation. A sequence of elasticity problems leading to the rough-faced crack in an infinite body under arbitrary loads will be defined and solved. Application of fracture criteria to the stress field around the crack will lead to predictions of fracture-initiating loads, which will then be compared with those cited in the literature for cracks of simpler geometry.

Keywords: Predictive Behavior Modeling, Structural Ceramics

95. Adherence of Coatings

FY 1988
\$20,000

DOE Contact: Robert B. Schulz, (202) 586-8051

ORNL Contact: C. J. McHargue, (615) 574-4344

University of Tennessee Contact: J. Sproul, (615) 974-5327

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

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

96. Dynamic Interfaces

FY 1988
\$182,000

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

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.

The need for lubrication at the ring/cylinder interface has been established due to the high friction coefficients and wear rates measured during dry sliding of a variety of monolithic ceramics and ceramic coatings. The maximum operating temperature with ceramics was found to be limited by the availability of suitable lubricants.

Current efforts for a second phase are addressing the performance of advanced toughened monolithic ceramics, thermal-spray coatings, surface modifications, and high temperature lubricants.

Keywords: Dynamic Interfaces, Wear, Structural Ceramics, Coatings and Films, Predictive Behavior Modeling, Monolithics, Adiabatic Diesels

97. Advanced Statistics Calculations

FY 1988
\$190,000

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;
- 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 and Technique Development

98. Physical Properties

FY 1988
\$75,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. Ray Johnson, (615) 576-6832
ORNL Contact: D. L. McElroy, (615) 574-5976

The objective is an improved understanding of the factors which determine the thermal conductiveness of toughened structural ceramics at high temperatures. 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.

Keywords: Structural Ceramics, Thermal Conductivity

99. Translucence Effects

FY 1988

\$20,000

DOE Contact: Robert B. Schulz, (202) 586-8051

ORNL Contact: D. L. McElroy, (615) 574-5976

Ricardo-ITI Contact: Thomas Morel, (312) 789-0003

The purpose of this task was to conduct analytical studies using detailed computer codes which describe a realistic engine thermal environment including gas-to-wall heat fluxes, as well as the combined radiation/conduction heat transfer through a thermal barrier layer. A detailed parametric study was carried out in which the following parameters were varied, and their effect on heat barrier effectiveness studied: (1) material absorption coefficient, (2) material conductivity, (3) material thickness, and (4) engine operating conditions. The results showed that translucence can have significant detrimental effects on heat barrier effectiveness under realistic diesel engine conditions.

Keywords: Structural Ceramics, Diesel Engines, Thermal Conductivity

100. Project Data Base

FY 1988

\$100,000

DOE Contact: Robert B. Schulz, (202) 586-8051

ORNL Contact: D. Ray Johnson, (615) 576-6832

ORNL Contact: B. L. P. Booker, (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. Although MOR-type data are the only test data included in the first hardcopy summary report, the system has been designed to provide maximum flexibility to allow the addition of other data as the data base grows.

Keywords: Database, Mechanical Properties, Structural Ceramics

101. Characterization of Transformation-Toughened Ceramics

FY 1988
\$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 task has several objectives. A main objective was 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 was initiated.

Results showed that MgO-PSZ is susceptible to overaging at 1000°C, with a dramatic decrease in the MOR and fracture toughness in 500 hours. Although the yttria-doped zirconias were also susceptible to overaging, the decrease in mechanical properties was not as dramatic as for the MgO-doped TZPs. Other studies at low temperatures indicated that within the 200-400°C temperature range, the TZP material became "destabilized," resulting in a large loss of mechanical properties and even catastrophic failure of the test sample.

Due to the inherent problems of TZPs at low and high temperatures, evaluation and characterization of these materials is 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

102. Fracture Behavior of Toughened Ceramics

FY 1988
\$210,000

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

Toughening and fatigue properties of transformation-toughened and whisker-reinforced materials are under examination. Emphasis is on understanding the effect of microstructure upon processes responsible for time-dependent variations in toughness and high-temperature strength. In addition, fundamental insight into the slow crack growth behavior associated with these materials is being obtained. Experimental results have been obtained on the high temperature fracture strength behavior in air of the alumina—20 vol % SiC whisker reinforced composites.

Keywords: Toughened Ceramics, Whiskers, Fracture, Flexure Test, Matrix, Zirconia, Alumina

103. Cyclic Fatigue of Toughened Ceramics

FY 1988
\$210,000

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 and demonstrate the capability of performing uniaxial tension-tension dynamic fatigue testing of structural ceramics at elevated temperature. A new, self-aligning grip system for tensile testing of ceramics was developed and patented. The technology has been transferred to private enterprise.

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

104. Rotor Materials Data Base

FY 1988

\$100,000

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 will be 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

105. Ceramic Corrosion Evaluation AGT

FY 1988

\$100,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. Ray Johnson, (615) 576-6832
NASA Contact: Carl A. Stearns, (216) 433-5504

Silicon carbide and silicon nitride specimens will be tested in a combustion rig simulating engine conditions. The combustion flow will be seeded with various impurities.

Keywords: Ceramics, Silicon Nitride, Silicon Carbide

106. Ceramic Durability Evaluation AGT

FY 1988
\$75,000

DOE Contact: Saunders B. Kramer, (202) 586-8012

NASA Contact: Sunil Dutta, (216) 433-3282

Garrett Contact: L. Lindberg, (602) 231-4001

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 will be evaluated.

Keywords: Time-Dependent Behavior, Silicon Carbide, Silicon Nitride, Glass Ceramics, Gas-Turbine Engine, High Temperatures

107. Environmental Effects in Toughened Ceramics

FY 1988
\$47,000

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 determine the environmental degradation processes operative in PSZ- and DTA-toughened ceramics using primarily the dynamic fatigue measurement. Flexural strength has been 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

108. High Temperature Tensile Testing

FY 1988
\$200,000

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. GTE SNW 1000 Si₃N₄ tensile samples are being tested using the new ORNL self-aligning grip system at three stressing rates. Fractography has indicated that fracture was transgranular at room temperature and the fracture origins were normally porosities and occasionally inclusions.

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

109. Standard Tensile Test Development FY 1988
\$120,000

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) 975-5772

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

Keywords: Creep, Structural Ceramics, Tensile Testing

110. Fracture Toughness Determination of Thin Coatings FY 1988
\$55,000

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.

Keywords: Fracture, Structural Ceramics

111. Non-Destructive Evaluation FY 1988
\$160,000

DOE Contact: Robert B. Schulz, (202) 586-8051

ORNL Contact: D. Ray Johnson, (615) 576-6832

ORNL Contact: W. A. Simpson, (615) 574-4421

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, Structural Ceramics, Ultrasonics

112. Ceramic Component NDE Technology

FY 1988
\$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 compounds. The NDE methods under study are X-ray, radiography, ultrasonics, scanning laser acoustic microscopy, thermo-acoustic microscopy.

Keywords: Ceramics, NDE, X-ray, Ultrasonics

113. Computed Tomography

FY 1988
\$90,000

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.

Keywords: Computed Tomography, NDE, Silicon Carbide, Silicon Nitride, Structural Ceramics, Green State

114. Nuclear Magnetic Resonance Imaging

FY 1988
\$160,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. Ray Johnson, (615) 576-6832
Argonne National Lab Contact: W. A. Ellingson, (312) 972-6068

This project will establish the feasibility of using NMR imaging systems to map organic B/P distributions in injection-molded green ceramics. It will also 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. In addition, the project will determine the sensitivity of NMR imaging methods to injection molding process variables as manifested in distribution of the organic.

Keywords: Nuclear Magnetic Resonance, Binder, Green State, Injection Molding, Reliability

115. NDE of Advanced Ceramics by Synchrotron Computer Tomograph FY 1988
\$100,000

DOE Contact: Robert B. Schulz, (202) 586-8051

ORNL Contact: D. Ray Johnson, (615) 576-6862

Radiation Science Contact: Allen S. Krieger, (508) 494-0335

Synchrotron radiation will be used in this project 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 has been 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, NDE, Structural Ceramics

116. Life Prediction FY 1988
\$1,000,000

DOE Contact: Robert B. Schulz, (202) 586-8051

ORNL Contact: C. R. Brinkman, (615) 574-5106

Allison Gas Turbine Division Contact: D. L. Vacarri, (317) 230-4313

The objective of this effort is to demonstrate that the useful life of ceramics used in either gas turbine or low heat-rejection diesel engines can be adequately predicted.

Keywords: Life Prediction, Structural Ceramics

117. Life Prediction FY 1988
\$500,000

DOE Contact: Robert B. Schulz, (202) 586-8051

ORNL Contact: C. R. Brinkman, (615) 574-5106

Garrett Auxiliary Power Division Contact: J. R. Smyth, (602) 220-3360

The objective of this effort is to demonstrate that the useful life of ceramics used in either gas turbine or low heat-rejection diesel engines can be adequately predicted.

Keywords: Life Prediction, Structural Ceramics

118. Spectroscopic Characterization

FY 1988
\$70,000

DOE Contact: Robert B. Schulz, (202) 586-8051

ORNL Contact: M. A. Janney, (615) 574-4281

University of Wisconsin Contact: M. A. Anderson, (608) 262-2470

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.

Keywords: Powder

119. Surface Adsorption

FY 1988
\$70,000

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.

Keywords: Powder

120. Thermodynamics of Surfaces

FY 1988
\$70,000

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.

Keywords: Powder

Technology Transfer and Management Coordination

121. Standard Reference Materials FY 1988
\$270,000

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.

Keywords: IEA, NIST, Reference Material, Powder Characterization, Structural Ceramics

122. Technology Transfer Assessment, Support Contracts, IEA FY 1988
\$87,000

DOE Contact: Robert B. Schulz, (202) 586-8051

ORNL Contact: D. Ray Johnson, (615) 576-6832

The purpose of this task is to facilitate the transfer of technology to private industry.

Keywords: Instrumentation and Technique Development, Technology Transfer, Assessment, Research, Subcontractors, Exhibits, Meetings

123. Management And Coordination FY 1988
\$865,000

DOE Contact: Robert B. Schulz, (202) 586-8051

ORNL Contact: D. Ray Johnson, (615) 576-6832

This effort assesses the ceramic technology needs for advanced automotive heat engines, formulates technical plans to meet these needs, and prioritizes and implements a long-range research and development program.

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

Device or Component Fabrication or Testing

124. Metal-Ceramic Joints AGT

FY 1988
\$ 0

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. Ray Johnson, (615) 576-6832
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 maximum temperature of interest for application of silicon carbide to metal and silicon nitride to metal-containing joints is 950°C. 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 and Welding, Metals, Structural Ceramics, AGT, Metal-Ceramic

125. Metal-Ceramic Joints AGT

FY 1988
\$ 0

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. Ray Johnson, (615) 576-6832
Battelle Contact: A. R. Rosenfield, (614) 424-4353

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 and Welding, Metals, Structural Ceramics, Metal-Ceramic

126. Ceramic-Ceramic Joints AGT**FY 1988
\$ 0**

DOE Contact: Robert B. Schulz, (202) 586-8051

ORNL Contact: D. Ray Johnson, (615) 576-6832

Norton Contact: Donald O. Patton, Jr., (508) 393-5963

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 and Welding, Structural Ceramics, Ceramic-Ceramic

127. Advanced Coating Technology AGT**FY 1988
\$40,000**

DOE Contact: Robert B. Schulz, (202) 586-8051

ORNL Contact: D. Ray Johnson, (615) 576-6832

GTE Contacts: V. K. Sarin, (617) 890-8460 and 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 is scheduled to begin in FY 1989.

Keywords: Coatings and Films, Chemical Vapor Deposition, Engines, Structural Ceramics, Silicon Carbide, Silicon Nitride, Adherence, Contact Stress

128. Advanced Coating Technology

FY 1988
\$150,000

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, Structural Ceramics, Corrosion

129. Wear Resistant Coatings

FY 1988
\$248,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. P. Stinton, (615) 574-4556
Caterpillar Contact: M. B. Beardsley, (309) 578-8514 and 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.

Keywords: Chemical Vapor Deposition, Coatings and Films, Engines, Structural Ceramics

130. Wear Resistant Coatings

FY 1988
\$244,000

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 were selected for further evaluation.

Keywords: Coatings and Films, Engines, Metals, Structural Ceramics, Wear

131. Thick Thermal Barrier Coatings FY 1988
\$246,000

DOE Contact: John 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 this 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

132. Thick Thermal Barrier Coatings FY 1988
\$145,000

DOE Contact: John Fairbanks, (202) 586-8066
NASA Contact: M. Murray Bailey, (216) 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

133. Sliding Seal Materials for Diesel FY 1988
\$75,000

DOE Contact: John Fairbanks, (202) 586-8066
NASA Contact: Richard Barrows, (216) 433-3388
Southwest Research Institute Contact: Shannon Vinyard, (512) 684-5111

The project is being 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 will be fabricated, tested, and evaluated in a test bed single cylinder engine with a ceramic cylinder liner.

Keywords: Carbides, Tribology, Ion-Implantation, Diesel Engine

134. High Temperature Solid Lubricant Coatings

FY 1988
\$50,000

DOE Contact: John W. Fairbanks, (202) 586-8066

NASA Contact: Hal Sliney, (216) 433-6055

Case Western Reserve University Contact: Joseph Prah, (216) 368-2000

High temperature wear resistant coating systems for use in the range of 1000°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

135. Advanced Turbine Technology Applications Project (ATTAP, AGT-100)

FY 1988
\$4,500,000

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 characterizations, process development, and component design and test.

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

136. Advanced Turbine Technology Applications Project (ATTAP, AGT-101)

FY 1988
\$4,500,000

DOE Contact: Saunders B. Kramer, (202) 586-8012

NASA Contact: Thomas N. Strom, (216) 433-3408

Garrett Turbine Engine Company 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.

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 knowledge and scientific advances into new options for the use of renewable energy, for electric energy delivery and control systems and for energy conversions. The Office manages programs in energy storage and electric energy systems 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 oil and gas fuels by nuclear and renewable energy sources, and will increase the reliability and efficiency of the energy economy. The goal is to provide reliable, inexpensive devices to correct the timing and location mismatch between energy sources and energy users that is presently corrected by the energy storage inherent in fossil fuels. The research is divided into three subprograms: Electrochemical Energy Storage, Battery Development, and Thermal Energy Storage.

Materials Preparation, Synthesis, Deposition, Growth or Forming

137. Incorporation of Phase Change Materials Into Building Construction Components

FY 1988
\$130,000

DOE Contact: E. Reimers, (202) 586-4563

ORNL Contact: J. Tomlinson, (615) 574-0768

University of Dayton Research Institute Contact: I. Salyer, (513) 229-2113

Efforts are underway to develop a gypsum wallboard system that contains a phase change material (PCM) for enhanced thermal storage capacity in the interior walls of lightweight building construction. Crystalline alkyl hydrocarbon (paraffins) have been identified as promising for the application. Suitably refined so that a single chain length species is present, these materials melt congruently and possess a low vapor pressure at room temperatures. Although several techniques for incorporating these materials into plasterboard have been studied, the simple process of suffusing the PCM directly into the interstices of the gypsum is being examined in more detail in full-size panels to determine the stability of the system. Efforts are also underway to address safety issues with the PCM-wallboard.

Keywords: Low-Temperature Service, Organics

138. Determination of the Effects of Dopants on Solid-State Phase Change Materials

FY 1988

\$40,000

DOE Contact: E. Reimers, (202) 586-4563

ORNL Contact: J. Tomlinson, (615) 574-0768

University of Nevada-Reno Contact: D. Chandra, (702) 784-4960

Techniques have been identified whereby the solid-solid transformation temperature of organic materials can be adjusted with only proportionate losses in the enthalpy of transformation. These techniques involve the use of interstitial and substitutional dopants that strain the crystal lattice of the host material without breaking hydrogen bonds. Successful development of this concept would facilitate the use of latent heat thermal storage in materials that remain solid—an advantage in many thermal energy storage applications where cost-effective containment of the storage material is a key issue. Differential scanning calorimetry, X-ray diffraction and thermal analyses are being performed on pentaglycerine doped with a range of additives to determine the manner in which dopants affect the crystal lattice so that optimal dopants can be identified.

Keywords: Organics, Low-Temperature Service, Consolidation of Powder, Crystal Growth

139. Corrosion-Resistant Coatings for High-Temperature, High-Sulfur Activity Applications

FY 1988

\$129,000

DOE Contact: A. Landgrebe, (202) 586-1483

Illinois Institute of Technology Contact: J. R. Selman, (312) 567-3037

The research project consists of three tasks: (1) optimize deposition of Mo and Mo₂C coatings; (2) chemical vapor deposition of Mo and TiN layers; and (3) corrosion behavior of Mo, Mo₂C, and TiN coatings. The optimize deposition of Mo and Mo₂C coatings task involved the investigation of electrochemical behavior of a FLINAK melt at a Mo electrode in a water-contaminated atmosphere. The chemical vapor deposition of Mo and TiN layers task included the purchase of plasma-enhanced equipment. The last task involved testing the corrosion behavior of Mo, Mo₂C coatings on steel/nickel inter-layer substrate in Na₂S₄ melt at 320°C.

Keywords: Chemical Vapor Deposition, Corrosion, Coatings and Films

140. Ceramics ResearchFY 1988
\$1,000,000

DOE Contact: A. Landgrebe, (202) 586-1483

LBL Contact: E. Cairns, (415) 486-5028

SNL Contact: R. Clark, (505) 844-6332

Work is being done on sodium/sulfur and lithium/iron sulfide batteries designed to operate at temperatures of several hundred degrees C. Materials for current collectors, separators, seals, and coatings to prevent corrosion are of concern. New superconducting ionic materials are being developed. Of special importance is the development of processing techniques to toughen beta alumina electrolytes and to make parts with more reproducible properties for use in sodium/sulfur batteries. Research is being conducted on the principles of ionic conduction in ceramics and the causes of electrolyte failure.

Keywords: Alloy Development, Alternate Materials, Corrosion, Joining and Welding, Fast Ion Conductors and Solid Electrolytes, Batteries

141. Metals and AlloysFY 1988
\$200,000

DOE Contact: A. Landgrebe, (202) 586-1483

LBL Contact: E. Cairns, (415) 486-5028

Aluminum alloys are being prepared and characterized for use as negative electrodes in aluminum/air batteries. Alloys of platinum are being studied for use as electrocatalysts in fuel cells and aluminum/air batteries.

Keywords: Alloy Development, Alternate Materials, Batteries

142. Organometallic CompoundsFY 1988
\$500,000

DOE Contact: A. Landgrebe, (202) 586-1483

Eltech Systems Corporation Contact: R. W. Fenn, (216) 357-4075

Macrocyclic compounds of transition metals are being investigated for use as electrocatalysts for air electrodes in fuel cells, and in aluminum/air and iron/air batteries.

Keywords: Alternate Materials, Fuel, Batteries

143. Polymers

FY 1988

\$100,000

DOE Contact: A. Landgrebe, (202) 586-1483

LBL Contact: E. Cairns, (415) 486-5028

Electronically and ionically conducting polymers are being synthesized, prepared as films, and characterized for use as electrodes, separators, and electrolytes in storage batteries and fuel cells.

Keywords: Polymers, Fast Ion Conductors and Solid Electrolytes, Batteries

144. Composite High Temperature Thermal Storage Media

FY 1988

\$140,000

DOE Contact: Eberhart Reimers, (202) 586-4563

ORNL Contact: John Tomlinson, (615) 574-0768

IGT Contact: Randy Petri, (312) 567-3985

The objective of this project is to develop advanced high temperature thermal storage media for industrial applications. The media consists of fired MgO ceramics containing metallic salt eutectics in the interstices of the ceramic material. Surface forces prevent leakage of the eutectic during thermal charge/discharge cycles. The materials are formed into pellets for use in packed bed heat recovery/storage systems. Further characterization of the Na/Br carbonate eutectic system (710°C) is underway, preliminary studies with complementary lower temperature eutectics have been initiated, and comprehensive project reports are being written.

Keywords: Composites, Industrial Waste Heat Recovery

145. Formation of Encapsulated Metallic Eutectic Thermal Storage Alloy

FY 1988

\$ 0

DOE Contact: Eberhart Reimers, (202) 586-4563

Ohio State University Contact: Prof. Robert Rapp, (614) 422-2491

The purpose of this project is to develop a prototype fabrication process for encapsulating carbonate salt pellets with a metallic coating to form a thermal storage pellet which retains some compressive strength (because of tension forces) when the salt is melted. This allows a packed bed, direct contact heat storage material with storage in latent as well as sensible heat. An effective way of producing pellets in mass and of the right size and uniformity is being studied. A pellet fabrication process to produce a storage media in the range of 700-800°C is under development.

Keywords: Composites, Materials Characteristics

Materials Properties, Behavior, Characterization or Testing

146. Development of Ice Self-Release Mechanisms FY 1988
\$30,000

DOE Contact: E. Reimers, (202) 586-4563

ORNL Contact: J. Tomlinson, (615) 574-0768

University of Missouri-Columbia/Kansas City Contact: W. Stewart, (816) 276-1283

Improved ice-making performance for cool storage systems can result from development of water additives that inhibit ice from sticking to evaporator surfaces. Early work identified additives and evaporator surface coatings that produced ice self-release from submerged evaporators due to buoyant forces. A series of experiments are underway to quantify the influence of those parameters that affect the self-release process.

Keywords: Low-Temperature Service (below 77°C), Instrumentation and Technique Development, Crystal Growth, Surface

147. Development of a Complex Compound Chill Storage System FY 1988
\$225,000

DOE Contact: E. Reimers, (202) 586-4563

ORNL Contact: J. Tomlinson, (615) 574-0768

Rocky Research, Inc. Contact: U. Rockenfeller, (702) 293-0851

Low-temperature chill storage can be accomplished through sorption between ammonia and salts. Prior work to develop solid-vapor complex sorption systems showed heat exchanger costs to be the major hurdle for a practical thermal storage system. In the current effort, catalytic inert solvents that reduce the heat exchange requirements for the complex are being studied in addition to advanced heat exchange surfaces. The goal of these efforts is to produce a heat and mass transfer technology of sufficient cost and performance to enable development of an operating low-temperature chill storage system based on ammoniated complex compounds.

Keywords: Low-Temperature Service (below 77°C), Organics

148. Evaluation of Heats of Mixing Systems for Thermal Energy Storage FY 1988
\$50,000

DOE Contact: E. Reimers, (202) 586-4563

ORNL Contact: J. Tomlinson, (615) 574-0768

NY Polytechnic Institute Contact: L. Stiel, (718) 643-5141

The purpose of this project is to identify and determine the heats of mixing of promising liquid-liquid and liquid-solid chemical systems for energy storage. Prior work to develop an analytical tool for determination of heats of mixing based on component activities and multi-component models identified several interesting aqueous systems based on amines, pyridines, and carbonates. Flow microcalorimetric equipment has been used to determine mixing enthalpies above and below the critical solution temperatures. Identification of suitable chemical systems with high heats of mixing are needed for successful development of thermal storage systems for building heating and cooling applications.

Keywords: Low-Temperature Service (below 77°C), Organics

149. Dendritic Zinc Deposition in Flow Batteries FY 1988
\$70,000

DOE Contact: A. Landgrebe, (202) 586-1483

Illinois Institute of Technology Contact: J. R. Selman, (312) 567-3037

Solution-side transport processes involved in acidic zinc deposition and their effect on electrode kinetics and deposit morphology were investigated. Corrosion kinetic parameters were estimated by using a nonlinear parameter estimation program. The effects of pH, rotation rate, bromine and charging current density on zinc dendrite growth history were studied. A mathematical model of the propagation of a two-dimensional wave surface was developed. The effects of secondary current distribution and the presence of a corrosion reaction on the propagation of electrode profile were analyzed.

Keywords: Corrosion, Structure, Batteries, Predictive Behavior Modeling

150. Fast Ion Conduction in Lithium Glasses FY 1988
\$100,000

DOE Contact: A. Landgrebe, (202) 586-1483

MIT Contact: H. Tuller, (617) 253-6890

Potassium borate glasses were found not to be dramatically less conductive than the corresponding Li and Na glasses because the potassium has a larger molar volume. Measurements of electrical conductivity, density and glass transition temperature have been extended to include previous compositions in the 33 percent (K₂O-KCl)-67 percent

B₂O₃ system as well as several new ones. Electrochemical studies with cells of the type Li-Al/glass/Li-Sn/glass/Li-Al have been resumed.

Keywords: Solid Electrolytes, Fast Ion Conductors and Solid Electrolytes

151. Polymeric Electrolytes for Ambient-Temperature Lithium Batteries FY 1988
\$50,000

DOE Contact: A. Landgrebe, (202) 586-1483

University of Pennsylvania Contact: G. Farrington, (215) 898-6642

A new discovery indicates that the cationic transport numbers of various poly(ethylene oxide) [PEO] complexes of divalent cation salts are strongly influenced by the thermal and hydration history of the complexes. It appears that fast cation transport can be "switched on and off" by appropriate treatment of these materials. Electrolytes formed with Cobalt(II)bromide and Ni(II)bromide were studied. In addition, because thermal history has influence on the conduction properties of these electrolytes, an investigation that involves simultaneous complex impedance analysis and differential scanning calorimetry is underway to learn more about the relationship between thermal history and conductivity.

Keywords: Polymers, Batteries

152. Exploratory Cell Research and Study of Fundamental Processes in Solid State Electrochemical Cells FY 1988
\$95,000

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. Dispersion of Na-β-Al₂O₃ powder into PEO-LiClO₄ was found to increase electrolyte conductivity by as many as three orders of magnitude at temperatures below the melting point. Exploratory cells fabricated using ultra-thin (30-70 μm) redox polymer (polyvinylferrocene) electrodes have been studied using impedance techniques to characterize the ion injection rate at PEO interfaces. Direct measurements of Li⁺ diffusivity in high molecular weight PEO samples have been made using microelectrode voltammetry.

Keywords: Polymers, Batteries

153. Corrosion, Passivity, and Breakdown of Alloys Used in High-Energy-Density Batteries

FY 1988

\$80,000

DOE Contact: A. Landgrebe, (202) 586-1483

Johns Hopkins University Contact: J. Kruger, (301)358-7732

Recent work has focused upon extending an earlier analysis of polarization and impedance data for Armco Fe and 1018 steel in solutions of various PC: water compositions with 0.5 M LiClO₄ as the electrolyte to two more PC: water ratios. The polarization curves showed that with increasing PC concentration up to 90 mole % PC, the E_{corr} , E_{pp} and i_{pass} values increased, indicating a more oxidizing environment and a less protective film. The impedance data indicate that increasing PC content lowers the general corrosion rate of the Armco FE, which may have implications with respect to the ability of the material to repassivate once its film is broken. In addition, tests aimed at determining the stability of the passivity indicated by the polarization curves were undertaken.

Keywords: Corrosion-Aqueous, Metals: Ferrous, Batteries

154. Materials for Fuel Cells

FY 1988

\$150,000

DOE Contact: A. Landgrebe, (202) 586-1483

BNL Contact J. McBreen, (516) 282-4513

Work has focused on conducting extended X-ray Absorption Fine Structure (EXAFS) studies on material relevant to fuel cells. This has included EXAFS studies of pyrolyzed iron and cobalt macrocyclics on Vulcan XC-72 carbon and carbon-supported platinum electrodes in phosphoric acid fuel cells. Results of the EXAFS studies of pyrolyzed Fe and Co TMPP indicate that in many cases at least three pyrolysis products are formed, including reduced metal and metal oxides. Removal of the metal and the oxides by chemical leaching revealed another component that is the catalyst.

Keywords: Fuel, Catalysts, Pyrolysis, Structure

155. Electrocatalysts for Oxygen Reduction and Generation FY 1988
\$177,000

DOE Contact: A. Landgrebe, (202) 584-1483

Case Western Reserve University Contact: E. Yeager, (216) 386-3626

Four catalyst systems were investigated: (1) macrocycle catalysts, (2) heat-treated macrocycles and nitrogen-containing polymers, (3) transition metal oxide systems, and (4) mixtures of metal oxides with either macrocycles or nitrogen-containing polymers.

Keywords: Catalysts, Polymers, Metals Surface, Composites

156. Materials Durability in the Zinc/Bromine System FY 1988
\$145,000

DOE Contract: J. Quinn, (202) 586-1491

SNL Contact: C. Arnold, (505) 844-8728

This program involves detailed chemical and mechanical characterization of materials and components that were aged in an accelerated manner or used in a typical battery environment. The first type of material investigated was polyvinyl chloride (PVC), the prime candidate for the fabrication of the battery's flow frame. Fourier transform infrared (FTIR) analyses of treated and untreated samples of PVC-1 and PVC-4 revealed the following: (1) PVC-4 is more stable than PVC-1, and (2) dehydrohalagenation, bromination, and oxidation occurred in both materials. Microhardness measurements indicate that the degradation is diffusion controlled and heterogeneous.

Keywords: Polymers, Batteries

157. Use of Micro Particles as Heat Exchangers and Catalysts FY 1988
\$32,800

DOE Contact: Eberhart Reimers, (202) 586-4563

LBL Contact: Arlon Hunt, (415) 586-5370

The focus of this project is on the issue of heat transfer between particles and gas since this was identified as important in understanding a broad range of energy storage and conversion systems. The first objective of the project was to investigate heat transfer mechanisms as a function of particle size and state of the gas. The goal of this study is to determine under what circumstances the particle temperature is moderately independent of the gas temperature and conversely those conditions when the particle temperature is "pinned" to the gas temperature. These two examples define the extremes in particle temperature and therefore delineate the range of applications of the process. Studies of the steady state heat fluxes in radiantly heated particle suspensions were initiated. Simplified analytic solutions of the heat transfer between very small particles

and gas were formulated. These analytical solutions facilitated rapid evaluation of the factors influencing the steady state temperatures and heat transfer rates between radiantly heated particles and the gas. Experiments include using iron, iron oxide particles, and carbonaceous particles in conjunction with possible reversible gas phase energy storage reaction couples such as SO_2/SO_3 . Project closed out in FY 1987 due to lack of funding.

Keywords: Catalyst, Metals, Semiconductors, Microstructure, Transformation, Surface Characterization and Treatment, Energy Storage

158. Evaluation of Heats of Mixing Systems for Thermal Energy Storage FY 1988
\$41,000

DOE Contact Eberhart Reimers: (202) 586-4563

ORNL Contact: John Tomlinson, (615) 574-0768

New York Polytechnic Institute Contact: Leonard Stiel, (718) 643-5141

The purpose of this project is to identify and determine the heats of mixing of promising liquid-liquid and liquid-solid chemical systems for energy storage. Prior work to develop an analytical tool for determination of heats of mixing based on component activities and multi-component models identified several interesting aqueous systems based on amines, piridines and carbonates. Flow microcalorimetric equipment has been assembled and is being used to determine mixing enthalpies above and below the critical solution temperatures. Identification of suitable chemical systems with high heats of mixing are needed for successful development of thermal storage systems for building heating and cooling applications.

Keywords: Organics, Predictive Behavior Modeling

159. Development of Solid/Vapor Ammoniated Complexes as Thermal Energy Storage Materials FY 1988
\$100,000

DOE Contact: Eberhart Reimers, (202) 586-4563

ORNL Contact: John Tomlinson, (615) 574-0768

Rocky Research Contact: Uwe Rockenfeller, (702) 293-0851

Prior research to identify and apply sorption reactions in storage heat pumps has identified issues critical to development of working systems. Heat exchanger designs that enhance solid/vapor reaction rates in ammoniated systems and additives that act as catalysts to speed reactions were identified and examined experimentally. Based on these efforts, preliminary designs of heat actuated and compressor actuated cool storage

systems were completed for multiply-complexing ammoniated salts. This work will serve as a basis for development of a chill storage system for low temperature industrial applications.

Keywords: Low Temperature Service (below 77°C), Structure

Materials Structure and Composition

160. New Lithium-Based Battery Materials FY 1988
\$202,000

DOE Contact: A. Landgrebe, (202) 586-1483

Stanford University Contact: R. Huggins, (415) 723-4110

Work continues in the area of negative electrode materials with the investigation of lithium activity alloys that undergo displacement reactions. In the area of positive electrode materials, the room-temperature electrochemical behavior of ternary-phase oxide bronzes in the Li-Mo-O system is examined on a ternary-phase triangle for comparison with the high-temperature (equilibrium) phase diagram. Work continues on the deposition of thin films using atmospheric pressure chemical vapor deposition and the use of Li-Si-S ternary phases as electrolyte or electrode materials.

Keywords: Batteries, Structure, Chemical Vapor Deposition

161. Spectroscopic Studies of Passive Films on Alkali and Alkaline Earth Metals in Nonaqueous Solvents FY 1988
\$67,000

DOE Contact: A. Landgrebe, (202) 586-1483

Case Western Reserve University Contact: D. G. Scherson, (216) 368-5186

Research efforts have focused on the nature of the reactions that take place upon exposure of a variety of organic solvents to sub-, mono-, and multi-layers of alkali and alkaline earth metals vapor that is deposited onto selected host metal substrates under ultra-high-vacuum (UHV) conditions. Careful analysis of the behavior of expected decomposition products generated by the reactions of non-aqueous solvents with alkali and alkaline earth metals using LEED, AES, TDS, HREELS, and UPS spectroscopy was conducted.

Keywords: Surface, Structure, Vapor Deposition, Coatings and Films, Batteries

162. Raman Spectroscopy of Electrode Surface in Ambient-Temperature Lithium Secondary Battery FY 1988

\$47,000

DOE Contact: A. Landgrebe, (202) 586-1483

Jackson State University Contact: H. Tachikawa, (601) 968-2171

In situ Raman spectroscopy of surface layers on lithium electrodes in LiAsF₆/propylene carbonate (PC) solution was completed. Several different lithium electrodes were examined, including lithium metal (ribbon), thin-film lithium electrodes deposited on nickel or silver electrodes. Information on Raman Spectra studies is used to understand the cycle life of rechargeable lithium electrodes in nonaqueous solutions.

Keywords: Surface, Structure, Batteries

Device or Component Fabrication, Behavior or Testing

163. Glass Electrolytes and Advanced Cell Concepts

FY 1988

\$150,000

DOE Contact: A. Landgrebe, (202) 586-1483

ANL Contact: I. D. Bloom, (312) 972-4516

This three-year project is entering its final year. Thus far, a fabrication process has been developed to produce ANL glass tubing in which glass tubing is drawn directly from the melt at 900-100°C. Short lengths of glass tubing have been produced using dry, CO₂-free gases as both the blanket and blowing gas and a Swagelok-tipped, mechanically guided blowpipe. As part of the fabrication process, a metal-to-glass seal was formed between the glass electrolyte tube and the Swagelok connector. Tubes fabricated in this fashion have been used in sealed, small-scale (10-30 mHh) Na/S cells.

Keywords: Solid Electrolytes

164. Proton Exchange Membrane Electrode Optimization

FY 1988

\$50,000

DOE Contact: A. Landgrebe, (202) 586-1483

LANL Contact: J. Huff, (505) 667-6832

Efforts were continued to characterize Nafion-impregnated electrodes with low Pt loading and to improve the interface between such electrodes and PEM electrolytes. Oxygen reduction reaction kinetics were investigated at Pt/ionomer interfaces to provide information needed to establish a base line for the estimation of Pt use in gas-diffusion

electrodes in contact with ionomer membranes. The hydrogen and oxygen absorption/desorption characteristics and the electrode kinetics of fuel cell reactions were examined at both uncoated and Nafion-coated Pt gauze test electrodes.

Keywords: Catalysts, Fuel

165. Electrode Fabrication and Fuel Cell Evaluation

FY 1988
\$10,000

DOE Contact: A. Landgrebe, (202) 586-1483

LANL Contact: J. Huff, (505) 667-6832

Improved electrode fabrication to attain high power densities in fuel cells is accomplished by: (1) impregnation of an optimum quantity of Nafion into a Prototech electrode, (2) optimization of the hot pressing of Prototech electrodes onto a Nafion membrane, (3) proper humidification of reactant gases, (4) localization of a high concentration of Pt near the electrode surface, and (5) use of high temperatures and pressures.

Theoretical analysis of the characteristic behavior of the porous gas-diffusion electrode showed that the current distribution was such that, at high current densities, most of the current is generated over a small depth, on the order of a few mm, from the front surface of the electrode.

Keywords: Fuel, Catalysts, Hot Pressing, Predictive Behavior Modeling

166. β -Alumina Electrolyte Development

FY 1988
\$ 0

DOE Contact: J. Quinn, (202) 586-1491

Ceramatec Inc., Contact: J. Rasmussen, (801) 486-5071

Electrolytes of partially stabilized and unstabilized zirconia-toughened materials were fabricated in which wet bag isostatic pressing was used as the method of green forming. Following fabrication, the electrolytes were characterized for mass density, ionic resistivity, burst strength of ring sections, visual characteristics, and dimensional characteristics. After characterization, the electrolytes were assembled into sodium/sulfur cells. During assembly, a number of electrolyte fractures occurred. The cells were then placed in test stands, brought to temperature, and cycled for operational life and freeze/thaw tolerance. Post-test characterization will include visual examination, surface chemistry analysis, ionic resistivity, burst strength, and residual strain.

Keywords: Batteries, Isostatic Pressing, Fracture

167. Advanced Membrane Development for the Zinc/Bromine System FY 1988
\$280,000

DOE Contact: J. Quinn, (202) 586-1491

SNL Contact: C. Arnold, (505) 844-8728

Microporous separators are currently used in all zinc/bromine battery technologies. The chief advantages of microporous separators are their low cost and low area resistivity. One serious disadvantage of microporous separators is their lack of selectivity. The initial approach to this problem is to impregnate and/or coat microporous separators with cationic polymers. Such treatments should bring about a reduction in the rate of bromine transport by two mechanisms: (1) through the polymer; and (2) physical closure of some fraction of the pores. Hybrid or composite membranes containing up to 20 percent (Sulfonated polysulfone) SPS by weight were prepared by impregnating a microporous separator with solutions of SPS in dimethylformamide. The important electrochemical properties of these membranes are area resistivity and bromine transport rate.

Keywords: Polymers, Composite, Batteries

168. Improved Chromium Platings for Sodium/Sulfur Cell Containers FY 1988
\$20,000

DOE Contact: J. Quinn, (202) 596-1491

SNL Contact: W. D. Bonivert, (415) 294-2987

The research emphasis will be on improving the current corrosion protection scheme of thermally producing a chromium layer, because the durability of this layer may not be sufficient for utility storage applications. Experimental progress was curtailed because improvements to the plating laboratory had to be made in order to comply with environmental regulations. During the remodeling, new plating bath chemistries were prepared and post-processing options for the electroplated chromium layers were explored. The possibility of plating chromium from fused salt baths was also investigated. This option will not be pursued because of the difficulty and the high cost associated with commercialization.

Keywords: Batteries, Corrosion

169. TES Media Evaluation FY 1988
\$40,500

DOE Contact: E. Reimers, (202) 486-4563

PNL Contact: J. Bates, (509) 375-2539

The ceramic/molten carbonate salt matrix TES media has been successively tested under laboratory conditions, but many aspects of the concept can only be investigated in

an industrial environment. These include inbed salt migration; inbed particulate accumulation; TES media degradation when simultaneously exposed to typical thermal, mechanical, and chemical conditions; thermal performance and ease of operation in an industrial environment; and identification of application-specific design and operating factors that may affect the concept's technical and economic feasibility. PNL will support ORNL in the design, installation, acceptance testing, and operation of the test facility. The design, fabrication, and installation should be completed by summer, followed by eight months of operation during which several forms of the ceramic/molten carbonate salt matrix will be tested.

Keyword: 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 to promote 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, Electric Systems, and Materials Research.

Materials Properties, Behavior, Characterization or Testing

170. Microfilamentary Superconducting Composite

FY 1988
\$100,000

DOE Contact: R. Eaton, (202) 586-1506

Ames Laboratory Contact: D. K. Finnemore, (515) 294-4037

Material processing procedures are developed to produce long slender filaments of copper oxide superconductors by forcing liquid through a nozzle with a supersonic stream of oxygen gas. The filaments are composed of the new high transition temperature copper oxide materials and combined with a ductile, high-conductivity normal metal for a stabilizer. A major part of this work is the diagnostic studies to demonstrate sample quality using TEM, SEM, optical microscopy, magnetization, and transport critical current studies.

Keywords: Composites, Fibers, Grain Boundaries, Superconductors

171. Practical Superconductor Development for Electric Power Applications FY 1988
\$500,000

DOE Contact: R. Eaton, (202) 586-1506

Argonne National Laboratory Contact: R. Weeks, (312) 972-4931

The conductor development program is a parallel approach 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.

Keywords: Superconductors, Composites, Coatings and Films, Structure

172. Practical Conductor Development for Electric Power Systems FY 1988
\$350,000

DOE Contact: R. Eaton, (202) 586-1506

Brookhaven National Laboratory Contact: A. Goland, (516) 282-3819

The various methods to be employed for fabricating composite conductors containing high- T_c oxides will be restricted to those which lead themselves to being 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.

Keywords: Composites, Coatings and Films, Superconductors

173. Films Processing Methods and Device Technology Development FY 1988
\$400,000

DOE Contact: R. Eaton, (202) 586-1506

Lawrence Berkeley Laboratory Contact: N. Philips, (415) 486-6062

Several approaches are undertaken to develop thin films suitable for the conductor development task. Three techniques are adapted and refined: sputtering, laser ablation, and sol-gel processing. The characterization of the electrical transport properties of superconducting films requires the measurement of resistivity as a function of current density, magnetic field amplitude and direction, temperature, and frequency. In addition to routine techniques, efforts are also focused on understanding the AC loss mechanisms.

Keywords: Superconductors, Coatings and Films, Crystal Growth

174. Thin Film Superconductors for Electric Power Systems FY 1988
\$200,000

DOE Contact: R. Eaton, (202) 586-1506
SERI Contact: R. McConnell, (303) 231-1019

The approach is to conduct research into fabrication process 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.

Keywords: Superconductors, Coatings and Films, Polymers, Crystal Growth, Structure

175. High Temperature Superconductor Materials and Power Device Development FY 1988
\$280,000

DOE Contact: R. Eaton, (202) 586-1506
SNL Contact: D. Scheuler, (505) 844-4041

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) never allowing it to form in the first place by controlling the solution-precipitation process; (2) decomposing the carbonate by heating to temperatures 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.

Keywords: Superconductors, Crystal Defects and Grain Boundaries, Structure, Consolidation of Powder, Powder Synthesis and Characterization

176. Fabrication Development of High Temperature Superconductor for Electric Utility Applications FY 1988
\$300,000

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, on powder consolidation and fabrication, and on vapor deposition. 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 question 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, Consolidation of Powder, Powder Synthesis and Characterization

177. Development of Practical Conductors Utilizing High-Temperature Oxides

FY 1988
\$300,000

DOE Contract: R. Eaton, (202) 586-1506

ORNL Contact: D. Kroeger, (615) 574-5177

The primary effort is toward reduction or elimination of grain boundary resistance, one of the recognized causes of the poor critical currents observed in sintered $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$. 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 variable and the effects of texturing in superconducting ceramics will permit the production of high- J_c superconducting materials.

Keywords: Superconductors, Crystal Defects and Grain Boundaries, Structure, Consolidation of Powder, Powder Synthesis and Characterization

178. Evaluation of Polymers for Electric Insulation

FY 1988
\$105,000

DOE Contact: R. Eaton, (202) 586-1506

ORNL 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.

Keywords: Insulators/Dielectrics - Polymeric, Creep, Fracture, Polymers

Materials Structure and Composition179. Fast-Response Zinc Oxide Varistor Material Development FY 1988\$40,000

DOE Contact: R. Eaton, (202) 586-1506

ORNL Contact: F.A. Modine, (615) 574-6287

Grain boundary barrier breakdown studies are studied. Electrical properties of ZnO varistors are measured as a function of microstructure. Special emphasis is given to response of varistors to very fast electrical pulses, conduction mechanisms at grain boundary barriers, relationship between charge and mass transport, and the degradation of varistor electrical performance.

Keywords: Grain boundaries, Semiconductors

Device or Component Fabrication, Behavior or Testing180. Fabrication of High-T_c and High-J_c Superconductors by Dynamic Compaction of Oriented High-T_c Powders and Processing Superconducting Materials Under High-O₂ Pressure FY 1988\$300,000

DOE Contact: R. Eaton, (202) 586-1506

LLNL Contact: W. Nellis, (415) 423-6665

Dynamic explosion compaction process for fabrication of superconductors is designed to produce the required microstructure and composite structure. Orientation of the crystal axes of the particles is achieved by pre-alignment in a magnetic field. In addition, optimization of sintering time with respect to processing parameters (elevated temperature and pressure) will produce fully dense superconducting materials without the required post-processing steps of sintering and annealing to regain oxygen stoichiometry.

Keywords: Superconductors, Consolidation of Powder, Extrusion, Grain Boundaries, Structure

181. Interfacial Aging Phenomena in Power Cable Insulation Systems FY 1988\$100,000

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 impurities, namely ionic, from the semi-conducting layers into the insulation are monitored.

Keywords: Semiconductors, Insulators/Dielectrics - Polymeric

182. Conducting Polymer Research for Electric Power Equipment Applications

FY 1988
\$200,000

ORNL Contact: S. J. Dale, (615) 574-4829

Westinghouse Contact: E. Schoch, (412) 256-1960

Conducting polymeric technology is assessed with the view of replacing the traditional stress grading materials within conducting polymers electrical equipment as cables, bushings, generators, and transformers, where electrical stress grading is an essential part of the design. Major considerations will include materials properties, material processing as well as impact on performance and projected economics.

Keywords: Polymers

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 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 dramatically improve 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

183. Thermochromic Materials Research for Optical Switching Films FY 1988
\$8,000

DOE Contact: M. M. Jenior, (202) 586-2998

Honeywell Contact: G. V. Jorgensen, (612) 378-4655

This project includes the development of a thermochromatic material that can be used on opaque surfaces to control insolation through building envelopes. This synthesized material will passively switch between a heat-transmitting state and a heat-reflecting state at specific design temperatures. Doped vanadium oxide (VO₂) coatings have been deposited on glass and sapphire substrates, and analyzed by measuring their sheet resistances and their spectral transmittances above and below their transition temperatures. The formulation for a paint that switches its reflectance has been developed based on undoped vanadium oxide pigment and silicone epoxy binder. Doping with tungsten decreases the pigments transition temperature.

Keywords: Coatings and Films, Metallic Glasses, Photothermal, Low Temperature Service

184. Electrochromic Films and Deposition Processes FY 1988
\$175,000

DOE Contact: M. M. Jenior, (202) 586-2998

SERI Contact: D. Blake, (303) 231-1202

This project involves the development of a laboratory-scale plasma-enhanced chemical vapor deposition (PE-CVD) process for producing practical, cost-effective electrochromic coatings for architectural glass. The development of a practical, multi-layer, solid-state electrochromic coating process will encourage industry to incorporate such a coating in solar aperture glazing products which can be used to improve the energy efficiency of buildings. In FY 1988, experiments on optimizing the conditions for producing tungsten oxide films at rates of up to 500 Angstroms per second were completed. In addition, researchers discovered molybdenum oxide films that exhibit a color-neutral darkening electrochromic transition, which shows promise as an architecturally acceptable color change for window applications, and a molybdenum oxyfluoride film that is electrochromically active but has a very low coloration in the visible region on the spectrum. The latter has potential as a counter electrode in window applications.

Keywords: Coatings and Films, Transformation, Chemical Vapor Deposition, Low Temperature Service

185. Electrochromic Glazings (Nickel-based)FY 1988

\$170,000

DOE Contact: M. M. Jenior, (202) 586-2998

LBL Contact: Steven Selkowitz, (415) 486-5064

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 FY 1988, the basic switching characteristics of devices using electrochromic nickel oxide were investigated. Films on conductive glass were made by both electrochemical and sputter deposition, vacuum evaporation, and sol-gen techniques. A basic polymer electrolyte suitable for nickel oxide devices was developed, refined, and evaluated. The switching characteristics of nickel oxide were improved by doping with lithium. The electrochromic properties of vanadium oxide were also studied.

Keywords: Coatings and Films, Low Temperature Service

186. Solid State Electrochromic "Smart" Windows (Tungsten-based)FY 1988

\$130,000

DOE Contact: M. M. Jenior, (202) 586-2998

EIC Contact: R. D. Rauch, (617) 769-9450

The purpose of this project is to develop an all solid-state thin film electrochromic coating for windows that can provide active control of solar insolation through windows by the application of a small DC electric current. The fabrication processes are intended to be appropriate for large areas using standard thin film vacuum deposition techniques. These "smart" windows will offer a means of regulating daylight, and solar input to and radiation heat loss from building interiors to improve energy efficiency. Thin film laminated electrochromic devices consisting of five layers were fabricated. The two outer layers are electrodes. The inner layers consist of an electrochromic material, an ion conductor, and a counterelectrode. The devices exhibit reversible electrochromic switching over approximately 100 cycles.

Keywords: Coatings and Films, Low Temperature Service

187. Electrochromic Materials for Controlled Radiant Energy in Buildings
(Tungsten-based)

FY 1988
\$230,000

DOE Contact: M. M. Jenior, (202) 586-2998

Tufts University Contact: R. B. Goldner, (617) 628-5000

The project involves development and modeling of all-solid optical switching devices based on 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 project 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) window 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-WO₃) 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 FY 1988, the first anodically-coloring EC films were synthesized. A structural model explaining lithium insertion into ITO was developed, and reversible changes in X-ray structure upon insertion/removal of lithium were demonstrated.

Keywords: Coatings and Films, Transformation, Low Temperature Service

188. Holographic Diffractive Structures for Enhanced Daylighting

FY 1988
\$110,000

DOE Contact: M. M. Jenior, (202) 586-2998

Advanced Environmental Research Group Contact: R. Ian-Frese, (617) 864-4982

This project focuses on the development of a low-cost holographic diffractive structure (HDS) system that maximizes the utilization of sunlight for daylighting. HDSs can 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 FY 1988, the performance of HDSs in a physical model and in several fenestration strategies was evaluated.

Keywords: Coatings and Films, Low Temperature Service

Materials Properties, Behavior, Characterization or Testing

189. Advanced Phase-Change Materials and Systems for Solar-Passive Heating and Cooling of Residential Buildings FY 1988
\$ 0

DOE Contact: Robert Hassett, (202) 586-8163
University of Dayton Contact: I. O. Salyer, (513) 229-2113

This project involves developing cost-effective methods for incorporating phase-change materials (PCMs) into construction materials (concrete, plasterboard, etc.). A series of commercially available crystalline alkyl hydrocarbon (C-18) materials can be used not only for passive solar thermal storage applications, but also for active solar applications, "cool" storage, and de-icing bridge decks. Collected radiation is often wasted because it cannot be stored in available building materials; if PCMs were incorporated into conventional materials, performance gains could be substantial. Accomplishments to date include the test and analysis of alkyl-hydrocarbon PCMs encapsulated in samples of conventional building materials (plasterboard, cement board, and plaster) and the development of low-cost methods for containing PCMs in building materials have been developed. This research also sought to improve the fire-retardant capabilities of the PCMs for conventional building applications, such as plasterboard. This contract was terminated in May 1988 as the research was to be continued under a subcontract to the Oak Ridge Laboratory. (This project is funded by the Office of Energy Storage.)

Keywords: Transformation, Low Temperature Service

190. Thermal Energy Storage in "Plastic Crystals" FY 1988
\$45,000

DOE Contact: Robert Hassett, (202) 586-8163;
University of Nevada-Reno Contact: D. Chandra, (702) 784-4960

The focus of this activity is to gain fundamental understanding of the nature of crystal structure changes in the lattice of solid-solid phase change materials (SSPCMs) and their effects on thermal properties of SSPCMs so that their transition temperatures can be lowered to near room temperature. The known pure organic SSPCMs are not suited for passive solar buildings because their transition temperatures are too high. A near room-temperature adjusted "plastic crystal," neopentolglycol (NPG), has been made

and its true crystal structure has been determined. The contract was terminated and all subsequent development efforts transferred to the Oak Ridge Laboratory.

Keywords: Plastic Crystals

191. Desiccant Materials/Dehumidifier Geometries Research FY 1988
\$150,000

DOE Contact: J. Goldsmith, (202) 586-8779

SERI Contact: A. Pesaran, (303) 231-7636

The objectives are: (1) generating data based on heat and mass transfer performance of promising dehumidifier geometry/material combinations and validating fundamental models that can be used as modules for overall systems-analysis computer programs; and (2) identifying the effect of pollutants abundant in residential areas on solid desiccant materials for dehumidifiers that may reduce their performance for solar air conditioning applications. FY 1988 activities included the collection of: (1) test data on equilibrium capacity of four promising desiccant materials; (2) experimental data on pressure drop and heat and mass transfer rates on promising material/geometry combinations (silica gel and lithium chloride with corrugated geometry) for dehumidifiers; and (3) information on the effect of residential pollutants on silica gel capacity and how to characterize such effects for different pollutants. A desiccant contamination test facility was designed and is under fabrication. The test facility is expected to be operational by mid-January 1989. It will be operated 24 hours a day for one year to obtain data on the degradation impact of tobacco smoke (the worst indoor airborne contaminant) on 100 samples of different desiccants.

Keywords: Polymers, Organics, Surface Phenomena, Desiccants

192. Advanced Desiccant Materials Research FY 1988
\$150,000

DOE Contact: J. Goldsmith, (202) 586-8779

SERI Contact: A. Czanderna, (303) 231-1240

Determining how the desired sorption performance of advanced desiccant materials can be predicted by understanding the role of their surface phenomena and materials modifications is the focus of this activity. 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 FY 1988, polystyrene sulfonic acid (PSSA) has been prepared with modifications for the molecular weight, percent sulfonation, and type of alkali salt (e.g., sodium salt (SS)). The modified PSSASS yields sorption isotherms with improved shape and capacity. A cross-linked hydrogel has been synthesized for sorption characterization. The quartz crystal microbalance (QCM) apparatus has been improved with the addition of a computerized data acquisition system. A Sartorius beam microbalance system has been designed and installed, and will be ready for use in 1989.

Keywords: Polymers, Surface Phenomena, Desiccants

193. Open-Cycle Absorption Solar Cooling

FY 1988
\$110,000

DOE Contact: John Goldsmith, (202) 586-8779

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 moisture 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, Adsorbents

194. Solar Cooling Research Facility

FY 1988
\$575,000

DOE Contact: M. Lopez, (415) 273-4264

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 the identification of the utility and application of desiccant materials and the development of innovative materials and systems. In FY 1988, the Diurnal Test Facility was completed and is being debugged. A moisture properties database and handbook was prepared, and algorithms developed for combined mass and heat transfer in buildings. The Radiant Barrier Facility was

constructed, and a draft ASTM standard for the "Use and Installation of Radiant Barrier Systems" was prepared.

Keywords: Low Temperature Service, Desiccants, Absorption

195. Evaluation of Photochromic Plastics

FY 1988
\$53,000

DOE Contact: M. M. Jenior, (202) 586-2998

American Optical Corporation Contact: N. Chu, (617) 765-9711

This project involves the evaluation of photochromic plastic materials for their potential application to architectural glazing in buildings designed to use or control solar energy. Spiroxazine photochromic materials are clear in the unactivated state. When activated by light at wavelengths in the ultraviolet (UV) region at or just below the visible region of the spectrum, this material absorbs strongly in the visible region. The material serves as a completely reversible optical switch or shutter activated automatically when exposed to sunlight. Photochromic materials as optical switching elements for apertures and daylighting systems have potential for increasing solar heat gain in the winter and rejecting heat in the summer and require no external power supply or electrical connecting circuitry. In FY 1988, the photochromic performance of spirooxazines was evaluated in four polymeric host materials: cellulose acetate butyrate (CAB), polyurethane, poly vinyl butyryl (PVB), and acrylic pressure-sensitive adhesive. Researchers also evaluated two types of light stabilizers (organonickel and hindered amine) that improve the photochromic durability of spirooxazines without impairing their photochromic functions.

Keywords: Low Temperature Service, Polymers, Coatings and Films

196. Daylighting Enhancement

FY 1988
\$80,000

DOE Contact: M. M. Jenior, (202) 586-2998

LBL Contact: Steven Selkowitz, (415) 486-5064

The objectives of this project 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 FY 1988, light guide research included development of an algorithm for optimizing a tracking collector's mechanical design; determination that thermal heat gain in plastic optical fibers should not be a problem; refinement of the optical theory underlying the collector's Fresnel lens design (and the filing of an initial patent

application for a mechanism that eliminates chromatic dispersion in the lens); and the development of software for completing the preliminary design. During FY 1989, the preliminary mechanical and optical system design will be completed, the evaluation of projected economic and energy-savings performance will be refined, and human factors relating to lighting quality will be addressed.

Keywords: Low Temperature Service, Coatings and Films

197. Research and Development of a Static Optical System to Reduce Apparent Motion of the Sun FY 1988
\$41,000

DOE Contact: M. M. Jenior, (202) 586-2998

Lighting Sciences, Inc., Contact: I. Lewin, (602) 991-9260

The objectives of this project are to design a lens system with high transmittance as well as desired directional control for maximum efficiency. Most daylighting techniques are hampered by the natural motion of the sun. Active collection systems have been developed, but are expensive and complex. Passive collection systems to date suffer from low efficiency. A system that could obtain sunlight from the full range of useful intensities and transmit it in a reduced angular range would work well with newly developed light pipes. It could also be used for fenestration, skylights, and other applications. In FY 1988, 10 prototype lenses were developed and analyzed. Based on this work, an optimized prototype lens was fabricated, tested, and analyzed.

Keywords: Coatings and Films, Low Temperature Service

198. Advanced Evacuated Tubular Concentrator Research FY 1988
\$53,000

DOE Contact: John Goldsmith, (202) 586-8779

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 FY 1988, a generic optical and thermal model with performance parameters suitable for IEA transient modeling of collector and system performance was defined. Also, the circumferential distribution of solar energy flux as input to the heat pipe option was determined. There are two flux peaks that are three times the average flux on the heat pipe. Distribution is a function

of the incidence angle; the flux becomes more uniform as the sun moves off zero. The determination of flux is critical if the heat pipe is an insert in a glass tube.

Keywords: Coatings and Films, Low Temperature Service

Solar Thermal Technology Division

Solar Thermal Technology is developing central receiver systems and parabolic dish systems to concentrate the sun's energy. This concentrated energy can then be used for industrial process heat, generating electricity, or producing fuels and chemicals. The combination of concentrated direct solar flux (to 14,000 suns) and high temperature (to 5000°F) can cause unique and beneficial material transformations of metals, alloys, ceramics, and fibers. In addition, solar induced degradation of materials such as silver polymer films and metals for use in solar thermal receiver systems is being studied.

Materials Preparation, Synthesis, Deposition, Growth or Forming

199. Silver/Polymer Reflector Research

FY 1988
\$1,240,000

DOE Contact: Martin Scheve, (202) 586-8110

SERI Contact: Paul Schissel, (303) 231-1226

Research is being conducted to develop silver/polymer reflector films that are resistant to ultraviolet and pollutant degradation, are cleanable, and have specular reflectances of 90 percent or more (within a 4-mrad cone angle). Useful film lives of 5 years or more are needed for solar thermal technology applications.

Solar concentrators account for about 50 percent of the installed cost of a solar thermal system. Research is being carried out on polymer-based reflectors because they can substantially reduce the life cycle costs of concentrators, and hence for solar thermal systems. Silver/polymer reflectors offer the advantages of lighter weight, reduced cost, and design flexibility compared with silvered glass.

This research focuses on testing, characterization, and evaluating polymer-coated silver mirrors. Silver is being deposited onto candidate commercially available polymer films to meet performance standards. Research is also being conducted to understand the mechanisms of degradation of the silvered polymer films, and to find suitable stabilizers for them.

Keywords: Polymers, Coatings and Films, Surface Characterization and Treatment, Corrosion, Radiation Effects, Reflectors, UV Degradation

Materials Properties, Behavior, Characterization or Testing200. Sol-Gel Protective Films for Metal Solar Mirrors

FY 1988

\$200,000

DOE Contact: Martin Scheve, (202) 586-8110
SERI 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 substrates. Optical measurements (hemispherical, diffuse and specular reflectance) were made to characterize changes in the mirror resulting from the application of the sol, 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 accelerated testing in acid. Two layer coating schemes of sol-gel films were also evaluated.

The planarizing ability of sol-gel films was investigated on several 400 series stainless steel substrates. The smoothing effects of the sol-gel planarizing films were evaluated by optical techniques, followed by deposition of a film of silver over the sol-gel planarized substrates. The silver film is covered with a protective sol-gel overcoat. It was found that the specular reflectance of the stainless steel substrates could be increased from initial values of 0.36-0.90 to final values of 0.93 by the application of the planarizing sol-gel films.

Sol-gel coated stainless steel substrates will be used in the next generation solar concentrators.

Keywords: Sol-Gel, Surface Preparation and Treatment, Corrosion Resistance, Solar Concentrators

201. High Flux Effects on Materials

FY 1988

\$350,000

DOE Contact: Frank Wilkins, (202) 586-1684
SERI Contact: Daniel O'Neill, (404) 894-3589

Research on the beneficial effects of high solar flux on materials 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 oxidative 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.

Keywords: Carbon Fibers, Surface Modification, Mechanical Property Enhancement

202. Surface Transformation of Metals FY 1988
\$50,000

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 energy, and that mechanical properties such as hardness and wear resistance could be improved.

Surface alloying of metal powders to metal substrates using intense solar flux was examined. It was found that alloy phases similar to those which can be induced by lasers were attainable with intense solar flux, and that the processing rate for metal surfaces could be greater with the solar beam than with lasers because the solar beam diameter is much larger.

Keywords: Surface Alloying, Surface Modification, Surface Phases

203. Materials for Applications in Regenerative Thermal Electrochemical (RTEC) Technology FY 1988
\$50,000

DOE Contact: Frank Wilkins, (202) 586-1684
SERI Contact: L. Marty Murphy, (303) 231-1050

Containment materials for RTEC technology were investigated. Materials needed for the technology must withstand high pressure ammonia, dilute acids, and temperatures from ambient to 1500°F. The materials must also be reasonably inexpensive, for commercial application of the RTEC technology. Preliminary investigations have identified graphite and carbon composites as suitable containment materials.

Keywords: Electrochemical Systems Materials, Photoelectrochemical Systems

204. Transport and Optical Properties of Molten Salt Blackeners FY 1988
\$50,000

DOE Contact: Sigmund Gronich, (202) 586-1623

SERI Contact: Daniel M. Blake, (303) 231-1222

The radiative, dielectric, and optical properties of cobalt oxide salt for possible use as darkeners for molten nitrate salts were measured. Flowing molten nitrate salts are used as a radiant heat absorption fluid in the Direct Absorption Receiver (DAR).

Keywords: Cobalt Salts, Molten Salts, Radiative Properties, Direct Absorption Receiver

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

205. Amorphous Silicon for Solar Cells

FY 1988
\$10,500,000

DOE Contact: Morton B. Prince, (202) 586-1725
SERI Contact: Bill Wallace, (303) 231-1380

This project performs applied research upon the deposition of amorphous silicon alloys to improve solar cell properties. Efficient solar energy conversion is hindered by improper impurities or undesired structure in the deposited films and the uniformity of the films over large, (1000 cm²) areas. The films are deposited by plasma enhanced chemical vapor deposition, (glow discharge), thermal chemical vapor deposition and sputtering. The long term goal of this effort is to develop the technology for 12 percent efficient solar cells with an area of about 1000 cm². Achieving that goal should enable amorphous silicon to be a cost-effective electrical generator.

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

206. Polycrystalline Thin Film Materials for Solar Cells FY 1988
\$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

207. Deposition of III-V Semiconductors for High-Efficiency Solar Cells FY 1988
\$2,000,000

DOE Contact: Morton B. Prince, (202) 586-1725
SERI Contact: John Benner, (303) 231-1396
SNLA Contact: David King, (505) 844-8220

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 20 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

208. Materials and Device Characterization

FY 1988
\$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 and Treatment, Microstructure and Solar Cells

Device or Component Fabrication, Behavior or Testing

209. High-Efficiency Crystal Silicon Solar Cells

FY 1988
\$2,000,000

DOE Contact: Morton B. Prince, (202) 586-1725

SERI Contact: John Benner, (303) 231-1396

SNLA Contact: David King, (505) 844-8220

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

210. High Temperature Elastomers for Dynamic Sealing Applications FY 1988
\$5,000

DOE Contact: R. LaSala, (202) 896-4198
BNL Contact: L. E. Kukacka, (516) 282-3065

This project which was completed in FY 1988, performed applied research to optimize a Y-267 EPDM elastomer formulation, developed earlier by GTD for static seal applications, for use in dynamic seal applications at temperatures up to 260°C. Elastomers for these conditions did not exist, and a successful development should substantially reduce drilling and completion costs. The effects of compositional changes on the properties of the elastomer were determined, and the formulation optimized to yield the specific sealing requirements. Prototype and full-scale testing was performed, a final report issued and technology transfer to industry initiated. Significant improvements in the cost and reliability of geothermal components should result.

Keywords: Organics, Material Degradation, Stress, Drilling, Seals and Bearings

211. Geothermal Waste Utilization and Disposal FY 1988
\$10,000

DOE Contact: R. LaSala, (202) 896-1146
BNL Contact: L. E. Kukacka, (516) 282-3065

This program which was completed in FY 1988 involved the development of processes for converting toxic constituents of geothermal wastes into nonleachable forms which can be used as general construction materials. Before the large-scale development of geothermal energy can occur, environmentally and economically acceptable methods for the disposal of large quantities of waste must be developed. The program involved the selection of encapsulating materials, and the fabrication and evaluation of waste

forms. If implemented, significant improvements in the economic and environmental aspects of geothermal energy should be accrued.

Keywords: Cements, Polymers, Bonding Agents, Material Degradation, Bulk Characterization, Waste Management

212. Materials for Non-Metallic Heat Exchangers FY 1988
\$110,000

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

213. Biochemical Concentration and Removal of Toxic Components from Geothermal Wastes FY 1988
\$225,000

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

214. Advanced High Temperature Geothermal Well Cements FY 1988
\$185,000

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 CO₂ at temperatures >150°C are also needed. Emphasis is being placed on high temperature rheology, phase chemistry, and the mechanical, physical, and chemical resistance properties of the cured materials.

Keywords: Cements, Material Degradation, Strength, Transformation, Bulk Characterization, Drilling

215. Corrosion in Binary Geothermal Systems FY 1988
\$10,000

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

216. Advanced High Temperature Chemical Systems for Lost Circulation Control

FY 1988
\$100,000

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

217. Medium Temperature Solid Electrolytes: Proton Conductors

FY 1988
\$155,000

DOE Contact: M. Gurevich, (202) 586-6104

BNL Contact: C. Linkous, (516) 282-7949

Stanford Contact: R. Huggins, (415) 723-4110

Fundamental investigations are being pursued on the synthesis and characterization of modified high temperature polymers that may serve as proton conductors and on non-aqueous, molten salt hydride-ion conducting electrolyte. This work is ongoing at BNL

and Stanford University, respectively. 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 H₂-permeable electrodes which can serve as electrodes for electrochemical structures which can be used in steam electrolysis.

Keywords: Polymers, Electrolytes

218. Hydrogen Production with Photoactive Semiconductor Catalysts FY 1988
\$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 H₂ production experiments.

Keywords: Semiconductors, Plasma Polymerization, Coatings

Materials Properties, Behavior, Characterization or Testing

219. High Temperature Steam Electrolysis FY 1988
\$50,000

DOE Contact: M. Gurevich, (202) 586-6104

Westinghouse R&D Center Contact: W. Feduska, (412) 256-1951

Westinghouse has conducted analytical investigations to identify possible causes of limited solid oxide electrolyte cell life when these cells operate in the steam electrolysis mode. A mathematical model has been developed which predicts current density and voltage. Current distributions are equated to thermal profiles in order to assess prospects of inducing thermomechanical stresses. Findings have suggested no problems along the

length of the cell tube; however, circumferential current distributions may induce stresses, particularly at the interface with interconnect material.

Keywords: Solid Oxide Electrolytes

220. Cold Storage of Hydrogen on Activated Carbon

FY 1988
\$76,000

DOE Contact: M. Gurevich, (202) 586-6104
Syracuse University: J. Schwartz, (315) 423-2807

H₂ storage enhancement on activated carbon has been demonstrated when platinum or palladium catalysts have been used. Substitution of non-noble metal catalysts (i.e., nickel) have proven unsuccessful due to poor metal dispersion and/or pore blockage. Further 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 H₂ storage system prototype fabrication.

Future efforts will be directed toward the design and fabrication of a Process Development Unit capable of storing up to 1 lb. of H₂.

Keywords: Hydrogen Storage, Catalysts

221. Hydrogen Production via Photoelectrolysis

FY 1988
\$60,000

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 H₂ and O₂. 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 H₂. 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

222. Novel Methods for Solar Hydrogen Production

FY 1988
\$340,000

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 to (1) 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. Future efforts will be 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 MnO₂. 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 1988 for the Division of Materials Sciences were \$172,500,000. This was allocated to 554 projects. Many projects cross the traditional categories and, for example, involve property-structure relationships. Nevertheless, the approximate funding distribution for FY 1988 was:

	<u>\$ (Millions)</u>
Materials Preparation, Synthesis, Deposition, Growth or Forming	21.0
Materials Structure and Composition	27.5
Materials Properties, Behavior, Characterization or Testing	80.8
Device or Component Fabrication, Behavior or Testing	--
Facilities	43.2

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 1988 (DOE/ER-0389 dated September 1988). 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; Collaborative Research Centers (descriptive information); cross-cutting indices: investigators, materials, techniques, phenomena, environment. Limited copies may be obtained by calling (301) 353-3427.

Division of Engineering and Geosciences

Materials Properties, Behavior, Characterization or Testing

223. Bounds on Dynamic Plastic Deformation FY 1988
\$125,000

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

224. Diffusion, Fluid Flow, and Sound Propagation in Disordered Media FY 1988
\$68,000

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

225. In-Flight Measurement of the Temperature of Small, High Velocity Particles FY 1988
\$133,000

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

226. Experimental Measurement of the Plasma/Particle Interaction FY 1988
\$319,000

DOE Contact: Oscar P. Manley, (301) 353-5822

Idaho National Engineering Laboratory Contacts: M. E. McIlwain, (208) 526-8818,
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

227. Integrated Sensor/Model Development for Automated Welding FY 1988
\$450,000

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 noncontact 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

228. Nondestructive Characterization of Fracture Dynamics and Crack Growth FY 1988
\$183,000

DOE Contact: Oscar P. Manley, (301) 353-5822

Idaho National Engineering Laboratory Contacts: J. A. Johnson, (208) 526-9021, B. A. Barna, (208) 526-6124, R. A. Allemeir, (208) 26-9588

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

229. Plasma Reduction of Metallic Oxide Particles

FY 1988
\$71,000

DOE Contact: Oscar P. Manley, (301) 353-5822

MIT Contacts: J. F. Elliott, (617) 253-3305 and J. Szekely, (617) 253-3236

The objective of this research is the characterization of reactions in composite carbon-metal oxide particles and the possible reduction of metal oxide particles injected into the tail flame of a thermal arc plasma. The experimental program consists of injecting particles in the size range of 5 to 50 microns into the plasma flame, and then extracting these particles with a quenching tool at various positions down stream from the injection point. The collected particles are examined by optical and electron microscopy to obtain information on the changes such as melting, evaporation, reduction, etc., that occur during the transit of the particles in the flame. Samples of powders with a very small size range will be employed in studies of evaporation and melting.

The temperature and velocity fields of the plasma flame are being calculated with a computer program that has been developed for that purpose. The rate of heat transfer from the flame to the particles will be determined in experiments in which particles with different, but always well characterized, thermo-physical properties are employed. By sectioning and analyzing these particles, it is possible to determine the extent of melting, and of vaporization that has occurred. The results will be compared with predictions by use of the computer model.

This work is closely coordinated with the plasma modelling and gas-particle studies in progress at MIT, and with measurements of particle trajectories and temperatures of particles passing through plasma flames that are in progress at the Idaho National Engineering Laboratory.

Keywords: Plasma Processing

230. High-Temperature Gas-Particle Reactions

FY 1988
\$125,000

DOE Contact: Oscar P. Manley, (301) 353-5822

MIT Contacts: J. F. Elliott, (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

231. Mathematical Modeling of Transport Phenomena in Plasma Systems FY 1988
\$95,000

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

232. In-Process Control of Residual Stresses and Distortion in Automatic Welding FY 1988
\$41,000

DOE Contact: Oscar P. Manley, (301) 353-5822

MIT Contact: Koichi Masubuchi, (617) 253-6820

The objective of this research is to develop the technology of in-process control of residual stresses and distortion in automatic welding. The program consists of the following phases:

Phase 1: In-process control of residual stresses and distortion in some weldments.

Phase 2: Development of technologies for minimizing and eliminating, if possible, tack welds.

Phase 2-1: Analytical and experimental studies of thermal stresses during welding and forces acting on tack welds.

Phase 2-2: GMAW process control to minimize interference from tack welds.

Phase 3: Plans for future advancement of the technology of in-process control of residual stresses and distortion.

Phase 2-2 has been added since July 1986. The research efforts thus far covered all phases but Phase 3, which will be done at the end of the program.

Keywords: Automatic Welding, Control

233. Multivariable Control of the Gas-Metal Arc Welding Process FY 1988
\$156,000

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

234. Metal Transfer in Gas Metal Arc Welding FY 1988
\$127,000

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

235. Modeling and Analysis of Surface Cracks

FY 1988

\$192,000

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

236. Thermal Plasma Processing of Materials**FY 1988
\$361,000**

DOE Contact: Oscar P. Manley, (301) 353-5822

University of Minnesota Contact: E. Pfender, (612) 625-6012

A combined analytical/experimental program is carried out directed towards a better understanding of the interaction of particulate matter with thermal plasmas. One of the major objectives of the work is the development and diagnosis of a new plasma reactor which should solve the problems of particle injection, particle confinement, and particle dwell time in the plasma. Finally, it is intended to use this reactor for materials studies involving superconducting alloys.

The modeling work is primarily concerned with a detailed assessment of the relative importance of the numerous effects which determine heat, momentum, and mass transfer to and from particles injected into thermal plasmas. Diagnostic methods for the plasma include emission spectroscopy, laser Doppler anemometry, current, voltage, and calorimetric heat transfer measurements. Product powders will be analyzed using scaling and transmission electron microscopy, x-ray and electron diffraction, and measurements of the transition temperature for superconducting compounds.

Keywords: Plasma Processing, Plasma Diagnostics

237. Transport Properties of Disordered Porous Media from the Microstructure**FY 1988
\$94,000**

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

238. Inelastic Deformation and Damage at High Temperature

FY 1988

\$125,000

DOE Contact: Oscar P. Manley, (301) 353-5822

Rensselaer Polytechnic Institute Contact: Erhard Krempl, (518) 266-6432

A combined theoretical and experimental investigation is performed to study the biaxial deformation and failure behavior of 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

239. Energy Changes in Transforming Solids

FY 1988
\$165,000

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

240. Nondestructive Testing

FY 1988
\$250,000

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 Å 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

241. Effective Elastic Properties of Cracked Solids

FY 1988
\$55,000

DOE Contact: Oscar P. Manley, (301) 353-5822
Tufts University Contact: Mark Kachanov, (617) 628-5000, ext. 2821

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

A new approach to many cracks problems based on interrelating the average tractions on individual cracks is introduced. Its advantages are that it yields simple

analytical results which are quite accurate up to very high crack densities and that it can be applied to crack arrays or arbitrary geometry. Relation between deterioration of elastic properties and "damage" is discussed.

Keywords: Fracture, Elasticity

242. Laser Diagnostics of Plasma Assisted Chemical Vapor Deposition (PACVD) Processes FY 1988
\$185,000

DOE Contact: Oscar P. Manley, (301) 353-5822

United Technologies Research Center Contact: W. C. Roman, (203) 727-7590

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 and (5) demonstrated CARS collibrator sensitivity PACVD reactor of 10m Torr.

Keywords: Coating, Plasma Diagnostics

243. Elastic-Plastic Fracture Analysis Emphasis on Surface Flaws FY 1988
\$439,000

DOE Contact: Oscar P. Manley, (301) 353-5822

Idaho National Engineering Laboratory Contact: W. G. Reuter, (205) 526-0111

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

244. Continuous Damage Theory FY 1988
\$54,000

DOE Contact: Oscar P. Manley, (301) 353-5822

University of Illinois Contact: D. Krajcinovic, (312) 996-7000

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 losing the physical insights provided by the micromechanical studies. Once the theory has been checked on some benchmark problems (for which the pertinent micro-mechanical 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

245. New Ultrasonic Imaging and Measurement Techniques for NDE FY 1988
\$250,000

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. New techniques for ultrasonic computer tomographic imaging (reconstruction) are being explored that utilize elastic wave scattering models and the new multiviewing instrumentation. This could be an important innovation in that images so obtained are expected to be free of distortions due to the effects of material anisotropy and complex sample surfaces encountered in some current imaging techniques.
2. Novel techniques are being explored that can be used to produce ultrasonic transducers with specialized features to significantly improve flaw and material property detection and characterization. One such technique is now in place for the development of practical Gaussian beam transducers. This transducer has many benefits including no sidelobes and no rapid fluctuations in the near field. The technique is being extended with the objective of discovering ways

to fabricate other acoustic transducers that show essentially diffractionless features over a substantial propagation distance.

3. Studies have been initiated using broadband unipolar pulse techniques developed earlier on this project to characterize "fuzzy" boundaries in materials. This measurement depends largely upon being able to detect acoustic impedance changes over a small but finite spatial dimension, a condition that is nearly impossible to observe using conventional ultrasonics. The detection and characterization of "fuzzy" boundaries is of importance in the control of various materials processes and in the study of two-phase systems.

Keywords: Nondestructive Evaluation, Ultrasonic, Fracture

246. Effects of Crack Geometry and Near-Crack Materials Behavior on Scattering of Ultrasonic Waves for QNDE Applications FY 1988

\$68,000

DOE Contact: Oscar P. Manley, (301) 353-5822

Northwestern University Contact: J. D. Achenbach, (312) 491-5527

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

247. Diffusion and Ion Transport in Multicomponent Electrolyte Solutions FY 1988
\$140,000

DOE Contact: G. Kolstad, (301) 353-5822, FTS 233-5822

LLNL Contact: D. G. Miller, (415) 422-8074, FTS 532-8074

We have measured the four ternary diffusion coefficients D_{ij} at 25°C of the representative system NaCl-MgCl₂-H₂O at 25°C at 25 compositions. These compositions are at the 5 total molarities of 0.5, 1.0, 2.0, 3.0, and 3.8 (near saturation). At each total molarity we used (NaCl)/MgCl₂ mole ratios of 1/3, 1/1, and 3/1, as well as near tracer of NaCl in MgCl₂ and near tracer of MgCl₂ in NaCl. This project is part of a major 10-lab international collaboration (Miller is the coordinator) in which activity data, transport numbers, conductances, and tracer diffusion coefficients are being obtained. These data will be used to calculate the ternary ionic Onsager coefficients l_{ij} . These, in turn, will be compared with predictions of new statistical mechanical theories which may be valid to 1 molar. The Onsager coefficients may also be used to test semi-empirical models which yield ternary l_{ij} from l_{ij} data from the constituent binaries; such semi-empirical models may be valid up to 2-4 molar. Since concentrated electrolyte solutions are involved in many DOE programs, estimation procedures are quite important.

Keywords: Diffusion, Ion Transport, Concentrated Electrolyte Solutions, Multicomponent Systems, Estimation Procedures

248. Reactive Flow Modeling FY 1988
\$100,000

DOE Contact: G. Kolstad, (301) 353-5822, FTS 233-5822

LLNL Contact: Craig Tarver, (415) 423-3259, FTS 543-3259

The ignition and growth reactive flow model in the DYNAZD hydrodynamic computer code was successfully applied to a wide variety of experiments on TATB-, HMX-, TNT- and PETN-based solid explosives and propellants. These experiments include: embedded pressure and particle velocity gauges, laser interferometry, wedge tests, corner turning tests, gap tests, and failure diameter measurements. The phenomenological reactive flow model is used laboratory- and world-wide, and can address most solid explosives vulnerability and performance scenarios. Considerable progress has been made on the next generation reactive flow model, which solves shock initiation and detonation problems in more fundamental ways such as reacting all the material with temperature dependent Arrhenius chemical kinetics, and is applicable to problems that the current model cannot directly address.

Keywords: Explosives, Shock Initiation, Detonation

Division of Advanced Energy Projects

249. Aerodynamic Focusing of Particles and Heavy Molecules

FY 1988

\$67,000

DOE Contact: Ryszard Gajewski, (301) 353-5995

Yale University Contact: Juan Fernandez de la Mora, (203) 432-4347

Theoretical predictions indicate that, by accelerating a gas-particle mixture through a converging nozzle, it is possible to concentrate dense beams of small uncharged particles into a narrow focus under previously unexplored conditions. Because high resolution aerodynamic focusing could be exploited in a variety of applications, including "direct writing," basic studies are proposed in order to assess its limits and potential technological impact. Experiments with micron-size aerosol particles (for which Brownian motion effects are negligible) will first examine the ratio between the diameters of the nozzle exit and the focal region size, for which theory predicts values well in excess of 100. These studies will be subsequently extended down to the molecular level, by substituting the suspended particles with neutral vapors of a heavy species (Au, Wf₆, etc.) diluted in gaseous H₂ or He. The non-negligible Brownian motion of the heavy component leads then to a finite diffusive broadening of the focal region and sets a limit to the writing resolution attainable. Two theoretical approaches are proposed to study this defocusing phenomenon, one based on Brownian-dynamics simulations and the other exploiting the smallness of the random velocity as compared with the mean velocity of the heavy molecules. The phenomenon will also be studied experimentally, first visually by laser-induced fluorescence (LIF) of I₂ molecules seeded in high-speed jets of H₂ and He and also by sampling from He-Hg jets through a small orifice in a plate and analyzing for the concentration of Hg.

Keywords: Aerosols, Laser-Induced Fluorescence

250. Superconductive Electric Motor

FY 1988

\$394,000

DOE Contact: Ryszard Gajewski, (301) 353-5995

Los Alamos National Laboratory Contact: David S. Phillips, (505) 667-5128

The goal of this program is to evaluate the concept of an electric motor utilizing superconducting ceramic elements, certainly in the field coils and probably in the armature. This motor will probably be "homopolar" in geometry, since that system minimizes the AC disturbance experienced by the conductors. It will probably be fabricated by "macro-composite" technology within or on top of normal ceramic structural members. Several technological difficulties seem to impede this development—they will be addressed in turn. First, the critical current densities in ceramic superconductors are disappointingly low, calling for investigation of improved flux pinning routes based on both precipitation and grain-size control. Second, the large scale composite ceramic

processing technology envisioned for this application is itself unusual and requires a body of chemical compatibility data not yet extant. Research is needed in high temperature phase equilibria to help identify plausible ceramic matrices. Finally, the basic motor geometries previously envisioned for use with lower temperature metallic superconducting windings are largely dominated by the refrigeration equipment required to attain those low temperatures. Both the relaxed geometries apparently permitted by the higher temperature ceramic conductors and the refrigeration requirements remaining must be considered in the final choice of a design.

Keywords: Superconductivity, Electric Motor

251. Gas Jet Deposition of Metallic, Semiconducting and Insulating Films FY 1988
\$154,000

DOE Contact Ryszard Gajewski, (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

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.

Division of Physical and Technological Research

The Physical and Technological Research Division conducts physical, chemical, and instrumentation research related to the health and environmental aspects of energy technology development. Included are support of physical and chemical characterization studies, atmospheric sciences research, research on measurement and dosimetry techniques, and fundamental radiation biophysics.

Materials Properties, Behavior, Characterization or Testing

252. Semiconductor Radiation Detector Technology

FY 1988

\$364,000

DOE Contact: G. Goldstein, (301) 353-5348/FTS 233-5348

LBL Contact: F. S. Goulding, (415) 486-6432/FTS 451-6432

This project is designed to develop the technology of radiation detectors with emphasis on semiconductor and other solid-state detectors. The work includes basic detector material studies, development of new types of detectors, and specialized electronic signal processing techniques. The foundation of modern spectroscopy using semiconductor detectors has been laid by this project. Recent work has focused on native defects in germanium and silicon and on defects produced by radiation damage and the relationship of these defects and detector performance. Work is in progress on multielement silicon detectors and "on-chip" techniques for readout from these detectors. Recent work has also resulted in some very significant developments in signal processing that improves both the energy resolution and counting-rate performance of spectrometers. The results produced by this project are rapidly used by a number of United States companies involved in materials, detector, and spectrometer systems development.

Keywords: Semiconductors, Radiation Effects, Instrumentation and Technique Development

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.

Materials Properties, Behavior, Characterization or Testing

253. Irradiation Damage in Ceramics for Fusion Applications

FY 1988
\$400,000

DOE Contact: T. C. Reuther, (301) 353-4963

LANL Contact: F. W. Clinard, Jr., (505) 667-5102

Ceramics are tested in neutron and other irradiation fields to identify appropriate materials for use in the environment of a fusion reactor. The testing program focuses on mechanical, thermal, and electrical properties of structural and insulating ceramics, and is carried out in collaboration with workers at other laboratories in the U.S. and overseas.

Keywords: Insulators/Dielectrics - Ceramic, Structural Ceramics, Radiation Effects, Magnetic Fusion

254. Neutron-Interactive Materials

FY 1988
\$2,600,000

DOE Contact: T. C. Reuther, (301) 353-4963

ORNL Contact: E. E. Bloom, (615) 574-5053

The economics and acceptability of magnetic fusion energy depend heavily upon the successful performance of structural materials used to construct the first wall and blanket. The mechanical and physical properties of a wide range of materials are determined following exposure to high levels of neutron damage in both mixed spectrum and fast fission reactors. Corrosion behavior of materials in liquid metal and aqueous media is evaluated. The cost and environmental impact of disposing of radioactive components are being addressed. New reduced-activation alloys (austenitic and ferritic steels, vanadium alloys) are being developed with radioactive decay characteristics which are sufficiently rapid to eventually allow near-surface burial of used components. The potential for reduced-activation manganese-stabilized austenitic steels to meet the first wall and blanket requirements of the International Thermonuclear Experimental Reactor (ITER) is being assessed. This work includes studies of welding, stress corrosion cracking, and the effect of low-temperature neutron irradiation on fracture toughness.

Keywords: Magnetic Fusion Energy, Structural Materials, Physical/Mechanical Properties, Corrosion, Reduced-Activation Alloys, ITER

255. Neutron-Interactive Materials (U.S./Japan)

FY 1988
\$1,300,000

DOE Contact: T. C. Reuther, (301) 353-4963

ORNL Contact: E. E. Bloom, (615) 574-5053

This is a collaborative program with the Japan Atomic Energy Research Institute to determine the effects of neutron irradiation on the mechanical properties of austenitic stainless steels for magnetic fusion energy first wall and blanket applications. Irradiations are carried out in the High Flux Isotope Reactor (HFIR) to simulate the neutronic and thermal environment typical of an intermediate fusion machine such as the International Thermonuclear Experimental Reactor (ITER). The neutron spectrum of the HFIR is tailored to reproduce the helium generation rate and displacement damage rate characteristic of ITER. Post-irradiation measurements include creep, swelling, fatigue, and tensile properties. The effects of generating high concentrations of helium typical of a commercial reactor are simulated by irradiating in an unmodified HFIR spectrum.

Keywords: Magnetic Fusion Energy, Austenitic Stainless Steels, Neutron Irradiation Mechanical Properties

256. Development of Vanadium-Base Alloys for Fusion Reactor Applications FY 1988
\$325,000

DOE Contact: T. C. Reuther, (301) 353-4963
ANL Contact: D. L. Smith, (312) 972-5180

Radiation resistant vanadium-base alloys with low long-term residual radioactivity are being developed for fusion reactor application. Work is focused on the V-Cr-Ti-Si systems and includes effects of nonmetallic impurities on mechanical properties, effects of neutron radiation, and chemical compatibility.

Keywords: Metals: Non-Ferrous, Refractory Metals, Corrosion, Hydrogen Attack, Radiation Effects, Mechanical Properties, Magnetic Fusion

257. Corrosion/Compatibility of Fusion Reactor Structural Materials FY 1988
\$250,000

DOE Contact: T. C. Reuther, (301) 353-4963
ANL Contact D. L. Smith, (312) 972-5180

Corrosion/compatibility investigations on the performance of candidate fusion reactor structural materials are conducted in both liquid metal and aqueous environments. Emphasis is placed on the effects of liquid metal and water chemistry, e.g., O, N, C, and H concentrations, on both corrosion and stress corrosion. Structural materials include vanadium-base alloys, and austenitic and ferritic steels. The liquid metal work focuses primarily on liquid lithium, but includes effort on the Pb-Li eutectic alloys.

Keywords: Metals: Non-Ferrous, Corrosion-Aqueous, Corrosion-Liquid Metal, Magnetic Fusion

258. Solid Breeder Materials FY 1988
\$290,000

DOE Contact: S. Berk, (301) 353-4171
ANL Contact: C. Johnson, (312) 972-7533

The lithium containing ceramics Li_2O , LiAlO_2 , Li_4SiO_4 , and Li_2ZrO_3 are receiving consideration as tritium breeder materials for fusion reactors. A data base of thermochemical thermophysical, and transport properties is being developed. Surface adsorption/desorption characteristics for $\text{H}_2/\text{H}_2\text{O}$ on LiAlO_2 and Li_4SiO_4 is being investigated. A computer model for tritium transport and release from candidate materials is being developed. The program continues to evaluate the implications of

current in-reactor experiments on material performance and on tritium transport and release. An international collaborative effort has been established that comprises in-reactor and laboratory property studies and the exchange of personnel.

Keywords: Lithium Ceramics, High Temperature Properties, Magnetic Fusion, Tritium, Transport Models

259. Tritium Oxidation Kinetics

FY 1988
\$340,000

DOE Contact: S. Berk, (301) 353-4171

ANL Contact: R. F. Mattas, (312) 972-8673

The rate of oxidation of pure tritium which has permeated through a stainless steel tube is being investigated. The oxidation rates are measured in an environment characteristic of a fusion reactor tritium breeding system. The oxygen concentration ranges from <1 to 2000 ppm, temperatures range from 350-550°C, tritium pressures range from 10^{-4} to 1 Pa, and hydrogen concentrations range from <0.001 to 20 ppm. Results indicate that high oxygen concentrations, in excess of 500 ppm, are required to yield a conversion to tritiated water of >99 percent.

Keywords: Metals: Ferrous, Surface, Magnetic Fusion

260. FLIBE (Fluorine-Lithium-Beryllium Salt)

FY 1988
\$77,000

DOE Contact: S. Berk, (301) 353-4171

ANL Contact: R. F. Mattas, (312) 972-8673

FLIBE, as a molten salt, is a potential tritium breeding material for fusion reactors. This project is examining the possibility of adding small amounts of MoF_6 to help control corrosion of the structural material, e.g., refractory metal, and to control tritium solubility in the FLIBE.

Keywords: Coatings and Films, Metals: Non-Ferrous, Corrosion-Molten Salt, Magnetic Fusion

261. Statistical Theory of Radiation Effects

FY 1988
\$105,000

DOE Contact: T. C. Reuther, (301) 353-4963

UCLA Contact: N. M. Ghomiem, (213) 825-4866

This work provides a fundamental understanding of the underlying physical phenomena which govern the interaction of radiation with structural and non-structural materials in a fusion environment. Since this environment is impossible to duplicate experimentally at the present time, computer simulations and theoretical models are developed to investigate the following problems.

1. Interaction of atomic collision cascades generated by fusion neutrons with materials;
2. Atomic clustering and microstructure evolution under irradiation;
3. Dislocation dynamics during high temperature deformation under irradiation.

Results of this research will identify critical irradiation and material variables which govern the irradiation response of materials in the following categories: (1) swelling, (2) radiation hardening, (3) radiation embrittlement, (4) loss of ductility, and (5) creep deformation.

Keywords: Metals: Ferrous, Creep, Crystal Defects, Radiation Effects, Structure, Magnetic Fusion

262. Welding of Low Activation and Fusion First Wall Materials

FY 1988
\$90,000

DOE Contact: T. C. Reuther, (301) 353-4963

Auburn University Contact: B. A. Chin, (205) 826-4575

This project is investigate the weldability of low activation ferritic alloys and the problems which occur during the welding of He containing previously irradiated materials. The low activation alloys which are being investigated are modifications of the 2.5, 9 and 12 Cr ferritic steels. Welding studies of irradiated materials are being conducted using tritium doped 316 and 12 Cr steels. The tritium is used to produce He in the material to simulate irradiation exposure without the associated activity caused during irradiation.

Keywords: Metals: Ferrous, Welding, Magnetic Fusion

263. Neutron Interactive Materials Program

FY 1988
\$1,555,000

DOE Contact: T. C. Reuther, (301) 353-4963, FTS 233-4963

PNL Contact: D. G. Doran, (509) 376-3238, FTS 444-3238

In support of the National Fusion Materials Program, a number of ferrous and non-ferrous low activation materials are being developed and tested for radiation sensitivity. Emphasis is on, but not limited to, alloys for first wall/blanket applications.

The short-term goal is to aid in meeting CIT/ITER design needs. The long-term goal is to develop an understanding of radiation effects in order to provide a sound basis for materials development.

The scope of the program includes alloy development, performance of irradiation experiments, coordination of Fusion MOTA irradiations, PIE of mechanical properties (especially tensile, fracture toughness and Charpy) and microstructure and their correlation, evaluation of environmental effects on crack growth processes, analysis and modeling, and coordination of other fusion materials program activities, including international ones such as the IEA initiative leading to a high energy, high flux neutron source for materials testing.

Keywords: Magnetic Fusion, Radiation Effects, Creep, Fracture, Structure, Metals:
Ferrous and Non-Ferrous

264. BEATRIX-II

FY 1988
\$1,150,000

DOE Contact: T. C. Reuther, (301) 353-4963, FTS 233-4963

PNL Contact: G. W. Hollenberg, (509) 376-5515, FTS 444-5515

The BEATRIX-II experiments in the FFTF reactor evaluate the *in situ* tritium release characteristics of lithium ceramics at high burn-up levels. High tritium release rates and stability are required for lithium ceramics to satisfy the fueling needs of D-T fusion reactors in the future. Lithium oxide is being evaluated in the present experiments with a temperature change canister and a temperature gradient canister. In the future, it is anticipated that another contender, Li_2ZrO_3 , will be irradiated along with canisters to evaluate the effect of irradiation on tritium permeation through barrier coated and bare stainless steel.

Keywords: Magnetic Fusion, Radiation Effects, Ceramics

265. Neutron Interactive Materials Calculations**FY 1988**

DOE Contact: T. C. Reuther, (301) 353-4963

LLNL Contact: M. Guinan, (415) 422-5776

The first goal of this project is the development of a new optimized (fully vectorized) molecular dynamics code for the Cray 2, utilizing recently development many-body potentials. Under the IEA-Annex II Agreement on Fusion, input from users in the U.S., EC, and Japan have contributed. We expect initial results in FY 1989.

Keywords: Radiation Effects, Radiation Theory, Low Activation Materials, Corrosion

**266. Damage Analysis and Fundamental Studies for Fusion
Reactor Materials****FY 1988****\$200,410**

DOE Contact: T. C. Reuther, (301) 353-4963

University of California Santa Barbara Contact: G. R. Odette, (805) 961-3525

The focus of this research program is to develop a fundamental understanding of the effects of neutron irradiation on the microstructural evolution and consequent mechanical properties and dimensional stability of structural materials for fusion reactors. It is the intent that this understanding be used to assist in predicting materials behavior in a fusion reactor from data that is largely derived from fission reactors. Work this year has continued to support the development of isotope tailoring experiments to systematically examine the effects of He/dpa on the microstructure and property evolution of austenitic and ferritic steels. We have also continued to develop techniques to extract fracture structure mode transition behavior with small (3mm diameter) discs, and we have examined micromechanical models of cleavage fracture in ferritic steels. The latter work has assisted in identifying an experimental program to address improving the resistance of ferritic steels to fracture in an irradiation environment.

Keywords: Radiation Effects, Microstructure, Fracture

267. Plasma-Materials Interactions**FY 1988****\$990,000**

DOE Contact: M. M. Cohen, (301) 353-4253

Sandia Contact: K. L. Wilson, (415) 294-2497

The interaction of hydrogenic plasmas with candidate first wall materials is evaluated in order to increase plasma-interactive component lifetime and to improve plasma performance in magnetic fusion energy reactors. Recent measurements have focused on the interaction of tritium plasmas with graphites, carbon fiber composites, and beryllium. Properties under study include tritium uptake and release kinetics, plasma

erosion rates, and the properties in redeposited materials. Laboratory simulations and measurements in existing magnetic fusion energy reactors are used to assess plasma-material interactions.

Keywords: Coatings and Films, Graphite, Composites, Metals: Non-Ferrous, Erosion, Hydrogen Attack, Surface, Magnetic Fusion

268. Aqueous Corrosion Studied in Support of the ITER Project FY 1988
\$300,000

DOE Contact: S. Berk, (301) 353-4171
RPI Contact: D. J. Duquette, (518) 276-6459

Aqueous corrosion studies are being performed on austenitic stainless steels in the annealed and sensitized conditions in lithium hydroxide and lithium nitrate solutions. Tests are being performed to categorize the localized corrosion and stress corrosion cracking resistance of the alloys. Electrochemical polarization coupled with slow strain rate techniques are being used in this study. These experiments are being performed to examine the use of stainless steels as structural materials for the International Thermonuclear Reactor (ITER). This project is in the initial phase of a multi-year effort.

Keywords: Metals, Corrosion-Aqueous, Magnetic, Fusion

269. Key Issues of Fusion Nuclear Technology Development FY 1988
\$ 0

DOE Contact: S. E. Berk, (301) 353-4171
UCLA Contact: M. A. Abdou, (213) 206-0501

Under this DOE contract, our activities covered the development of a computer model for tritium transport inside solid breeders, including the key transport mechanisms of grain and grain boundary diffusion, surface adsorption/desorption and diffusion through interconnected porosities. An important objective of this effort is to use the code in conjunction with experimental data from irradiated solid breeder experiments to obtain and understand fundamental transport properties of solid breeder ceramics.

Also included in this contract was the conceptualization and analysis of thermal conductance gap for solid breeder blankets for the next fusion technology test reactor. A packed bed configuration was proposed based on its attractive features. An experimental and modeling program was planned to address the key issues of conductance predictability and controllability for such a configuration.

Keywords: Ceramics, Transport, Predictive Behavior Modeling, Thermal, Modeling, Fusion

270. Thermal Convection Loop Experiments and Analysis of Mass Transport in Lithium/Fe-12Cr-1MoVW Systems FY 1988
\$200,000

DOE Contact: S. E. Berk, (301) 353-4171
UCLA Contact: M. A. Abdou, (213) 206-0501

For lithium-cooled fusion blankets, compatibility between the coolant and structural material imposes restrictions on the operating parameters, such as temperature and lithium purity. Experimental data on mass transport in the lithium/Fe-12Cr-1MoVW system were obtained from two thermal convection loops which spanned the temperature range relevant to fusion. It was found that mass transport and deposition, as measured by specimen weight change, were not simple functions of temperature for the entire temperature range investigated. At low temperatures, the mass transfer behavior and surface morphology were dominated by impurity reactions of nitrogen and carbon in the lithium with the steel. Below 450°C, nitrogen levels were sufficiently high to allow the formation of the adherent, protective corrosion product Li_9CrN_5 . In this regime, weight losses were insensitive to temperature. At high temperatures, the nitrogen content of the lithium is not sufficient to allow formation of the protective layer, and in this regime the weight changes were strongly dependent on temperature. The corrosion above 580°C was exponentially related to temperature, with an activation energy of dissolution of 63.7 kJ/mole. The experimental effort was supported by analysis of the mechanisms and processes of mass transport and deposition. Physical models and descriptions of the processes were developed, and limitations on the amount of carbon in lithium to prevent carbide precipitation were determined. Recommendations for the development of an alloy more resistant to attack by lithium were made.

Keywords: Corrosion, Liquid Metal

271. Solid Breeder Materials Program FY 1988
\$395,000

DOE Contact: S. E. Berk, (301) 353-4171, FTS 233-4171
PNL Contact: G. W. Hollenberg, (509) 376-5515, FTS 444-5515

A wide variety of lithium ceramics: Li_2O , LiAlO_2 , Li_4SiO_4 , Li_2ZrO_3 , Li_8ZrO_8 , etc., in the form of pellets, spores and single crystals from national laboratories in Europe, Japan and the United States are being irradiated in closed capsules. High tritium release rates and stability are required of these lithium ceramics so that they may be used for fueling D-T fusion reactors. Post-irradiation examination of the materials

includes measurement of swelling, tritium and helium retention, and microstructural changes. Experiments to date have revealed the stability of Li_2ZrO_3 during irradiation and significant swelling in Li_2O at high temperatures and burn-ups.

Keywords: Magnetic Fusion, Radiation Effects, Ceramics

272. High Heat Flux Irradiations

FY 1988
\$60,000

DOE Contact: M. M. Cohen, (301) 353-4253, FTS 233-4253

PNL Contact: O. D. Slagle, (509) 376-3424, FTS 444-3424

A variety of metals, composites and coated material are being irradiated in the FFTF reactor in order to evaluate their irradiation stability. These potential high heat flux materials must be able to survive thermal structural and plasma interactive challenges in fusion reactors during normal operation of the plasma even after irradiation to high neutron fluences. Unirradiated carbon/carbon composites are being irradiated now. The effect of non-isotropic fiber swelling/shrinkage on structural integrity and the degradation of thermal conductivity is of specific interest.

Keywords: Composites, Radiation Effects, Magnetic Fusion

273. Materials Studies for Magnetic Fusion Energy Applications at Low Temperatures

FY 1988
\$400,000

DOE Contact: D. Beard, (301) 353-4958

NIST Contact: R. P. Reed, (303) 497-3870

The program objectives are: (1) development of suitable structural alloys, insulators, and joining techniques for fusion magnets; (2) mechanical and physical property study and characterization of candidate materials; (3) establishment of appropriate low temperature measurement and material standards; (4) and efficient information transfer to magnet programs using handbooks, workshops, reports, and collaborative programs.

The focus of structural alloy research is the development of nitrogen-strengthened austenitic steels with improved strength and toughness at 4 K. The development of weld procedures and filler metals to achieve matching strength and toughness has placed emphasis on ductile fracture at low temperatures. Structural insulator research focuses on fiberglass-reinforced, epoxy matrix composites and emphasis is now placed on development of radiation-resistant insulators. For compact-ignition tokamak reactors,

high-strength/high-conductivity copper alloys have been studied. Property measurements at low temperatures include tensile, fracture toughness, creep, fatigue, fatigue crack-growth rates and elastic.

Keywords: Composites, Insulators, Metals: Ferrous and Non-Ferrous, Tensile, Creep, Fatigue, Fracture, Radiation Effects, Welding, Magnetic Fusion, Cryogenic Temperatures

Instrumentation and Facilities

274. Beam Plasma Neutron Source

FY 1988
\$60,000

DOE Contact: T. C. Reuther, (301) 353-4963

LLNL Contact: F. H. Coensgen, (415) 422-1166

A conceptual design of a plasma based D-T 14 MeV neutron source will be initiated for use in development of low-activation, long-lived fusion reactor materials. This facility will be designed to produce uncollided 14 MeV neutron wall loads in the range of 5 to 10 MW/m and for continuous operation.

Keywords: Fusion, Irradiation, Magnetic Fusion, Materials

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, 1988 (DOE/ER-0378), Abstracts of Phase II Awards, 1988 (DOE/ER-0379), and Abstracts of Phase II Awards, 1987 (DOE/ER-0337). 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

275. Technical Support to West Valley Demonstration Project FY 1988
\$800,000

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 in (a) characterizing high-level waste materials from West Valley storage tanks; (b) characterizing potential operating conditions of an ion exchange process that removes cesium from the high-level waste supernate; (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); and (d) characterizing the individual process operations to show control of the process and the final waste form composition.

Keywords: Ion Exchange, Borosilicate Glass, Process Control, Radioactive Waste Host

Materials Properties, Behavior, Characterization or Testing

276. Materials Characterization Center Testing of West Valley Formulation Glass

FY 1988
\$480,000

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. Finally, the MCC is providing assistance to West Valley related to enhancing the quality of their analytical data.

Keywords: Radioactive Waste Host

277. Development of Test Methods and Testing of West Valley Reference Formulation Glass

FY 1988
\$750,000

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 reference formulation glass waste forms for the West Valley Demonstration Project; and (c) studying means to maximize the region of acceptable quality around the point of optimal durability for the borosilicate glass waste form.

Keywords: Radioactive Waste Host

278. Process and Product Quality Optimization for the West Valley Waste Form

FY 1988
\$255,000

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 and (b)

developing methods for control of product quality during routine manufacture of the West Valley Demonstration Project waste form.

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 assure 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, notwithstanding 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 a net fiscal year appropriation of \$0. Total obligations for all uranium enrichment activities in FY 1988 was \$934 million.

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 1988 was \$17,462,000. 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 plants operate on the principle that lighter weight gaseous isotopes have slightly higher average velocities and thus can be made to diffuse through a porous barrier more rapidly than heavier species. Two streams can be created, one enriched in the lighter isotope and one depleted. Because enrichment for a single cycle, or stage, is very small, a cascade of stages is required. For example, a plant constructed for producing 4 percent assay U-235 would contain about 1200 stages. Although many other methods for enrichment are still being investigated and another production technique is being used in parts of Europe, diffusion

plants today still provide approximately 90 percent of the world's enrichment services. 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

279. Gaseous Diffusion: Barrier Quality

FY 1988
\$2,755,000

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

280. Gaseous Diffusion: Materials and Chemistry Support

FY 1988
\$2,975,000

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

Atomic Vapor Laser Isotope Separation (AVLIS)

The AVLIS process is based on utilizing the differences in the electronic spectra of atoms 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 metal product is as a liquid that is allowed to solidify upon withdrawal.

In June 1985, DOE selected AVLIS for further development and possible future deployment into the uranium enrichment enterprise. The primary emphasis for AVLIS in FY 1988 was to continue activities that will enable an integrated operation of full-scale lasers and separators in 1991/1992 for a series of mass balance enrichment runs. This demonstration will provide a base of technical and economic information adequate to accomplish three goals: (1) support a detailed design for an AVLIS production plant,

(2) establish a high confidence plan for integration of AVLIS into the nuclear fuel cycle, and (3) allow an AVLIS production deployment decision. Available resources in FY 1988 were focused on this goal and the activities included operation of large test beds and key subsystems. Procurement of the second phase of the Laser Demonstration Facility continued. In addition, a one-half scale separator facility continued operation in for FY 1988 to demonstrate enrichment and to provide component development and design data for a full scale separator. The AVLIS materials activities in FY 1988 were largely in support of the separator system and uranium processing activities. The latter technologies will have strong economic leverage for an 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 AVLIS metal feed and product into the existing uranium oxide/fluoride nuclear fuel cycle.

281. AVLIS: Separator Materials FY 1988
\$8,267,000

Selection and testing of candidate structural and component materials and coatings for the AVLIS separator system. Fabrication of components and subsystems for AVLIS process integrated enrichment tests.

Keywords: Enrichment, Uranium, Laser Isotope Separation, Atomic Vapor Laser Isotope Separation (AVLIS)

282. AVLIS: Uranium Processing FY 1988
\$3,465,000

Design, fabrication and operation of uranium electrolysis cells for AVLIS feed. Bath chemistry, solubility and construction materials studies. Design and operation of prototype AVLIS product purification equipment. Flowsheet development and demonstration of schemes for converting purified product into commercial nuclear fuel oxides.

Keywords: Enrichment, Uranium, Laser Isotope Separation, Atomic Vapor Laser Isotope Separation (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

283. Fuel Process Development

FY 1988
\$960,000

DOE Contact: J. E. Fox, (301) 353-3985

GA Technologies Contact: O. M. Stansfield, (619) 455-2895

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 defective particle fractions. 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

284. Fuel Materials Development

FY 1988
\$635,000

DOE Contact: J. E. Fox, (301) 353-3985

GA Technologies Contact: O. M. Stansfield, (619) 455-2895

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

285. Fuel Development and Testing

FY 1988
\$2,120,000

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.

Keywords: Fuel, Ceramics, Coatings, Microstructure, Radiation Effects, Diffusion, High Temperature Service

286. Graphite Development

FY 1988
\$155,000

DOE Contact: J. E. Fox, (301) 353-3985
GA Technologies Contact: R. Vollman, (619) 455-3310

This work supports the selection, characterization, and qualification of graphite materials for applications in HTGRs. These efforts are focused on the development of an improved 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 element of this work is the development of graphite materials behavior and failure criteria required for reliable design analyses.

Keywords: Graphite, Ceramics, Irradiation Effects, Strength, Corrosion, High Temperature Service

287. Graphite Development and Testing

FY 1988
\$736,000

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 an improved 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

288. Metals Technology Development FY 1988
\$35,000

DOE Contact: J. E. Fox, (301) 353-3985

GA Technologies Contact: W. R. Johnson, (619) 455-2905

This work includes activities to characterize and qualify the metallic materials selected for applications in the HTGR system. Tasks involve work to identify and produce 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

289. Structural Materials Development FY 1988
\$715,000

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 support the design of 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

290. Advanced Gas Reactor Materials Development**FY 1988
\$290,000**

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

291. Fuel Performance Demonstration FY 1988
\$5,300,000

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 140,000 MWD/T burn-up and will continue irradiation to cladding breach. Program plans to complete initial off-normal testing in EBR-II, including RBCB and fabrication variable tests.

Keywords: Breeder Reactor, Actinides, Fuel

292. Pyroprocess Development FY 1988
\$4,625,000

DOE Contact: David L. Hoof, (301) 353-2964/FTS 233-2964
ANL Contact: Leslie Burris, (312) 972-4383/FTS 972-4383

Establish technical feasibility of the proposed pyroprocesses including electrorefining, halide slagging, and waste treatment processes. Program will select optimum cathode concept/configuration for electrorefining process, conduct engineering scale (20-40 kg) demonstration of electrorefining with uranium, and run laboratory-scale demonstration of waste treatment processes.

Keywords: Waste Treatment, Electrorefining, Pyroprocesses

293. Fuel Safety Experiments and Analysis FY 1988
\$4,000,000

DOE Contact: John Lewellen, (301) 353-3684/FTS 233-3684
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

294. Core Design Studies

FY 1988
\$1,800,000

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 PRISM and SAFR, 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. Support the conversion of EBR-II and FFTF to metal-fueled cores. Conduct reference metal core designs for SAFR and PRISM. Conduct FFTF metal core reactivity coefficients and neutronics performance evaluation. Evaluate impact of actinide self-consumption in closed fuel cycle. Determine bias factors and uncertainties for FFTF metal core.

Keywords: Actinides, Reactor Design, Breeding Ratio, Metal Core

295. Fuel Cycle Studies

FY 1988
\$3,800,000

DOE Contact: David L. Hoof, (301) 353-2964/FTS 233-2964

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

296. LMR Technology R&D FY 1988
\$5,500,000

DOE Contacts: John Lewellen, (301) 353-3684/FTS 233-3684 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

297. Structural Design/Life Assurance Technology FY 1988
\$500,000

DOE Contact: Andrew Van Echo, (301) 353-3930/FTS 233-3930

ORNL Contact: Jim Corum, (615) 574-0718/FTS 624-0718

Provide methods, rules, and criteria needed to resolve life assurance deficiencies with regard to welds, geometric discontinuities, and creep-fatigue loadings. Provide structural design methods, rules, and criteria, supported by results of tests and analyses, needed to qualify modified 9 Cr-1 Mo steel for LMR service. Provide comprehensive plan, including structural and material testing requirements, initiate development of flaw assessment procedures applicable to modified 9 Cr-1 Mo steel components and LMR service conditions. Program will initiate test for developing flaw assessment procedure for modified 9 Cr-1 Mo steel. Provide comprehensive plan for development of flaw assessment procedures applicable to modified 9 Cr-1 Mo steel components under LMR service conditions. Provide recommendations regarding design use of creep-fatigue failure criterion based on ductility exhaustion. Evaluate simplified creep-fatigue method for modified 9 Cr-1 Mo. Run second thermal shock failure test of modified 9 Cr-1 Mo steel cylinder. Evaluate concerns about weldments and notch-like geometric discontinuities.

Keywords: Fatigue, Failure Testing, Joining and Welding, Creep

298. Modified 9 Cr-1 Mo Steel Design Properties**FY 1988
\$390,000**

DOE Contact: Andrew Van Echo, (301) 353-3930/FTS 233-3930

ORNL Contact: Phil Rittenhouse, (615) 574-5103/FTS 624-5103

Continue long-term creep-rupture tests on base metal, weldments, and castings. Perform mechanical property surveillance tests on thermally aged and fabricated materials. Continue long-term creep-fatigue interaction and mean-stress tests. Initiate creep-crack propagation tests in support of flaw assessment procedures. Program will initiate creep-crack propagation experiments. Report effects of long-term thermal aging on tensile and toughness behavior. Report metallographic and mechanical property results relative to hot cracking during bending of pipes.

Keywords: Creep, Fatigue, Tensile Testing, Toughness

299. Nondestructive Testing Technology for Heat Exchangers**FY 1988
\$130,000**

DOE Contact: David L. Hoof, (301) 353-2964/FTS 233-2964

ORNL Contact: Robert W. McClung, (615) 574-4466/FTS 624-4466

Investigate materials, design, and fabrication modifications necessary for operation of 400°F eddy-current and ultrasonic probes in sodium. Determine optimum instrument parameters for operation of 400°F probes. Demonstrate ultrasonic problems with improved 400°F operation. Determine optimum operating parameters for high temperature probes. Establish probe material and design modifications needed for operation in sodium.

Keywords: Nondestructive Testing, Eddy Currents, Ultrasonic

300. Nuclear Systems Materials Handbook**FY 1988
\$30,000**

DOE Contact: C. Chester Bigelow, (301) 353-4299/FTS 233-4299

ORNL Contact: Martin F. Marchbanks, (615) 574-1091/FTS 624-1091

Continue mechanical property correlations development and incorporate into the Nuclear Systems Materials Handbook (NSMH). Prepare NSMH pages describing baseline creep properties of modified 9 Cr-1 Mo steel. Prepare NSMH pages describing continuous cycling fatigue behavior of modified 9 Cr-1 Mo steel. Prepare NSMH pages describing effects of thermal aging on modified 9 Cr-1 Mo steel. In FY 1988, the program was phased out.

Keywords: Mechanical Properties, Creep, Fatigue

301. MOTA Fabrication and Operation

FY 1988
\$1,278,000

DOE Contact: Andrew Van Echo, (301) 353-3930/FTS 233-3930

WHC Contact: Roger W. Powell, (509) 376-4529/FTS 444-4529

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.

Keywords: Irradiation, Environmental Testing

302. Absorber Development

FY 1988
\$193,000

DOE Contact: C. Chester Bigelow, (301) 353-4299/FTS 233-4299, Andrew Van Echo, (301) 353-3930/FTS 233-3930

WHC Contact: Robert D. Leggett, (509) 376-2505/FTS 444-2505

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 (EFPD). Provide report on absorber performance to date in FFTF.

Keywords: Control Rods, Nuclear Absorbers

303. FFTF Metal Fuel Testing

FY 1988
\$1,025,000

DOE Contact: Andrew Van Echo, (301) 353-3930/FTS 233-3930

WHC Contact: Robert D. Leggett, (509) 376-2505/FTS 444-2505

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, Metals: Non-ferrous

304. Core Demonstration Experiment (CDE)

FY 1988
\$2,393,000

DOE Contact: Jacob Glatter, (301) 353-3921/FTS 233-3921

WHC Contact: Robert D. Leggett, (509) 376-2505/FTS 444-2505

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, Metals: Non-ferrous

305. International Collaboration

FY 1988
\$161,000

DOE Contact: Jacob Glatter, (301) 353-3921/FTS 233-3921

WHC Contact: Robert D. Leggett, (509) 376-2505/FTS 444-2505

This project includes completing fabrication of the Dispersion Strengthened Ferritic Steel (DSF-1) fuel test with cladding types agreed to with DOE and PNC, monitoring irradiation performance in FFTF of PNC fuel (MFA-1 and -2) and blanket (MBA-1) assemblies, characterizing production lots of MA-957 cladding, reconstituting MOTA NAM-1 test specimens and shipping 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

306. Development of Improved Thermoelectric Materials for Space Nuclear Power Systems FY 1988
\$200,000

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 $1 \times 10^{-3} \text{C}^{-1}$ over the temperature range of 300-1000°C.

During FY 1988, 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

307. Development of an Improved Process for the Manufacture of DOP-26 Iridium Alloy Blanks FY 1988
\$730,000

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.

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).

Initial scale-up to a nominal 2" diameter x 8 kg consumable arc melt extrusion billet size was proven technically feasible as evidenced by the successful high temperature impact test of uranium simulant fuel clad impact test hardware produced from the improved sheet process blanks.

Reproducibility of good quality nominal 2" diameter consumable arc cast ingots proved to be a problem due to equipment inadequacies. Scale-up to a 2½" diameter x 10 kg ingot size coupled with minor surface conditioning appears to have mitigated the ingot quality problem. Procurement of a state-of-the-art consumable arc melting furnace was initiated. Optimization of the extrusion and rolling processes was initiated.

Keywords: Consumable Arc Melt, Extrusion, Noble Metal

308. Carbon Bonded Carbon Fiber Insulation Manufacturing Process Development and Product Characterization FY 1988
\$600,000

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.

Procurement in production quantity of all raw materials including the new rayon fiber was completed. Process optimization studies which were about 70 percent complete are continuing into FY 1989. Equipment relocation in a dedicated centralized area was completed. Procurement of a computer-aided image analyzer for simplification of X-Ray (film) inspection was initiated. Process and product qualification is scheduled for completion in FY 1989.

Keywords: Insulators/Thermal, High Temperature Service, Fibers

Device or Component Fabrication, Behavior or Testing

309. Nondestructive Testing Methods Development and Application to Thermoelectric Materials and Devices FY 1988
\$170,000

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

310. Characterization of State-of-the-Art Improved Silicon-Germanium Thermoelectric Device/Materials and Silicon-Germanium Materials Development FY 1988
\$500,000

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., close packed arrays of couples) device is being studied. Long-term stability of thermal and electrical properties of thermoelectric materials and devices will be studied.

In addition, exploratory studies of the potential of mechanical alloying for producing unique high performance Silicon-Germanium type thermoelectric materials was initiated.

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 \$67 million in FY 1988 including approximately \$37 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

The objectives of the Commercial Spent Fuel Management (CSFM) Program are to encourage and expedite the implementation of existing and new spent nuclear fuel storage technologies; to accelerate the availability of dry storage and rod consolidation technologies through licensed cooperative demonstrations at reactor sites and unlicensed testing at Federal facilities; and to provide the planning for a Federal capability to store up to 1900 MT of spent fuel for those utilities that the NRC determines cannot reasonably provide increased at-reactor storage when needed.

Materials Properties, Behavior, Characterization or Testing

311. Development of Criteria for Nuclear Spent Fuel Storage in Air FY 1988
\$650,000

DOE Contact: C. R. Head, (202) 586-9606
PNL Contact: E. R. Gilbert, (509) 375-2533

This project performs applied research to characterize the oxidation behavior of commercial UO_2 spent nuclear fuel. In case a few spent fuel assemblies containing fuel rods with undetected reactor induced breached cladding are placed into dry storage, this research will assure that dry storage conditions will not permit significant oxidation of the exposed UO_2 . Laboratory tests are being conducted to determine the oxidation behavior of spent fuel and unclad UO_2 . The tests are in the range of 135 to 230°C and the test matrix was statistically designed to provide data to determine acceptable fuel temperatures and storage criteria. Test variables also include an imposed gamma field, typical of that in a dry storage cask, and moisture and burnup levels bracketing those encountered in a dry storage cask.

Keywords: Fuel, UO_2 Oxidation, Interim Dry Storage

312. Development of Zircaloy Deformation and Creep Rupture Models for Predicting Cladding Behavior During Interim Dry Storage FY 1988
\$49,000

DOE Contact: C. R. Head, (202) 586-9606
PNL Contact: E. R. Gilbert, (509) 375-2533

This project predicts the temperature-time conditions to which commercial LWR spent fuel can be exposed during interim dry storage without undergoing significant creep rupture of the Zircaloy fuel cladding. It uses the existing data base on nonirradiated Zircaloy cladding to develop theoretical models for deformation and creep rupture for

spent fuel interim dry storage conditions, and uses the models to predict the envelope of acceptable temperature-time storage conditions. Models of deformation include diffusional creep, grain boundary sliding, and diffusion controlled dislocation creep. Models of degradation by creep include transgranular cracking, triple point cracking, and cavitation. A comparison of predictions with the Federal Republic of Germany deformation and creep rupture data on spent fuel rods and irradiated Zircaloy cladding provide a means of verifying the predictions for these prototypic cases. A computer program to predict allowable storage temperature-time histories using deformation and fracture map methodology was converted to mainframe and popular PC formats. Documentation of the program was prepared and will be published in FY 1989.

Keywords: Cladding Rupture, Fuel, Zircaloy Cladding

313. PWR and BWR Spent Fuel Assembly Crud Composition, Characterization, and Effects on Operations

FY 1988
\$12,000

DOE Contact: C. R. Head, (202) 586-9606

PNL Contact: W. J. Bailey, (509) 375-2615

In FY 1986 two PWR and two BWR spent fuel assemblies were acquired in order to disassemble these assemblies and retrieve individual fuel rods. Two PWR fuel assemblies have been disassembled to remove 24 fuel rods. The pulling forces required for fuel rod removal were monitored during the disassembly operations, qualitative observations were made and a videotape prepared.

In FY 1988 these operations were completed on a BWR spent fuel assembly. Upon the completion of disassembly operations, the fuel rods were examined with a periscope and observations made about the fuel rod crud. These observations included uniformity of deposition, thickness, and the difficulty of removing the crud. A letter report was issued summarizing the results of these activities in FY 1988. A technical paper will be prepared and published in FY 1989.

Keywords: Disassemble, Fuel, Crud

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 1988.)

Materials Properties, Behavior, Characterization or Testing

314. Waste Package Environment FY 1988
\$935,000

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

315. Waste Form Testing FY 1988
\$2,951,000

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

316. Metal Barrier Testing FY 1988
\$2,162,000

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

317. Other Engineered Barrier Waste Package Components FY 1988
\$64,000

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

318. Integrated Testing FY 1988
\$1,281,000

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

319. Waste Package: Performance Assessment FY 1988
\$622,000

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

320. Research on Geochemical Modeling of Radionuclide Interaction with a Fractured Rock Matrix FY 1988
\$1,189,000

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: Geochemical Modeling, Computer Modeling, Rock-Water-Waste Interaction

Device or Component Fabrication, Behavior or Testing

321. Waste Package: Design, Fabrication and Prototype Testing FY 1988
\$908,000

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

322. Waste Package Environment Field Tests FY 1988
\$1,595,000

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

323. Microstructure Investigations of Nodular Cast Iron FY 1988
\$25,000

DOE Contact: F. Falci, (301) 353-3595
SNL Contact: K. B. Sorenson, (505) 844-5360

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

324. Composition Investigation of Nodular Cast Iron FY 1988
\$25,000

DOE Contact: F. Falci, (301) 353-3595
SNL Contact: K. B. Sorenson, (505) 844-5360

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

325. Generate Material Property Database for Nodular Cast Iron FY 1988
\$100,000

DOE Contact: F. Falci, (301) 353-3595
SNL Contact: K. B. Sorenson, (505) 844-5360

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

326. Mosaik Brittle Fracture Test Program FY 1988
\$100,000

DOE Contact: F. Falci, (301) 353-3595
SNL Contact: K. B. Sorenson, (505) 844-5360

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

327. Investigate Thickness Effects on Impact and Toughness Properties of Ferritic Steel FY 1988
\$80,000

DOE Contact: F. Falci, (301) 353-3595
SNL Contact: K. B. Sorenson, (505) 844-5360

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

328. Investigate the Feasibility of Using Depleted Uranium as a Structural Component in Cask Construction FY 1988
\$5,000

Doe Contact: F. Falci, (301) 353-3595
SNL Contact: K. B. Sorenson, (505) 844-5360

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

Instrumentation and Facilities

329. Evaluate Current NDE Methods for Applicability to Thick Section Nodular Cast Iron FY 1988
\$20,000

DOE Contact: F. Falci, (301) 353-3595
SNL Contact: K. B. Sorenson, (505) 844-5360

Sandia has contracted with the National Institute of Standards and Technology to perform an evaluation of current NDE procedures. The nature of nodular cast iron requires a study limited to this candidate material. The nodularity of the graphite tends to inhibit NDE sensitivity. The thick-walled nature of the casks pose additional restrictions on the sensitivity of NDE procedures.

Keywords: Nondestructive Evaluation, Nodular Cast Iron

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 Waste Research and Development

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 Plant 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 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) is being prepared to support selection of a disposal strategy for Hanford high-level, transuranic and tank wastes. The Preferred Alternative recommends proceeding with disposal of double-shell tank waste, retrievably-stored transuranic waste and encapsulated cesium and strontium. Further development and evaluation is recommended 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, 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

330. Waste Form Qualification FY 1988
\$4,550

DOE Contact: Ken Chacey, (301) 353-4970 and Marv Furman (509) 376-7062
Westinghouse Hanford Company Contact: Seve 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 is generated which is 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)

331. Immobilization/Volume Reduction/In-place Stabilization FY 1988
\$5,200

DOE Contact: Ken Chacey, (301) 353-4970 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 Implantation and Microsensors 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, microsensors, ion-solid microanalysis/channeling, defects and hydrogen in solids, and laser and electron beam annealing. 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 modification and analysis of these near-surface and interfacial regions. Fundamental understanding of physical and chemical principles, materials properties and microfabrication technologies are combined to develop new approaches to sensing such parameters as radiation, hydrogen and other gases, pressure, magnetic fields, liquid viscosity, optical signals and corrosion. A major aspect of the work is thus to develop an underlying understanding and control of defects, hydrogen-materials interactions alloying processes, sensing functions, 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

332. Ion Implantation Studies for Friction and Wear FY 1988
\$500,000

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.

Keywords: Ion Implantation, Friction, Wear, Amorphous Metals

333. Silicon-Based Radiation Hardened Microelectronics FY 1988
\$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 SiO₂ and at the Si-SiO₂ 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

334. New Concepts in Microsensors FY 1988
\$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 propagation, 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. Surface acoustic

waves have been exploited to make new sensors for various vapors, thin films, and the viscosity of liquids. 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.

Keywords: Microsensors, Microcircuitry

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

335. Plasma Etching

FY 1988
\$400,000

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

Fundamental studies are carried out 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

336. Plasma-Enhanced Chemical Vapor Deposition

FY 1988
\$200,000

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

Fundamental studies are carried out 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. 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

337. Laser-Controlled Etching and Deposition of Materials FY 1988
\$200,000

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

338. Surface Chemistry of Organometallics for Compound Semiconductor Epitaxy FY 1988
\$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 ($\text{Ga}(\text{CH}_3)_3$, $\text{Al}(\text{CH}_3)_3$, 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

339. Metallorganic Chemical Vapor Deposition

FY 1988
\$400,000

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 ($\text{Ga}(\text{CH}_3)_3$, $\text{Al}(\text{CH}_3)_3$, etc., and Group V hydrides (AsH_3 , PH_3 , etc.) or alkyls ($\text{As}(\text{CH}_3)_3$, $\text{P}(\text{C}_2\text{H}_5)_3$, 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

Condensed Matter and Surface Science Department, 1130

The mission of Department 1130 is to provide fundamental understanding and strong technology bases in two main areas: (1) shock wave and explosives physics and chemistry; (2) electronic and structural properties; (3) surface science of materials. Current areas of emphasis include shock-induced solid state chemistry, shock initiation of heterogeneous explosives, shock-activated thermal battery, PVF_2 stress gauge, phase transitions in ferroelectrics, high T_c modification and control of surface properties, the superconductors, defects in semiconductors, modification and control of surface properties, the early stages of oxidation and corrosion, adhesion of metals to polymers.

Materials Properties, Behavior, Characterization or Testing

340. Shock Physics and Chemistry

FY 1988
\$500,000

DOE Contact: A. E. Evans, (301) 353-3098

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 PVF₂ 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

341. Electronic and Structural Properties

FY 1988
\$400,000

DOE Contact: A. E. Evans, (301) 353-3098
Sandia Contact: B. Morosin, (505) 844-8169

The magnetic properties and crystal structures of high T_c superconductors are being investigated in order to gain new insights into the mechanisms responsible for the superconductivity and to guide the development of new superconductors. Radiation-induced defects and their deep electronic levels in silicon and compound semiconductors are being studied to understand the physics and the role of these defects in device degradation.

Keywords: High T_c Superconductors, Semiconductors, Defects, Deep Levels

342. Surface Science

FY 1988
\$400,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
SNLA Contact: T. A. Michalski, (505) 844-5829

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 oxidation and corrosion of metals and semiconductors, the nature of the adhesion of polymers to metals and how to improve it, and the mechanisms by which gaseous species are dissociated at the surface and transported to the insulator-semiconductor interface in MIS gas sensors. Novel chemical vapor deposition techniques are being developed to produce more uniform and reliable multicomponent pyrotechnics.

Keywords: Surface Physics, Field Ion Microscopy, Auger Electron Microscopy, UV Photoemission Spectroscopy, Oxidation, Corrosion, Adhesion, Pyrotechnics

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. 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

343. Materials Growth by Molecular Beam Epitaxy (MBE) FY 1988
\$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/InAs and InGaAs/GaAs 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

344. Materials Growth by MOCVD FY 1988
\$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

345. Strained Layer Superlattices for IR Detectors FY 1988
\$300,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098

Sandia Contacts: S. R. Kurtz, (505) 844-5436; 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. Detection to 12 μm has been demonstrated.

Keywords: Strained-Layer Superlattices, Infrared Detectors

346. Novel Processing Technology for Semiconductor Technologies FY 1988
\$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 Schottky barrier and Ohmic contact formation, passivation layer development, and development of new metallurgical techniques for deposition of reactive alloys.

Keywords: Semiconductor Devices

347. Thin Film Superconductors FY 1988
\$300,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098

Sandia Contact: D. S. Ginley, (505) 844-8863

Thin films at the high temperature superconductors in the Y-Ba-Cu-O and Ti-Ca-Ba-Cu-O systems are being prepared by MBE, E-beam evaporation and sputtering. Oriented and random films with T_c s to 112K are being produced. Patterning and contacting technology for the films is also being developed.

Keywords: Thin Films, Superconductors: High Temperature, Coatings and Films

Solid State Research Department, 1150

The mission of Department 1150 is to provide a basic understanding of solid materials with an emphasis on electronic properties. The department provides supporting experimental and theoretical research both on materials of current interest as well as on systems of importance in emerging technologies. Current studies include hydrogen and

helium in metals, high temperature superconductivity, high temperature devices, surface science, high performance semiconductors, and fundamental studies of disordered materials.

Materials Properties, Behavior, Characterization or Testing

348. Superconductivity FY 1988
\$540,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
Sandia Contact: J. E. Schirber, (505) 844-8134

Transport 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

349. Semiconductors FY 1988
\$540,000

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 studies of electronic properties of boron carbide at high temperatures. Defects in semiconductors. Physics of light-hole devices based on strained layer superlattices.

Keywords: Superconductivity, Ceramics, Predictive Behavior Modeling

350. Surface Science FY 1988
\$500,000

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, Predictive Modeling

351. Disordered MaterialsFY 1988
\$500,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098

Sandia Contact: D. W. Schaefer, (505) 844-7937

Application of polymeric synthesis routes to ceramic materials. Gas phase materials processing. Gelation in foam precursors and sol-gel glasses. Fundamentals of film formation.

Keywords: Glass-Ceramics, Sol Gel Process, Thin Films

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 Forming352. Dyed Antireflective Photoresist MaterialFY 1988
\$100,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098

SNL Contact: C. Renschler, (505) 844-8151

Photopatterning of photoresist materials on reflective substrates can be highly problematic. Reflective notching and standing wave effects can give rise to irregular geometries which lead to device failure. We have developed a photoresist formulation

containing small concentrations of a dye molecule which eliminates this problem. The material is a modification of standard photoresist formulations; the fact that it has virtually identical properties allows its direct substitution into production runs without significant modifications of processing facilities or techniques.

Keywords: Polymers, High Temperature

353. Sulfonated Aromatic Polysulfones FY 1988
\$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 for batteries. The new materials have been shown to exhibit significantly enhanced coulombic efficiencies and stabilities compared with inexpensive commercial membranes, but have a large cost advantage compared with fluorinated materials. Aging and resistivity tests are continuing. Future work will also involve sulfonation of other high-stability polymers including polyphenylene, as well as in preparation of commercial microporous membrane materials with the new cation-permeable polymers. This latter work is aimed at enhancing the efficiency of commercial separate membrane systems.

Keywords: Polymers, Coatings and Films, Batteries

354. Carbon Foams FY 1988
\$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.

Keywords: Carbon Foam

Materials Properties, Behavior, Characterization or Testing355. Radiation Hardened DielectricsFY 1988

\$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

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. The Division carries out aging studies, compatibility studies, and coordinates these activities with designers and quality assurance staff. To support these programs, the division carries out in-depth studies on radiation chemistry, photochemistry, surface chemistry, and spectroscopy on polymeric systems.

Materials Preparation, Synthesis, Deposition, Growth or Forming356. Polysilanes, Photoresists, Photoconductors, and Non-Charring DielectricsFY 1988

\$150,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098

SNL Contacts: J. M. Zeigler, (505) 844-0324, P. Walsh, (505) 844-8547 and R. G. Kepler, (505) 844-7520

Improved polysilane self-developing photoresists have been synthesized which have a silyl side group replacing the typical alkyl groups of our previously discovered materials. These materials are under investigation for use as positive working, reactive ion etch resistant non-solvent developed photoresists for use in simplified microelectronic circuit

and PC board manufacture. Time resolved spectroscopy experiments are being conducted to understand the fundamental photochemistry and photophysics behind the self-development process. Other polysilanes show promise as photoconductors for electrophotographic applications. Photophysical studies are being carried out to understand the mechanism of charge carrier generation and transport in these "sigma-conjugated" polymers. The high temperature resistance and non-charring behavior of these materials makes them potentially attractive as dielectric materials. Melttable, crosslinkable polysilanes are being developed for that application. The electronic properties of different polysilanes are being investigated for use of these polymers as nonlinear optical materials.

Keywords: Insulators/Dielectrics-Polymeric, Photoresistant

357. Mechanistic Studies of Polysilane Synthesis

FY 1988
\$20,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098

SNL Contact: J. M. Zeigler, (505) 844-0324

Fundamental studies of the mechanism of reductive coupling of dichlorosilanes to polysilanes with sodium metal are being carried to develop improved synthetic methods which increase yields and provide greater control over molecular weight distributions. This work has shown that silyl radicals are the predominant intermediates on the pathway to high polymer, that the molecular weight distribution is controlled by diffusion effects, and that the molecular weight distribution is subject to a large number of subtle reaction parameter effects. The improved synthesis procedures which resulted are currently being patented. We have also shown that the yield of polysilane is fundamentally limited by chain "back-biting" side reactions inherent in the coupling chemistry.

Keywords: Polymers, Predictive Behavior Modeling

358. Chemistry of Plasma Etching and Deposition Processes

FY 1988
\$130,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098

SNL Contacts: J. M. Zeigler, (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 which 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

359. Materials Structure, Dynamics, and Property Studies by Multinuclear Pulsed NMR Spectroscopy FY 1988
\$75,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098

SNL Contacts: J. M. Zeigler, (505) 844-0324 and R. A. Assink, (505) 844-6372

Multinuclear nuclear magnetic resonance spectroscopy of liquid and solid samples is being applied to several materials related problems. The ^{13}C and ^1H 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

360. Studies of Adhesion at the Molecular Level by Surface Science Techniques FY 1988
\$210,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098

SNL Contacts: J. M. Zeigler, (505) 844-0324 and J. A. Kelber, (505) 844-5436

Mechanisms of polymer-polymer and polymer-metal adhesion are being studied by a combination of surface sensitive techniques including ESD, PSD, XPS, and Auger spectroscopies. Particular emphasis is being placed on the observation of the interactions between metaloxide surfaces and amine-cured epoxies. Results to date indicate that amine-cured epoxies undergo strong specific chemical interactions via the Natorn sites with oxidized Cu and Al surfaces even when applied under "real world" conditions.

Work is continuing on understanding such chemical interactions in detail, as well as the effects of moisture exposure on such long term interactions.

Keywords: Polymers, Surface, Adhesion

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

361. Microporous Foam Development FY 1988
\$157,500

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098

SNL Contact: J. H. Aubert, (505) 844-5604 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

362. Development of Removable Encapsulants FY 1988
\$157,500

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098

SNL Contacts: 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

363. Mechanical Properties of Encapsulants

FY 1988

\$21,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098

SNL Contact: D. Adolf, (505) 844-4773

The crucial thermophysical properties for determining the level of thermally generated stresses in polymeric encapsulants are the coefficient of thermal expansion, the bulk modulus, and either the shear or tensile modulus. We have measured these properties as a function of temperature for the common encapsulants used in our weapons facilities. Previously, the bulk modulus had been estimated from room temperature tensile modulus measurements and estimates of Poisson's ratio. We have directly measured the bulk modulus using a tri-axial testing facility and see significant differences from the historical values. In addition, the frequency dependence of the shear modulus was measured allowing modelling of the viscoelastic behavior of these materials.

Keywords: Polymeric Encapsulants, Organic, Tests, Bulk Modulus

364. Deformation of Kevlar Fabrics

FY 1988

\$73,500

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098

SNL Contacts: R. H. Ericksen, (505) 844-8333 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

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 inhomogeneous materials, contacts to electronic materials, dielectrics, and special materials and processes.

Materials Properties, Behavior, Characterization or Testing

365. Nonlinear Optical Materials FY 1988
\$100,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098

SNL Contacts: R. G. Kepler, (505) 844-7520 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

366. Hydrogen Effects in Silicon FY 1988
\$100,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098

SNL Contacts: R. G. Kepler, (505) 855-7520 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 then 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

367. Rapid Thermal Processing of Gate Oxides FY 1988
\$100,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098

SNL Contacts: R. G. Kepler, (505) 844-7520 and W. K. Schubert, (505) 846-6548

High quality thin SiO₂ 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, 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

368. Development of Automated Methods for Chemical Analysis FY 1988
\$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/Fourier transform-mass spectrometer (CG/FTMS) system has recently been installed and will be used for support of a variety of applied and basic research programs, such as development of 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. Metals 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

369. Thermomechanical Treatment of U Alloys

FY 1988
\$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 are being investigated in U-Ti and U-Nb 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

370. Advanced Methods for Electron Optical, X-ray and Image Analysis

FY 1988
\$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 microscopy 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

371. Advanced Methods for Surface and Optical Analysis FY 1988
\$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 Preparation, Synthesis, Deposition, Growth or Forming

372. Analytical Electron Microscopy of Engineering Alloys

FY 1988
\$130,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098

SNL Contact: A. D. Romig, (505) 844-8358

Analytical Electron Microscopy (AEM) allows the local chemistry within a thin foil to be determined with high resolution. This cannot be done in engineering (complex) alloys in a straightforward manner because of the difficulty in interpreting x-ray peaks in multicomponent systems. Techniques have been developed using Monte Carlo simulations on a computer to sort out all of the measured effects and to allow quantitative analysis. These quantitative measurements allow diffusion properties to be measured and, in turn, the kinetics of such metallurgical phenomena as precipitation to be

determined. Work has been extended to examine quantitatively segregation of impurities to defects (grain boundaries, stacking faults, dislocations).

Keywords: Metals: Ferrous and Non-Ferrous, Joining and Welding, Transformation, Electron Beam Methods, Weapons

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

373. Toughness of Ductile Alloys FY 1988
\$330,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098

SNL Contacts: R. J. Salzbrenner, (505) 846-9949 and J. A. VanDenAvyle, (505) 844-1016

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

374. Friction and Wear of Modified Surfaces FY 1988
\$230,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098

SNL Contacts: R. J. Bourcier, (505) 844-6638 and A. D. Romig, (505) 844-8358

The improvement of friction and wear behavior using surface modification has been a very productive approach that includes many traditional methods (e.g., carburizing or nitriding). Recent work in ion implantation has shown that this technique can both decrease friction and improve wear, although the mechanism by which this occurs is not

understood. It is known that an amorphous layer is formed and current work is aimed at understanding the metastable metallurgy of near-surface regions. Microhardness historically has been used to characterize these modified surfaces but this has been without a thorough understanding of low-load indentation testing. Finite element modeling techniques are being used to help separate artifacts caused by very low loads from the influence of a modified surface layer. Successful modeling will allow us to begin to model the friction process itself. Work has been conducted on nitrogen-implanted stainless steel and aluminum-implanted nickel.

Keywords: Metals: Ferrous and Non-Ferrous, Erosion/Wear/Tribology, Ion Implantation, Weapons

375. Alloy Deformation Response and Constitutive Modeling FY 1988
\$300,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098

SNL Contacts: W. B. Jones, (505) 844-4026 and R. J. Bourcier, (505) 844-6638

All complex structures are now designed using finite element computer codes which can now handle both exotic geometries and plastic/creep deformation. Constitutive models which embody both time-dependent and time-independent inelastic behavior need to be developed which have a basis in the metallurgy and dislocation substructural characteristics of the alloys used. Also important is the long-time microstructural stability of alloys and how to incorporate this into the models. Stainless steels are being studied using both uniaxial and biaxial testing techniques in order to characterize alloy response. Models are being developed which represent the deformation mechanisms operating and can be formulated for inclusion into finite element codes.

Keywords: Metals: Ferrous, Creep, Fatigue, Nuclear Reactors, Predictive Behavior Modeling, Weapons

376. Corrosion FY 1988
\$1,150,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098

SNL Contact: N. R. Sorensen, (505) 844-1097

Glassy alloys can exhibit exceptionally good corrosion resistance. We are conducting a program to determine how certain glassy alloys derive this resistance to corrosion and why they require less alloyed chromium than conventional stainless steels. This understanding could lead to better utilization of chromium in conventional stainless alloys. By using ion implantation, we are also separating and identifying the relative contributions of alloy structure and composition to corrosion behavior. We have shown that P is detrimental to corrosion resistance at low Cr levels because it stimulates

dissolution but the alloy cannot passivate. However, P is beneficial at higher Cr levels because this enhanced dissolution actually promotes passive film formation.

Keywords: Metals, Amorphous Materials, Glassy Alloys, Corrosion

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

377. Vacuum Arc Remelting

FY 1988
\$60,000

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

378. Aluminum Laser Welding

FY 1988
\$40,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098

SNL Contact: J. L. Jellison, (505) 844-6397

Designers are selecting aluminum alloys for many new components. Welding methods for joining these alloys are limited, particularly where heat input must be minimized. Laser welding processes are being characterized. Current emphasis is on

determining the role of metal evaporation on composition, mechanical properties, and hot-cracking. Future work will be directed towards minimizing melt-freeze cycles during welding. A CW laser system is under development to provide improved processing capabilities.

Keywords: Metals: Non-Ferrous, Joining and Welding, Conventional Solidification

379. Welding of Nickel-Based Alloys FY 1988
\$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

380. Plasma Arc Welding FY 1988
\$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

381. Laser Welding

FY 1988
\$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

382. Development of Materials for Magnetic Fusion Reactors

FY 1988
\$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

383. Development of Hard, Wear-Resistant Coatings for Mechanical Applications

FY 1988
\$80,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098

SNL Contact: J. K. G. Panitz, (505) 844-8604

As a continuation and conclusion to an earlier study, amorphous NiCrFeSiB and NiCrSiB alloy coatings with varying amounts of Ni and Cr were deposited using a dual beam ion system. The coatings were bombarded with a beam of argon ions at beam energies from 0 to 350 eV at varying current densities during deposition. These coatings displayed disappointing friction and wear properties with high (>1) coefficients of friction and a short wear life. However, these coatings displayed superb resistance to C1-corrosion. The coatings which contain higher concentrations of Cr displayed superior corrosion resistance.

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.

Keywords: Carbon Coatings, Erosion/Wear/Tribology

Materials Properties, Behavior, Characterization or Testing

384. Modification of Mechanical Properties by Ion Implantation

FY 1988
\$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

Device or Component Fabrication, Behavior or Testing

385. Process Control Ultrasonic Cleaning of Delicate Parts FY 1988
\$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

386. Plasma Oxidation and Reduction Studies FY 1988
\$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

387. Ion Beam Reactive Deposition System

FY 1988

\$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

388. Deposition and Evaluation of Titanium Nitride Films

FY 1988

\$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

389. In Situ Friction, Wear, and Electrical Contact Resistance Systems FY 1988
\$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.

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.

Materials Preparation, Synthesis, Deposition, Growth or Forming

390. Ceramic Processing

FY 1988
\$2,600,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
SNL Contact: B. C. Bunker, (505) 844-8940

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

391. Electrophoretically-Deposited Coatings

FY 1988

\$150,000
DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
SNL Contacts: A. K. Hays, (505) 844-9996 and D. J. Sharp, (505) 844-8604

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

392. Glass and Glass-Ceramic Development**FY 1988
\$2,500,000**

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098

SNL Contacts: F. P. Gerstle, Jr., (505) 844-4304 and D. H. Doughty, (505) 844-1933

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

Materials Properties, Behavior, Characterization or Testing**393. Fracture of Ceramics****FY 1988
\$680,000**

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098

SNL Contact: F. P. Gerstle, Jr., (505) 844-4304

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

394. Optical Diagnostics for Materials Processing

FY 1988
\$240,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098

SNL Contacts: A. K. Hays, (505) 844-9996 and H. C. Peebles, (505) 846-3454

Optical diagnostics are being developed to map the temperature, composition, and velocity profiles as a function of time to species present in the atmosphere during standard ceramic and metallurgical processes (e.g., welding, vacuum arc remelting, and plasma spraying). This information is necessary to obtain a scientific understanding of the phenomena that govern these processes. Present efforts include the study of plumes formed during the Nd:YAG laser welding of aluminum and iron alloys and plasmas formed in the interelectrode gaps of VAR furnaces. Present work includes developing optical diagnostics for chemical vapor deposition of ceramic films.

Keywords: Optical Diagnostics, Welding, Vacuum Arc Remelting

Sandia National Laboratories - Livermore

Materials Preparation, Synthesis, Deposition, Growth or Forming

395. Powder Metallurgy

FY 1988
\$200,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098

SNL Contacts: J. A. Brooks, (415) 294-2051; 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

396. Advanced Electrodeposition Studies

FY 1988

\$100,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098

SNL Contacts: H. R. Johnson, (415) 294-2822, W. D. Bonnert, (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 develop 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

397. Metal Forming

FY 1988

\$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 particular, 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

398. Advanced Organic Materials FY 1988
\$200,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098

SNL Contacts: D. L. Lindner, (415) 294-3306, J. G. Curro, (505) 844-3936, W. R. Even, (415) 294-3217 and C. B. Frost, (415) 294-2048

Recent developments in our understanding of the relationship between microstructure and macroscopic properties has led to the ability to produce polymeric 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. Studies are presently centered on understanding the relationship between processing conditions, cooling rate, solution composition, and solidification direction in controlling the microstructure. We have begun determining the relationship between these unique microstructures and physical and mechanical 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. 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

399. Particulate Technology FY 1988
\$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

400. Tritium Getter Technology

FY 1988
\$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 quick 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.

Keywords: Hydrogen Getters, Tritium

401. Molded Desiccant Foam

FY 1988
\$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

402. Plasma Processing

FY 1988
\$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 TLM, 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

403. Tritium and Decay Helium Effects on Crack Growth in Metals and Alloys

FY 1988
\$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 thermo-mechanical 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

404. Joining Science and Technology FY 1988
\$400,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098

SNL Contacts: J. A. Brooks, (415) 294-2051, K. W. Mahin, (415) 294-2051 and J. R. Springarn, (415) 294-3307

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 of important parameters, including microanalytical analysis of 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, the measurement and modeling of mechanical properties of brazed joints, and the design, testing, 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 binary alloy systems.

Keywords: Joining and Welding, NDE, Microstructure, Metals, Transformation, Solidification, Modeling

405. Composites: Characterization and Joining

FY 1988
\$150,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098

SNL Contacts: J. B. Woodard, (415) 294-3115, B. C. Odegard, (415) 294-2789 and
J. R. Springarn, (415) 294-3307

The stability, compatibility, and joining of polymer matrix composite materials are being investigated in conjunction with efforts at Sandia National Laboratories, Albuquerque. The work focuses on graphite-fiber-reinforced composites and includes both thermosetting and thermoplastic matrix materials. The measurements of moisture saturation levels for several resin systems has agreed well with previous investigators. Characterization of water adsorption sites in thermosetting matrix materials will be studied by autoradiography after exposure of samples to tritiated water. The influence of matrix materials and post-cure thermal processing on adsorption sites and the coefficient of moisture expansion will be investigated. Condensable 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). 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

406. Compatibility, Corrosion, and Cleaning of Materials

FY 1988
\$30,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098

SNL Contacts: D. L. Lindner, (415) 294-3306, H. R. Johnson, (415) 294-2822 and
D. K. Ottesen, (415) 294-2787

Examination of surfaces to determine compatibility, corrosion, and cleanliness is being carried out using sophisticated 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 to peer inside small

diameter tubes and identify wall-surface contamination. This method has been shown to be applicable to production environments. Other methods are also being investigated with transfer of this technology to production agencies as a goal.

Keywords: Compatibility, Corrosion, Cleaning, FTIR

407. Tritium-Metal Interaction

FY 1988
\$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 $\leq 10 \mu\text{m}$ spatial resolution.

Keywords: Metals: Ferrous and Non-Ferrous, Surface, Defects/Grain Boundaries, Tritium

408. Measurement of Multilayer Thin Film Structures

FY 1988
\$50,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098

SNL Contact: R. 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

409. Helium in Metal Tritides

FY 1988
\$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 422-2360 and
D. F. Cowgill, (505) 844-7480

The evolution of helium in metal tritides is being studied by NMR, gas sampling and dilatometry techniques. NMR measurements carried out over the past year have been used to determine the helium bubble content in aged Pd and were successful in observing solid to liquid and liquid to gas phase transitions of the trapped He in these bubbles. A new, ultra-sensitive sampling system is under construction to measure, in real time, the evolution of He from aging tritides as a function of environmental conditions. In addition, the physical size changes in metal tritides is being measured to determine the lattice expansion due to the evolution of helium in the metal lattice. Initial results have been obtained for Pd.

Keywords: Tritium, Tritium Decay, Metal Tritides

410. Analysis of Defects and Interfaces in Metals

FY 1988
\$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 boundary 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

411. New Spectroscopy FY 1988
\$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

412. Tritium Facility Upgrade for Materials Characterization and Testing FY 1988
\$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 ^3He 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 limitations 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 quadrupole mass spectrometer permits a degree of sample preparation and characterization prior to PCT study.

Keywords: Spectrometer, Tritium Charging, Mechanical Testing, Scanning Electron Microscopy

413. New Analytical Techniques FY 1988
\$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

Lawrence Livermore National Laboratory

Materials Preparation, Synthesis, Deposition, Growth or Forming

414. Ion Beam Modification of Materials FY 1988
\$110,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098

LLNL Contact: R. G. Musket, (415) 422-0483/FTS 532-0483

Ion implantation can lead to unique layers inside materials. The nature of the layers formed can often be predicted, and the layers can dramatically change the interaction of the material with its environment. Recently, an essentially pure subsurface layer of aluminum has been formed in beryllium using ion implantation. For 200 keV Al⁺ implanted to a dose of 1.1×10^{18} Al/cm² combined with post-implant annealing at 570°C for one hour, Auger sputter profiles of individual grains revealed layers containing at least 98 at.% aluminum. Cross-sectional transmission electron microscopy measurements showed the presence of a crystalline aluminum layer inside the beryllium with very sharp interfaces with the beryllium. The 170-nm-thick aluminum layer was centered about 400 nm below the beryllium surface. This study provided the first documented evidence for creation of a pure elemental layer inside a host material using ion implantation.

Keywords: Metals: Non-Ferrous, Ion Implantation

415. Inorganic AerogelsFY 1988
\$600,000DOE 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 18 cm at selected densities over the range of 0.03 to 0.55 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

416. Synthesis Project (Explosives)FY 1988
\$250,000DOE 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. These materials have been a target for several other explosive synthesis groups in the U.S. and abroad. 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

417. Synthesis and Reactivity of Transition Metal Fluorocarbon Complexes FY 1988
\$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, $(CF_3)AuXU_2(L)$ ($X=Br, I$). 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

418. Sputtering (Plutonium Alloys) FY 1988
\$241,000

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 1×10^{17} atoms/cm²-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 1×10^{17} atoms/cm²-s with energies between 20 and 1000 eV. The triode "split-target" configuration will be used to synthesize wide ranges of Pu-solute

compositions to determine how specific elements influence the stability of Pu-rich alloys. Specific systems to be studied include Pu-G, Pu-Sc, and Pu-Yb.

Keywords: Sputtering, Actinides

419. Organic Aerogels

FY 1988
\$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 30-100 Å, cell sizes of less than 1000 Å, and surface areas of 400-700 m²/g. This microstructure is retained even after carbonization at 1100°C.

Keywords: Organic Aerogels, Sol-Gel, Laser Fusion Targets

420. New Ionomer Synthesis

FY 1988
\$9,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098

LLNL Contact: M. O. Riley, (415) 422-6865/FTS 532-3045

One objective of this research was to synthesize ionomers which could be used as inexpensive spectral filters for laser applications. Of particular interest were optically clear materials having absorptions at 1 micron, for use as amplified spontaneous emission absorbers on laser amplifiers. UV cut-off flash lamp filters capable of replacing presently used cerium doped quartz filters were also of interest. Preliminary flash lamp testing and absorption spectra characterization indicated some promise for these materials. A second goal was to prepare highly loaded ionomers. A limit of about 20 wt % metal was observed; this could be extended to about 25 wt % by preparation of (nominally) hybrid halato-ionomer structures. These materials were characterized by FTIR, DSC, TGA, and dynamic mechanical spectrometer.

Keywords: Ionomers, Spectral Filters

421. Polymer Foam Development

FY 1988
\$1,600,000

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 foams are needed to act as a wick to liquid DT in a spherical shell configuration for direct drive laser fusion targets. The foams 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. Three foams are under development which meet the basic requirements. A polystyrene foam is made by polymerizing an inverse emulsion of water-in-styrene. Resorcinol-formaldehyde foam is made by a condensation polymerization in aqueous solution followed by a supercritical drying. Cellulose acetate foam is made by dissolving cellulose acetate in benzyl alcohol at elevated temperature, lowering the temperature to produce a phase separation, and finally supercritically drying. The foam materials are characterized for cell size by SEM and uniformity by X-ray radiography. The foams have also been tested for hydrogen wettability, the effects of DT exposure and thermal contraction measured from room temperature to 20K.

Keywords: Polymer Foams, Low-Density Materials, Laser Fusion Targets

422. Atomic Engineering

FY 1988
\$64,000

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; (4) to develop techniques for *in situ* monitoring of Atomically Engineered materials during synthesis.

Keywords: Thin Films, Multilayer Technology

Materials Structure and Composition423. Theory of the Structure and Dynamics of Molecular Fluids FY 1988

\$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

424. Site-Specific Chemistry Using Synchrotron Radiation FY 1988

\$180,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098

LLNL Contact: Joe Wong, (415) 423-6385

We have performed a number of extended X-ray absorption fine structure (EXAFS) and X-ray absorption near-edge structure (XANES) experiments on BL 10-2 at Stanford Synchrotron Radiation Laboratory soon after this new powerful wiggler beamline became operational. These experiments include (a) site selective detection with optical EXAFS; (b) 3d and rare-earth substitutions in high T_c superconductors; (c) interface structure of a monolayer of Hf on a multilayer and (d) Cr^{3+} sites in fluoride laser crystals. The wiggler beam profile was also measured with a CCD imager. Such 2-dimensional CCD images were the first recorded of any synchrotron beam.

Keywords: Site-Specific Chemistry, Superconductors

425. Capillary Structures (in Foams) FY 1988

\$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

426. Plutonium Pyrochemical Research

FY 1988
\$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 initial emphasis of this study is to determine experimental $\Delta G^\circ F$ values for Pu-Si compounds, because such data currently is not available and Si is an important constituent of Pu residual wastes. We plan to obtain first approximate thermodynamic data by studying exchange reactions of Pu silicides with other silicides of comparable stability, such as the reaction $3\text{Mo}_3\text{Si} + 5\text{Pu}(\ell) = \text{Pu}_5\text{Si}_3 + 9\text{Mo}$ which, depending on the direction of reaction, allows us to set upper or lower limits on $\Delta G^\circ F$ for Pu_5Si_3 . Comparisons will also be made with silicides for Cr, W, and U. Currently, a clean atmosphere arc-melter has been set up and pure Pu_5Si_3 has been prepared. Reaction mixtures will be studied next. For quantitative $\Delta G^\circ F$ determinations, we plan to study vapor pressures of Pu silicides by Knudsen cell effusion.

Keywords: Plutonium Silicides, Plutonium Thermodynamics, Pyrochemical Processing, Plutonium Residual Wastes, Knudsen Cell Effusion

427. Low Density Material Aggregate Networks

FY 1988
\$186,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098

LLNL Contact: Lucy M. Hair, (415) 423-7823/FTS 543-7823

We successfully made gels using tertiary-amine-catalyzed epoxy novolac systems. On conversion to foams, it was shown that they indeed have the porous, nodular structures expected from an aggregate gel precursor, with the largest cells being 1-2 microns in diameter. We were able to achieve target densities of from 30 to 100 mg/cm^3 by varying epoxy monomer and amine catalyst concentrations. High-temperature post-curing of the foams was found to significantly improve elasticity and strength. The epoxy-novolac foams were also able to be carbonized, a step which increases stability of the material. We modeled the general process of aggregate gel formation through development of a computer code that simulates random Brownian motions of spheres in solution and causes them to stick together upon collision. By varying the number, size and porosity of the spheres, structures similar to the "aggregate networks" were formed.

Keywords: Foams, Gels, Computer Modeling

428. Electronic Structure in Superconducting Oxides

FY 1988

\$23,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098

LLNL Contact: M. J. Fluss, (415) 423-6665/FTS 543-6665

Positron annihilation analysis is used to measure electronic structure and other properties in solid materials at arbitrary temperatures. Positron lifetime measurements were made on several samples of superconducting oxides and conventional superconductors. A distinct change in the annihilation lifetime in the superconducting state was observed for all samples of superconducting oxides and no change was seen in similar measurements on conventional systems. These data are one of the few indications that electronic properties are changed in the superconducting state. Electronic structure and the existence of a Fermi surface in superconducting oxides and related compounds were explored both experimentally and theoretically using high resolution angular correlation measurements and LACO cluster calculations.

Keywords: Superconductors, Electronic Structure, Positron Annihilation

429. Theory of Superconducting Oxides

FY 1988

\$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 pairing 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

430. A New, First-Principles Method for the Calculation of the Electronic Structure of Surfaces and Grain Boundaries

FY 1988
\$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 a new, first-principles method, based on multiple scattering theory, for the calculation of the electronic structure of surfaces and grain boundaries. This method also allows us to study structurally complex materials such as the α phase of Pu. We have carried out calculations of the density of states (DOS) of unrelaxed and relaxed $\Sigma 5$ grain boundaries in Cu, as well as of α Pu, the latter within a nonrelativistic treatment. We are currently engaged in extending our codes to incorporate charge self-consistency and relativistic effects.

Keywords: Electronic Structure, Grain Boundary, Surface

Materials Properties, Behavior, Characterization or Testing

431. Nuclear Spin Polarization

FY 1988
\$770,000

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. 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 indicates 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 500 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. We are still looking world-wide for someone who can try HD polarization at 70-94 GHz (as a model for DT) sooner with existing equipment.

Keywords: Spin Polarization, Electron Spin Resonance

432. Measurement of Tritium Permeation Through Resistant Materials at Low Temperatures

FY 1988

\$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. By testing copper in annealed and unannealed foils and in single crystal discs, we found that permeation through copper foils at temperatures up to 100°C is controlled by transport through defects in the metal lattice; above 100°C permeation through the metal lattice controls. The permeation rate in annealed or single crystal copper at 50-170°C is consistent with Arrhenius extrapolation of literature data at higher temperatures, but the permeation rate in unannealed copper at 50°C is 10 times faster. Because the transport through lattice defects is slower than permeation through the metal lattice at high temperatures, but is not thermally activated, transport along defects becomes dominant at lower temperatures. Measurements on several other metals (aluminum, beryllium, cadmium, gold, iridium, lead, molybdenum, rhenium, silver, and tungsten) at 50°C also showed that extrapolation of high temperature data is not valid at this low temperature; presumably transport along defects is again dominating the total permeation rate.

Keywords: Permeation, Tritium, Liquid Scintillation Counting

433. Catalytic Properties of Actinide Compounds

FY 1988

\$185,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098

LLNL Contact: C. A. Colmenares, (415) 422-6352/FTS 532-6352

All the experimental work on the electronic structure and reactivity of U, UNi₂, and UNi₅ with O₂ and CO has been interpreted, and three papers written summarizing our results. Two of these have been submitted for publication. This work was carried out during a three-month visit of C. Colmenares to the European Institute for Transuranium Elements (West Germany) in the Fall of 1986. The techniques used were ultraviolet and X-ray photoelectron spectroscopies (UPS and XPS, respectively) and X-ray induced Auger photoelectron spectroscopy (AXES).

Because of the good results obtained previously with an oxidized UFe₂ catalyst for the hydrogenation of CO, a synthetic U_xFe_yO_z catalyst was prepared for us, by

Dr. D. Perry of the Lawrence Berkeley Laboratory, to study the same reaction and compare results. The major components of this catalyst were α - Fe_2O_3 , U_2O_5 and α - U_3O_8 (X-ray diffraction), but XPS showed that the surface was mostly iron (~27 atom%) as Fe_2O_3 with a small amount of uranium present as U_3O_8 (~3 atom%). The catalytic activity of this U/Fe oxide for the hydrogenation of CO was tested with a 1CO:1 H_2 gas mixture under similar conditions as those for the UFe_2 catalyst. A 5 percent carbon conversion was effected and alkanes from C_1 to C_8 produced in contrast to UFe_2 , which produced mostly methanol under the same conditions. This is due to a difference in the surface species of the two catalysts (UF_{2+x} and Fe_2O_3 are present in oxidized UFe_2). Studies have been initiated to study the reaction of U, UNi_2 and UNi_5 with hydrogen and H_2/CO mixtures.

Keywords: Actinides, Actinide Intermetallic, Electronic Structure, Reactivity, Catalytic Properties, Hydrogenation of CO

434. Pretransformation Behavior in Alloys

FY 1988

\$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

435. Interfacial Bonding in Multilayer X-ray Mirrors

FY 1988

\$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

436. $\Delta N=O$ Spectroscopy Using Multilayer Gratings FY 1988
\$162,000

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 $\lambda < 250 \text{ \AA}$ 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 $^{(s)}1/2^{(2p)}(1/2) \text{ } ^3P_O \rightarrow ^{(s)}1/2^{(2s)}1/2 \text{ } ^3S_1$ 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

437. Multilayer X-ray Optics Development FY 1988
\$220,000

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 thicknesses 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, exploratory 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

438. Thin Film Studies

FY 1988
\$160,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098

LLNL Contact: Troy W. Barbee, Jr., (415) 423-7796

The multilayer diffraction gratings studied were prepared by multisource magnetron sputter deposition onto 2000 nm period laminar amplitude grating substrates. The grating structures were anisotropically etched in <110> single crystal silicon and patterned using standard microlithography techniques. Multilayers of tungsten/carbon, rhodium/carbon, molybdenum/silicon and 304 stainless steel/silicon having periods of 2.5 to 20 nm have been fabricated onto these diffraction grating substrates and characterized using facilities at the Stanford Synchrotron Radiation Laboratory.

Keywords: Multilayer-Optics, Diffraction Gratings, Microlithography, Thin Films

439. In Situ Reversed Deformation Experiments

FY 1988
\$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.

Keywords: Metals, Structure, Mechanical Properties, Fatigue

440. Dislocation Microstructure of Aluminum and Silver Deformed to Large Steady-State Creep Strains FY 1988
\$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 ($\approx 1/4 \mu\text{m}$ 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

441. Delayed Failure of Silver-Aided Diffusion Bonds FY 1988
\$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 faying 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

442. Constitutive and Failure Behavior of Metals at High Rates of Tensile Strain

FY 1988
\$225,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098

LLNL Contact: W. H. Gourdin, (415) 422-8093/FTS 532-8093

The electromagnetically launched expanding ring provides a means of studying the constitutive and failure behavior of metals in tension at strain-rates of 10^4S^{-1} without the wave effects that can influence results obtained using other techniques such as the split Hopkinson pressure bar. A pulsed solenoid is used to induce a counter-rotating current in a specimen ring thereby producing a large body force that expands the ring rapidly. Poor electrical conductors can be launched with high conductivity pusher rings which are stripped away after maximum expansion speed is reached. Differentiation of the expansion speed history, measured with a velocity interferometer, gives the ring deceleration during free expansion from which, with the equation of motion, the flow stress can be calculated. Failure behavior is studied with framing camera records and collected fragments. The technique has been applied to tantalum and oxygen-free electronic (OFE) copper of various grain sizes. The stress-strain data obtained is in excellent accord with the literature and the effect of initial condition (grain-size) is clearly evident in copper. The data are being used to evaluate constitutive models for these materials.

Keywords: Metals, Expanding Rings, Constitutive Properties, Failure, High Strain-Rate

443. High Strain Rate Mechanical Testing

FY 1988
\$129,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098

LLNL Contact: D. H. Lassila, (415) 423-9537/FTS 543-9537

Considerable progress has been made in establishing capabilities to perform high rate mechanical testing using the Hopkinson bar technique. A new sample geometry is being developed for the testing of soft materials, for example copper, in tension. The strain determination in the tensile sample is performed by using high elongation strain gages and a high speed framing camera. The tensile Hopkinson bar apparatus is being

employed in a study of the effects of constitutive behavior on deformation stability at high strain rates.

Keywords: Metals, Strain Testing, Tensile Testing, Mechanical Testing

444. Theoretical and Experimental Studies of Solid Combustion Reactions FY 1988
\$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

445. Fracture Behavior of Refractory Metals and Alloys in Liquid Actinides FY 1988
\$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

446. Integrated Engineering Applications Software (IDEAS) Project FY 1988
\$107,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098

LLNL Contact: N. Nguyen, (415) 422-7458/FTS 532-7458

The objective of this project is to automate mechanical testing as well as to provide engineers and technicians in the section a tool to aid them in their everyday engineering functions. The automatic data acquisition will reduce error, increase efficiency, and provide more consistent test results. Because the data are stored by the computer, the engineers can easily manipulate and analyze the data in detail using the IDEAS tools.

Keywords: Instrumentation and Technique Development

447. High Temperature Metal Alloy Radiant Property Measurements in Conjunction with Advanced Surface Spectroscopy FY 1988
\$48,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098

LLNL Contact: M. A. Havstad, (415) 423-2598/FTS 543-2598

We seek to advance our fundamental understanding of the radiant properties (emissivity, absorptivity, and reflectivity) of metals by using spectroscopic tools never before applied to radiant property measurements. These tools permit detailed analysis of the atomic composition of the metal surface and enable us to correlate surface condition with variations in the radiant properties. Data from well-characterized, pure surfaces then allow computation of more fundamental quantities, such as index of refraction and extinction coefficient. With these, the radiant properties can be more fully understood. We have collected data on solid uranium samples of particular interest to the Laser Isotope Separation (LIS) program. Our apparatus and experimental techniques have been refined to give acceptable precision with small molten samples of highly reactive liquids. When making the optical reflection measurements, we have concentrated on making the surfaces of the liquid metals very nearly flat and pure. The crucibles must survive the attack of the molten metals long enough for the measurements to be made.

Keywords: Metals, Surface, Instrumentation and Technique Development

448. Modeling and Experimental Measurement of Residual Stress FY 1988
\$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

449. A Study of Residual Stress for Epoxy-Resin Composites FY 1988
\$185,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098

LLNL Contact: W. Feng, (415) 422-8701/FTS 532-8701

The residual stress for epoxy-resin composites due to curing is studied. A micro-mechanics model is developed. The epoxy is assumed to be a viscoelastic material. The constitutive equations for viscoelastic materials are written in the incremental form and a recurrence formula is obtained. Accelerated tests for determining the viscoelastic material properties of polymeric materials at temperatures below the glass transition temperature are presented. The mechanical time- and temperature-dependent material properties of an epoxy are determined. With test durations of a few hours, the relaxation function for F263 epoxy over many decades is obtained. From the macro-mechanics point of view, the curvatures, resulting from curing of thin flat asymmetric laminates, are related with the residual strains obtained from the micro-mechanics model. An experimental apparatus has been designed to determine the residual stress and to verify the accuracy of the analytical results. These results are used for determining the residual stress and for improving the integrity of composite structures.

Keywords: Composites, Encapsulants, Predictive Behavior Modeling

450. Failure Characterization of Composite Materials

FY 1988
\$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 IM6 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

451. Polymer Adhesion Science and Mechanics

FY 1988
\$35,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098

LLNL Contacts: S. J. DeTeresa, FTS 532-6466, J. D. LeMay, FTS 543-3599,
D. M. Hoffman, FTS 532-7759 and R. E. Lyon, FTS 543-8323

It was originally proposed to study the contribution of surface energy and mechanical energy to the performance of polymer adhesion bonds. Preliminary double-torsion adhesion fracture tests of an epoxy/poly(methylmethacrylate) system were conducted in the presence of low surface energy liquids under both steady-state crack propagation and quasi-static conditions. Steady-state crack propagation tests were shown to yield inconclusive results for the dependence of adhesive fracture energy on surface energy. However, changes in quasi-static fracture energies were shown to depend on surface energy in a manner predicted by simple thermodynamic analysis. Furthermore, measurements of the adhesive shear strength between an epoxy and several polymer substrates revealed a relationship between strength and thermodynamic work of adhesion.

Keywords: Polymer Adhesion, Fracture

452. Surface Modification to Reduce Abrasion and FrictionFY 1988
\$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 are determining enhanced resistance to particulate abrasion of surfaces covered by ceramic-like "hair." We will also examine the possible effects of such "hair" in reducing drag of bodies moving through liquids.

Conventional approaches to protection of surfaces against high abrasion and impact loads have used either extremely hard coatings or compliant elastomeric coatings. The former are vulnerable to impact damage while the latter are severely limited in thermal range and chemical environment. It is possible to combine the desirable properties of both in a structure in which hard material can be simultaneously compliant by virtue of a very large L/D ratio, i.e., "hair." We have demonstrated the good performance of carbon fibers in resisting damage from impacting particles.

The possible effect of reduced drag reduction in water of a surface covered with carbon "hair," at high R_o is being investigated.

Keywords: Abrasion, Carbon Fibers, Ceramics, Fibers, Protective Coatings

453. Numerical Modeling of Crack GrowthFY 1988
\$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

Device or Component Fabrication, Behavior or Testing

454. IC Protective Coatings

FY 1988

\$700,000

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 generation of these materials, and they are presently in place in ComSec (secure communications) equipment. Current development efforts are devoted to the third and fourth generation coatings.

Keywords: IC Protection, Protective Coatings

455. Characterization of Solid-State Microstructures in High Explosives by Synchrotron X-ray Tomography

FY 1988

\$50,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098

LLNL Contact: W. C. Tao, (415) 423-0499/FTS 543-0499

We have successfully performed non-invasive, detailed characterization of defect structures within PETN and HMX single crystals by computerized tomographic and topographic (CT) methods utilizing synchrotron X-radiation (SR). We have demonstrated the feasibility of using microtomography to study pore distributions in materials of similar X-ray absorption as HE. In collaboration with Prof. Bonse, we have developed an ultra small angle camera at HASYLAB in West Germany, which allows us to measure scattering intensity in both x and y with a point source geometry. We have extended the defect size to 2-3 μm using this camera system. We have demonstrated the performance of the USAXS camera on an analog materials to HE. Latex SEM calibration spheres covering the size range from ~ 0.1 -1.5 μm give scattering curves predicted from theory. The problem of determining pore sizes in HE materials is simply the inverse problem of scattering from the latex spheres. After the initial mapping of the HE crystal defects by CT with SR, the single crystals are suspended in an impedance matching medium and subjected to shock loading to determine their initiation sensitivity. Two experimental methods are employed in this phase of the study: microphotography and infrared emission. Coupled with both streak and frame cameras, microphotography allows us to examine a single crystal under shock loading with a spatial and temporal resolution of one micron and one nanosecond, respectively. Measuring the infrared emission vs. time yields information on the rate of chemical energy released. To study the influence of defect microstructure on shock wave propagation and energy coupling into the shock front, we have devised a simple barrel matrix attached to a single electric gun laminate to measure the wave profile as a function of HE crystal thickness. The breakout time

and position of the shock wave on the surface of the HE crystal are recorded by a streaking camera.

Keywords: Synchrotron, X-ray, High Explosive, Single Crystal, Initiation Characterization, Defect Microstructure

456. Optical Diagnostics of High Explosives Reaction Chemistry FY 1988
\$200,000

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. Substantial progress has been made in the first area. This progress includes increasing signal to noise in the CARS experiments of nitromethane to greater than 100. Additionally, high pressure burn rates of nitromethane have been measured to pressures in excess of 30 GPA. Four shots on a two-stage gas gun used to study carbon precipitation in shocked benzene have provided results that are very encouraging with regard to using light scattering as a general tool for examining particulate formation in a variety systems of greater applied interest.

Keywords: Reaction Zone Chemistry, High Explosive Carbon Particle Formation, Time Resolved Diagnostics

457. Application of Laser Gaging Technology to Mechanical Testing FY 1988
\$41,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098

LLNL Contact: D. R. Lesuer, (415) 422-9633/FTS 532-9633

This project investigated the application of a non-contacting laser gaging system as a means of obtaining accurate strain data during tensile testing under conditions which prohibit the use of conventional strain gages and extensometers (i.e., elevated temperatures). A special apparatus and the necessary software were developed for moving the laser up and down, allowing the laser to continuously scan the specimen gage section and measure the axial as well as the radial strains. Various tensile tests were conducted at room temperature, 150°C, and 300°C; in all cases, we obtained accurate strain data. Use of the Zygo laser system evaluated in this project is limited by its repeatability. Optra, Inc., has introduced a two frequency laser extensometer system into the market. A preliminary evaluation of this laser has showed promising results however,

a single system is not capable of measuring axial and radial strains simultaneously. In addition, Zygo has developed a new laser which has better resolution and higher accuracy than the model we evaluated. We will examine the new Zygo laser and continue to follow the progress of Opra laser development for applications to testing in hostile environments.

Keywords: Mechanical Testing, Tensile Testing

Instrumentation and Facilities

458. Scanning Tunneling Microscope FY 1988
\$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

459. Scanning Tunneling Microscopy (STM) and Atomic Force Microscope (AFM) as a Detector FY 1988
\$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

460. Tritium Facility Upgrade

FY 1988
(\$11,900,000)¹

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 20 percent complete. Scheduled project completion is in December 1989 (first quarter FY90) and presently has \$1.8M remaining of the total \$7.8M approved funding.

Keywords: Facilities, Tritium

461. Decontamination and Waste Treatment Facility (DWTF)

FY 1988
(\$6,600,000)¹

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 FY88, 16 percent of the \$41.3 million authorized funds has been expended. Title 2 final design is complete. An environmental impact statement (EIS) has been prepared, issued for public comment, and is in process. Applicable permits (RCRA and Air Quality) have been submitted and are under review by the regulatory agencies. 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

¹Line-Item Construction Project: not included in subtotal or total.

Los Alamos National Laboratory

Materials Preparation, Synthesis, Deposition, Growth or Forming

462. Actinide Alloy Development

FY 1988
\$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

463. Plutonium Oxide Reduction

FY 1988
\$150,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098

LANL (Contract No. W-7405-ENG-36) Contact: K. Axler, (505) 667-4085/FTS 843-4045

The thermodynamics of interactions among the components used in the pyrochemical processing of plutonium are determined along with the relevant phase relations.

Keywords: Radioactive Materials, Plutonium, Thermodynamics, Phase Diagrams, Direct Oxide Reduction, Electrorefining, Molten Salt Extraction

464. Replacement Noble-Metal Alloys

FY 1988
\$75,000

DOE Contact: G. Bennett, (301) 353-3197/FTS 233-3197

LANL (Contract No. W-7405-ENG-36) Contact: T. George, (505) 667-4931/FTS 843-931

New noble-metal based alloys are being developed to provide improved containment for plutonium oxide used in space power systems. The thermodynamics, phase relations and phase stabilities are being determined, so that the compatibility regimes can be calculated.

Keywords: Plutonium, Containment, Phase Diagrams

465. Whisker Reinforced Structural Ceramics FY 1988
\$200,000

DOE Contact: E. E. Hoffman, (615) 576-0735/FTS 626-0735

LANL (Contract No. W-7405-ENG-36) Contact: P. D. Shalek, (505) 667-6863/
FTS 843-6863

Long SiC whiskers are being grown by the vapor-liquid-solid (VLS) process for use as directional reinforcement for ceramic materials of interest to the Fossil Energy Materials Program. The main subtasks involved in this work are (1) growing of adequate quantities of high quality long whiskers for textile development while continuing to improve the process and its control, (2) improvement of whisker beneficiation, and (3) development of a staple yarn of satisfactory whisker density which can be woven.

Keywords: Ceramics, Whiskers, Composites, Textiles

466. Ion-Beam Implantation FY 1988
\$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

467. Electroplating Low Atomic Number Materials FY 1988
\$120,000

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

468. Three New Conducting Polymers FY 1988
\$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

One polyphenylguinoxaline and two polypyrrones, heretofore unknown materials, have been synthesized and all show unique electrically conductive properties when treated with appropriate doping agents. These new polymers all show better thermal stability than polyacetylene.

Keywords: Polyphenylguinoxaline, Polypyrrones, Conducting Polymers

469. New Highly Conductive Doped Polyacetylene FY 1988
\$150,000

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 new, unique, cesium electride has been found to induce a high level of electrical conductivity in polyacetylene films. This dopant has also been found to significantly improve the stability of polyacetylene. Canal polymerization of polyacetylene using an organic crystal matrix is being explored. This gives a highly oriented polymer.

Keywords: Conducting Polymers, Polyacetylene

470. Liquid Crystal Polymer Development FY 1988
\$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 will be made to synthesize a liquid crystal polymer with strength in three dimensions. This will be a unique polymer with a number of possible applications.

Keywords: Liquid Crystal Polymers

471. Surface Property Modified Plastic Components FY 1988
\$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

472. Low-Density, Microcellular Plastic Foams FY 1988
\$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

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.

Keywords: Foams, Polyolefins, Polyurethanes, Silicones, Polyesters

473. Target Coatings FY 1988
\$600,000

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

474. Physical Vapor Deposition and Surface Analysis FY 1988
\$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.

Keywords: Coatings and Films, Physical Vapor Deposition, Sputtering, Ion Plating, Corrosion, Nondestructive Evaluation

475. Fluidized Bed Coatings FY 1988
\$200,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098

LANL (Contract No. W-7405-ENG-36) Contact: D. W. Carroll, (505) 667-2145/
FTS 843-2145

Techniques have been developed for low-temperature deposition of tungsten, molybdenum, rhenium, and nickel on hollow substrates of spherical and cylindrical shapes. Ultra-thin, free-standing shapes have been fabricated.

Keywords: Coatings, Metals, Chemical Vapor Deposition

476. Electrodeposition of Metallic Glasses FY 1988
\$25,000

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 techniques. Thick amorphous deposits are possible by electrodeposition in contrast to the thickness limitations of the

rapid quenching technique. Applications include: hard coatings, corrosion-resistant coatings, coatings for weapons physics experiments and inertial confinement fusion components.

Keywords: Metallic Glasses, Amorphous Alloys, Electrodeposition, Metals

477. Polymers and Adhesives FY 1988
\$800,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098

LANL (Contract No. W-7405-ENG-36) Contact: W. A. May, Jr., (505) 667-6362/FTS 843-6362

The objective of this project is to identify potential weapons engineering and physics applications for plastic materials, select or develop appropriate materials, develop low cost fabrication techniques compatible with contractor production capabilities, and to characterize promising materials on a timely basis to provide optimum material choices for new weapons designs. Materials development projects include: highly filled polymers, reinforced composites, cushioning materials, and high-explosives-compatible adhesives.

Keywords: Adhesives, Composites, Polymers, Near-Net-Shape Processing, Surface Characterization and Treatment, Weapons

478. Tritiated Materials FY 1988
\$485,000

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.

Keywords: Tritium, Metal Tritides, Li(D,T), Tritiated Materials, Radioactive Materials

479. Salt Fabrication

FY 1988
\$530,000

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 and hot-isostatic pressing techniques to near-net-shape, 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

480. Slip Casting of Ceramics

FY 1988
\$100,000

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

481. Whisker Growth Technology

FY 1988
\$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

482. New Hot Processing Technology

FY 1988

\$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

483. Glass and Ceramic Coatings

FY 1988

\$10,000

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

Ceramic 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.

Keywords: Enamels, Ceramic Coatings, Metals, Radiation Effects, Accelerator Technology

484. Cold Pressing, Cold Isostatic Pressing and Sintering

FY 1988

\$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 , 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

485. Plasma-Flame Spraying Technology : FY 1988
\$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

486. Rapid Solidification Technology FY 1988
\$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

487. Superplastic Forming FY 1988
\$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

488. Microwave Sintering/Processing FY 1988
\$120,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098

LANL (Contract No. W-7405-ENG-36) Contact: J. 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 and glass. The method involves the use of very high frequency microwaves which suscept 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

489. Predictions of Super Strong Polymers FY 1988
\$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

490. High Energy Storage Material FY 1988
\$150,000

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/trifluoroethylene 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

491. High Temperature Superconductors for Electric Utility Applications FY 1988
\$275,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098

LANL (Contract No. W-7405-ENG-36) Contact: G. Maestas, (505) 667-1372/
FTS 843-1372

Preparation of superconducting ceramics into useful "generic conductor" configurations requires substantial improvements in critical current density along with provisions for both electrical and mechanical stabilization of the conductor. These combined goals are approached by classical powder synthesis and consolidation and by direct melting routes; the two depend on the same fundamental phase stability criteria and are synergistic. Primary attention is focused on the thallium-bearing systems.

Keywords: Superconductors, Tapes, Wires

492. Synthesis of Porous Glass Structures FY 1988
\$20,000

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 high surface area, porous glass fibers and rods from a silicon alkoxide gel. The porous glass structures are then used in the development of real-time chemical analysis sensors. Initial efforts involve the incorporation (attachment) of pH sensitive organic species into the porous glass to produce development pH sensors.

Keywords: Glass, Sol Gel, pH Sensors

Materials Structure or Composition

493. Actinide Surface Properties FY 1988
\$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) 667-2345/
FTS 843-2345

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

494. Neutron Diffraction of Pu and Pu Alloys FY 1988
\$237,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098
LANL (Contract No. W-7405-ENG-36) Contact: S. E. Bronisz, (505) 667-4665/
FTS 843-4665

Physical structure of plutonium is being studied by neutron diffraction at the Los Alamos WNR pulsed neutron source. A time-of-flight technique is used to measure diffraction at elevated temperatures and pressures.

Keywords: Alloys, Radioactive Materials, Transformation, Microstructure

495. Surface, Material and Analytical Studies FY 1988
\$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

496. Modeling of Interfaces in Ordered Intermetallic Alloys FY 1988
\$550,000

DOE Contact: S. M. Wolf, (202) 586-5377/FTS 896-5377

LANL (Contract No. W-7405-ENG-36) Contact: P. J. Hay, (505) 667-3663/FTS 843-3663

The ECUT Materials by Design effort has developed models to predict the cohesive properties of interfaces in ordered Ni-Al alloys and the role of solute atoms such as B and S in altering these properties during brittle fracture at grain boundaries. A hierarchy of models encompassing electronic structure calculations, interatomic potentials, atomistic simulations and phenomenological models of crack propagation has been implemented. The theoretical modeling effort complements the current ECUT experimental program in intermetallic alloy development at ORNL.

Keywords: Metals, Alloys, Intermetallics, Modeling, Grain Boundary, Structure

Materials Properties, Behavior, Characterization or Testing

497. Mechanical Properties of Plutonium and Its Alloys FY 1988
\$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

498. Phase Transformations in Pu and Pu Alloys FY 1988
\$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

499. Isobaric Expansion of Actinides FY 1988
\$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

500. Plutonium Shock Deformation FY 1988
\$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

501. Dielectric Loss Measurements in Ceramics FY 1988
\$400,000

DOE Contact: T. C. Reuther, (301) 353-4963/FTS 233-4963

LANL (Contract No. W-7405-ENG-36): H. M. Frost (505) 667-1290/FTS 843-1290

Ceramic insulators are required for high-frequency heating systems in fusion reactors, where intense radiation fields will be encountered. In this work loss tangent and dielectric constant measurements are made on irradiated materials to characterize damage effects and point the way toward development of improved insulators.

Keywords: Dielectric Properties, Ceramics, Radiation Damage, Electrical Insulators, Fusion Reactors, Radiation Damage

502. Nondestructive Evaluation FY 1988
\$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

Nondestructive evaluation techniques are developed that produce quantitative estimates of material properties. Multivariate analysis is applied to welding processes. Tomographic techniques are used to extend radiographic inspections.

Keywords: Nondestructive Evaluation, Radiography, Ultrasonic Microscopy, Tomography

503. Powder Characterization FY 1988
\$45,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098

LANL (Contract No. W-7405-ENG-36) Contact: G. J. Vogt, (505) 667-5432/
FTS 843-5432

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

504. Shock Deformation in Actinide Materials FY 1988
\$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

505. Dynamic Mechanical Properties of Weapons Materials FY 1988
\$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

506. Dynamic Testing of Materials for Hyper-Velocity Projectiles FY 1988
\$80,000

DOE Contact: A. E. Evans, (301) 353-3098/FTS 233-3098

LANL (Contract No. W-7405-ENG-36) Contact: G. T. Gray, III, (505) 667-5452/
FTS 843-5452

Soft-shock deformation and spall testing of high density materials. Microstructural characterization of shock-deformed material and fractography on spall fracture surfaces. Dynamic and quasi-static compression and tension tests.

Keywords: Shock Deformation, Spall Strength, Microstructure, Strength

507. Mechanical Properties FY 1988
\$300,000

DOE Contact: F. V. Nolfi, (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

508. Radiation Damage in High-Temperature Superconductors FY 1988
\$305,000

DOE Contact: R. J. Gottschall, (301) 353-3428/FTS 233-3428

LANL (Contract No. W-7405-ENG-36) Contact: F. W. Clinard, Jr., (505) 667-5102/
FTS 843-5102

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 changes in electrical and magnetic properties.

Keywords: High-Temperature, Superconductors, Radiation Damage, Atomic Displacements, Ionization Damage, Properties

509. Insulators for Space Reactor Applications FY 1988
\$92,000

DOE Contact: S. Samuelson, (415) 273-4253/FTS 536-4253

LANL (Contract No. W-7405-ENG-36) Contact: F. W. Clinard, Jr., (505) 667-5102/
FTS 843-5102

Insulators for thermionic convertors (used to generate electricity in fission reactors) face a severe environment, including high temperatures, a DC electric field, and an intense neutron flux. In this program candidate materials are exposed to that environment, and degradation effects monitored by measurements made during and after testing.

Keywords: Space Reactor, Thermionic Convertor, Electrical Insulators, Ceramics, Radiation Damage, Properties

510. Structural Ceramics**FY 1988
\$345,000**

DOE Contact: R. J. Gottschall, (301) 353-3428/FTS 233-3428

LANL (Contract No. W-7405-ENG-36) Contact: D. S. Phillips, (505) 667-5128/
FTS 843-5128

Mechanistic studies of crack propagation in model SiC-whisker reinforced glass matrix composites. Identification and modification of indigenous whisker surface species with implications for both mechanism and magnitude of toughening from crack tip-whisker interaction. Photoelastic characterization of both local and long-range stress fields resulting from whisker incorporation, crack incorporation, and crack-whisker interaction.

Keywords: Structural Ceramics, Fracture Toughness, Surface Science, Crack Propagation, Whiskers

Device or Component Fabrication, Behavior or Testing**511. Radiochemistry Detector Coatings****FY 1988
\$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

512. Target Fabrication**FY 1988
\$1,500,000**

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687

LANL (Contract 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

513. Filament Winder

FY 1988
\$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

514. Polymeric Laser Rods

FY 1988
\$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

515. High Energy Density Joining Process Development FY 1988
\$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

516. Arc Welding Process Development FY 1988
\$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 Varstraint 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, Varstraint, Video

517. Solid State Bonding FY 1988
\$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

AR&TD Fossil Energy 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

518. Fundamental Study of Aluminizing and Chromizing Processes FY 1988
\$50,000

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

519. Fabrication Development of Nickel-Iron Aluminides FY 1988
\$172,000

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: V. K. Sikka, (615) 574-5112/FTS 624-5112

The purpose of this task is to develop the fabrication technology for nickel-iron aluminides in sufficiently large heat sizes to provide assurance that the alloys can be fabricated by standard industrial processes.

Keywords: Alloys, Aluminides, Fabrication

520. Development of Iron Aluminides FY 1988
\$144,000

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: 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 Fe₃Al with an optimum combination of strength, ductility, and corrosion resistance for use as components in advanced fossil energy conversion systems.

Keywords: Alloys, Aluminides

521. Development and Evaluation of Advanced Austenitic Alloys FY 1988
\$268,000

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 intermetallic 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 7600°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 crackings 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 varestment 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

522. Evaluation of the Fabricability of Candidate Advanced Austenitic Alloys

FY 1988

\$100,000

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

523. Consolidation of Rapidly Solidified Aluminide Metal Powders

FY 1988

\$150,000

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

524. Investigation of Electrospark Deposited Coatings for Protection of Materials in Sulfidizing Atmospheres FY 1988

\$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

525. Short Fiber Reinforced Structural Ceramics FY 1988

\$225,000

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 investigate the utility of whisker reinforcement technology for producing structural ceramic composites of improved strength and fracture toughness. The program consists of two technical tasks. The first is to optimize an existing Los Alamos whisker growth process to produce alpha-phase silicon nitride ($\alpha\text{-Si}_3\text{N}_4$) whiskers and beta-phase silicon carbide ($\beta\text{-SiC}$) whiskers of uniform size, optimum strength, and in quantities suitable for composite use. The second task will involve evaluating the contribution of the whiskers in selected ceramic-matrix composites.

Keyword: Ceramics, Whiskers, Composites

526. Fabrication of Fiber-Reinforced Composites by Chemical Vapor Infiltration (CVI)**FY 1988****\$181,000**

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 and R. A. Lowden, (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 Si₃N₄ have been identified as being most promising. Fiber dimensions, geometry, packing density, binder type and concentrations, and other processing variables have been evaluated experimentally.

Initial experimental efforts focused on the use of a vacuum-forming molding process to form a low-density fiber bed suitable for vapor infiltration. Once the fiber bed was formed, dried, and heat treated, the matrix of the composite was formed by CVI using a high-temperature furnace. A novel scheme (patent applied for) of forcing the coating gases to flow through the fiber bed was tested in an attempt to increase the deposition rate over rates normally obtained when flowing the deposition gases across the surface to be coated. In addition, depending on the deposition reaction, a vacuum may be used to assist the flow of gases through the fibrous parts. 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

527. Characterization of Fiber-CVD Matrix Interfacial Bonds FY 1988
\$120,000

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

528. Microwave Sintering of Ceramics FY 1988
\$144,000

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 primary purpose of this program is to conduct coordinated research and development on ceramic materials with major emphasis on the microwave processing of new ceramics at ORNL.

Keywords: Ceramics, Microwave Sintering

529. Development of Advanced Fiber Reinforced Ceramics FY 1988
\$100,000

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 to be used is amorphous fused silica or modified silica glass and the focus will be the development of fiber reinforced silica. Parameters to be studied will 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

530. Modeling of Fibrous Preforms for CVD Infiltration

FY 1988

\$45,000

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

531. Improved Ceramic Composites Through Controlled Fiber-Matrix Interaction FY 1988
\$200,000
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

The fiber-matrix interface plays a key role in the performance of ceramic matrix composites; however, the nature of these interfaces and their relationship to composite properties, structure, and process/environmental history is not well understood. The purpose of this work is to understand and control the fiber-matrix interface to improve the performance of ceramic matrix composites in fossil energy systems. The principal objectives are to: (1) develop a basic understanding of fiber-matrix interfaces, (2) relate this understanding to the composite materials, properties, structures, processes, and environments, and (3) apply this knowledge to modify or control the fiber-matrix interface.

Keywords: Composites, Fiber-Reinforced

Materials Structure and Composition

532. Analytical Characterization of Coal Surfaces and Interfaces FY 1988
\$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. Much of the efforts will be directed to the development of equipment and techniques followed by interpretation in a manner most useful to design engineers. 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 Testing533. Transfer Model Predicting Thermomechanical Behavior of Refractory Linings to Industry FY 1988\$40,000

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: D. A. Patterson, (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

534. Transformation, Metallurgical Response and Behavior of the Weld Fusion and Heat Affected Zone in Cr-Mo Steels for Fossil Energy Applications FY 1988\$ 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 Tennessee, Department of Materials Science and Engineering (Contract No. DE-AC05-84OR21400, Martin Marietta Energy Systems, Inc., Subcontract No. 12B-07685CX77) Contact: C. D. Lundin, (615) 974-5310

The objective of this research was to develop fundamental information on the metallurgical behavior of the heat affected zone of welds in chromium-molybdenum alloys. This was accomplished by: (1) documenting formation behavior under the welding conditions that involve rapid heating and cooling, (2) determining the metallurgical transformation products in the heat affected zone and weld fusion zone, (3) determining the sensitivity of the materials to heat affected zone cracking, (4) determining the sensitivity of the materials to phenomena such as reheat cracking and/or hot cracking, and (5) determining the influence of the various heat affected zone regions on the creep rupture behavior.

Keywords: Materials Processing, Materials Characterization

535. Mechanical Properties and Microstructural Stability of Advanced Austenitic Alloys FY 1988
\$85,000

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

536. Analysis of Hydrogen Attack on Pressure Vessel Steels FY 1988
\$ 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 at Santa Barbara, Department of Chemical and Nuclear Engineering (Contract No. DE-AC05-84OR21400, Martin Marietta Energy Systems, Inc., Subcontract No. 19X-22276C) Contact: G. R. Odette, (805) 961-3525

Physical models were developed that describe the initiation and development of methane damage in carbon steel, C-Mn-Si steels, 2 1/4 Cr-1 Mo steel, and weldments. Nelson diagrams were predicted and were consistent with available data. The model is particularly useful in establishing the relative importance of microconstituents, deformation mechanisms, and fracture mechanisms to the hydrogen attack process. In this sense it will guide the development of modified low alloy steels for optimum resistance to hydrogen attack. The role that stress and plastic strain transients play in the hydrogen attack phenomena was examined. Such information is vital because the

current design rules for hydrogen service restrict the use of the Nelson curves to situations where the stresses do not exceed the primary stress intensities provided in the ASME Boiler and Pressure Vessel Code.

Keywords: Hydrogen Effects

537. Development of a Design Methodology for High-Temperature Cyclic Application of Materials Which Experience Cyclic Softening

FY 1988

\$ 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 Illinois, Department of Mechanical and Industrial Engineering (Contract No. DE-AC05-84OR21400, Martin Marietta Energy Systems, Inc., Subcontract No. 19X-55904C) Contact: D. L. Marriott, (217) 333-7237

The objective of this project is to develop a design methodology for high-temperature cyclic conditions, taking into account the effects of strain softening. Since the problem of cyclic softening is generic to a wide class of medium- to high-strength low alloy steels, it is not the main purpose of this investigation to examine specific characteristics of any one steel but to investigate the general behavior of components subject to the cyclic softening phenomenon. The specific objectives of the project are: (1) the development of simplified methods of component analysis to evaluate overall and local effects of cyclic softening on time-dependent deformations, (2) the development of an improved understanding of the mechanisms of interaction between intermittent cyclic stresses and reduction of resistance to creep deformation, (3) an evaluation of the possible effects of cyclic softening on the initiation and propagation of defects, (4) an evaluation of the possible effects of cyclic softening on the procedure for determining allowable design stresses for high-temperature design, and (5) provision of input into the material effort to extend life in existing power plants by examining the relation between material damage parameters and component performance criteria, for possible use in remnant life assessment.

Keywords: Materials, Cyclic Softening

538. Investigation of the Weldability of Ductile Aluminides

FY 1988

\$50,000

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 (ORNL) and Colorado School of Mines (CSM) and is conducted as a PhD thesis project by a CSM student working at CSM and at ORNL.

Keywords: Joining and Welding, Materials Characterization

539. Corrosion Studies of Iron Aluminides FY 1988

\$22,000

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

540. Fireside Corrosion Tests of Candidate Advanced Austenitic Alloys, Coatings, and Claddings FY 1988

\$60,000

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. [In Process]) 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

541. Microstructural Studies of Advanced Austenitic Steels FY 1988
\$36,000

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

542. Joining Techniques for Advanced Austenitic Alloys FY 1988
\$43,000

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

543. Corrosion and Mechanical Properties of Alloys in FBC and Mixed-Gas Environments

FY 1988
\$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 7500°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.

Work being conducted under this task provides a basic understanding of the corrosion behavior of commercial and model alloys after exposure to multicomponent gas mixtures. The information on scale thickness, intergranular penetration, and morphological changes developed in this task provides a rational basis for the extrapolation of corrosion rates as a function of temperature, alloy composition, and chemistry of the gas environment. The corrosion experiments by a thermogravimetric technique in mixed-gas atmospheres on selected commercial high-chromium alloys and on model alloys fabricated with compositional variations will establish the role of different alloying elements on the mechanisms of scale development and adhesion and on breakaway phenomena leading to scale failure. The project on heat exchanger materials involves development of corrosion information in the low- and medium-Btu gasification atmospheres. The experiments are conducted with internally cooled tube specimens of selected commercial materials and some commercial coatings. The critical variables, such as gas temperature and metal temperature, are independently controlled

in the ranges of interest in practical systems. The gas temperatures will range from 850 to 1100°C, a range that encompasses the raw gas outlet temperatures of dry ash and slagging gasifier types. The results from this program will establish the process variable envelopes for various commercial materials for use in heat exchanger applications. Incoloy 800H plates welded with low-nickel filler metals have been fabricated, and they will be examined for their corrosion resistance in mixed-gas atmospheres. Nickel aluminides and iron-nickel aluminides developed at Oak Ridge National Laboratory will be examined for their sulfur resistance by using thermal gravimetric analysis and post-exposure analysis of specimens.

Keywords: Corrosion, Gasification, Creep Rupture, Fluidized Bed Combustion

544. Investigation of Corrosion-Resistant Oxide Scales on Iron-Based Alloys in Mixed-Gas Environments

FY 1988

\$177,000

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 Cr₂O₃- and Al₂O₃-forming iron-based alloys in mixed oxidant (O₂, SO₂, H₂S, H₂O) 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., SiO₂ 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

545. Investigation of Corrosion Mechanisms of Coal Combustion Products on Alloys and Coatings

FY 1988
\$ 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 Pittsburgh (Contract No. DE-AC05-84OR21400, Martin Marietta Energy Systems, Inc., Subcontract No. 19X-43346C) Contact: G. H. Meier, (412) 624-5316

The objective of this research project was to investigate the formation and breakdown of protective oxide scales in mixed oxidant gases. The results of this research will support the development of improved heat exchanger materials for applications in: (1) heat recovery systems for coal conversion plants (particularly gasification), and (2) coal-fired, industrial and utility boilers. The materials used in this study were model alloys selected for their ability to form single oxides of chromium, aluminum, and silicon. The temperature range was 500°C to 700°C and the test environments contain mixed oxidants (O₂, CO₂, SO₂, H₂, and Cl₂). Specific objectives included determination of the effect of surface pretreatment and preoxidation on the structure and properties of oxide scales, and the correlation of these treatments and the resulting structures and properties with the breakdown of the scales in mixed oxidant gases. Loss of scale protection by mechanical means (cracking, spalling, etc.) and by transport of corroding species (S and Cl) was considered.

Keyword: Corrosion

546. Investigation of the Effects of Microalloy Constituents, Surface Treatment, and Oxidation Conditions on Development and Breakdown of Protective Oxide Scales

FY 1988
\$270,000

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

547. Investigation of the Effects of Microalloy Constituents, Surface Treatment, and Oxidation Conditions on Development and Breakdown of Protective Oxide Scales

FY 1988

\$250,000

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 Cr₂O₃ formers and Fe-25Cr-6Al which is an Al₂O₃ 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

548. Investigation of the Effects of Microalloy Constituents, Surface Treatment, and Oxidation Conditions on Development and Breakdown of Protective Oxide Scales

FY 1988

\$211,000

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

549. A Study of Erosive Particle Rebound Parameters FY 1988
\$40,000

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

550. Studies of Materials Erosion in Coal Conversion and Utilization Systems FY 1988
\$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

551. In-Situ Scanning Electron Microscopy Studies of Erosion and Erosion-Corrosion FY 1988

\$177,000

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

552. Solid Particle Erosion in Turbulent Flows Past Tube Banks FY 1988

\$40,000

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

553. Study of Particle Rebound Characteristics and Material Erosion at High Temperatures

FY 1988

\$ 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 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

554. Development of Nondestructive Evaluation Techniques and the Effect of Flaws on the Fracture Behavior of Structural Ceramics

FY 1988

\$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 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

555. Joining of Silicon Carbide Reinforced Ceramics FY 1988
\$150,000

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

556. Nondestructive Evaluation of Advanced Ceramic Composite Materials FY 1988
\$150,000

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 Si₃N₄ 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

557. Structural Reliability and Damage Tolerance of Ceramic Composites FY 1988
\$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) 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.

Keywords: Ceramics, Glasses, Materials Characterization

558. Mechanical Properties of Ceramic Fiber-Ceramic Matrix Composites FY 1988
\$50,000

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. [In Process]) 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

559. Ceramic Catalyst Materials FY 1988
\$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-ACO4-76DP00789) Contact:
D. H. Doughy, 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 will focus 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

560. Materials and Components in Fossil Energy Applications (Newsletter) FY 1988
\$115,000
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

561. Assessment of the Causes of Failure of Ceramic Filters for Hot-Gas Cleanup
in Fossil Energy Systems and Determination of Materials Research and
Development Needs FY 1988
\$ 0 (PF)
DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman,
(615) 576-0735/FTS 626-0735
Acurex Corporation (Contract No. DE-AC05-84OR21400, Martin Marietta Energy
Systems, Inc., Subcontract No. 11X-57964C) Contact: J. W. Sawyer, (415) 961-5700

The purpose of this project was to determine the principal causes of failure of ceramic filters used for removal of fine particles from high-temperature, high-pressure gas streams in coal conversion and utilization systems such as fluidized-bed combustors, direct

coal-fired gas turbines, and coal gasification systems. As part of this project, the current practice for design and engineering of ceramic filters was researched, and the current use for such filters in industrial and utility applications similar to those in the fossil energy systems listed above was described. Materials failure experience was examined, and causes of failure of ceramic filters were determined through conversations with manufacturers and users and through laboratory failure analyses. Materials research and development that would improve the reliability of these filters, and design features of current filters that contribute to materials failure, were identified.

Keywords: Gas Cleanup, Filters, Ceramic, Assessment

562. Assessment of Potential Applications of Ceramic Composites in Gas Turbines

FY 1988
\$ 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

563. Mechanisms of Galling and Abrasive Wear

FY 1988
\$75,000

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

564. Fabrication of Commercial-Scale Fiber-Reinforced Hot-Gas Filters by Chemical Vapor Deposition FY 1988

\$100,000

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. [in process]) 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, in collaboration with ORNL.

Keywords: Ceramics, Composites, Filters

565. Development of Ceramic Membranes for Gas Separation FY 1988

\$150,000

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 (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

566. Investigation of the Mechanical Properties of CVD Infiltrated Ceramic Composite Tubular Components

FY 1988

\$85,000

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

567. Thermomechanical Modeling of Refractory Brick Linings for Slagging Gasifiers

FY 1988

\$62,000

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 will include cyclic multiaxial nonlinear constitutive law, temperature-dependent heat conduction, and temperature-dependent creep laws, is to be developed for refractory brick and mortar. The model will be 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 will be made for vessel configuration, material property combinations, and optimum heating schedules.

Keywords: Refractory Liners

568. Evaluation of Candidate Materials for Solid Oxide Fuel Cells FY 1988
\$150,000

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 to find and develop highly electronically conducting oxides for use as cathodes in solid oxide fuel cells (SOFC). Specifically, the work involves determining the effects of rare earth additions on the electrical transport properties of candidate materials. In addition, the study will develop an understanding of the crystallographic, microstructural, and phase equilibrium factors that influence transport properties. The electronic conductivity, transference numbers, and Seebeck coefficient are measured as functions of temperature and oxygen partial pressure. An important part of this investigation involves the study of the stability of a particular oxide in the environments and temperature ranges of SOFC fabrication and operation as well as the compatibility of the oxide electrode with the other cell components. This latter criterion includes both chemical compatibility and relative thermal expansion coefficients.

Keyword: Fuel

569. Gas Separations Using Inorganic Membranes FY 1988
\$200,000

DOE Contacts: J. S. Halow, FTS 923-4109 and E. E. Hoffman, (615) 576-0735/
FTS 626-0735

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

570. Ceramic Fiber-Ceramic Matrix Hot Gas Filters : FY 1988
\$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 (to be issued under the AR&TD Fossil Energy Materials Program), with an industrial organization. By collaboration between ORNL and the industrial partner (selected by competitive bidding), full-size candle filters will be produced.

Keywords: Ceramic Composites, Filters

571. Identification of Materials for Hot-Gas Filter Tubesheets FY 1988
\$137,000

DOE Contacts: J. W. Byam, FTS 923-4533 and E. E. Hoffman, (615) 576-0735/
FTS 626-0735

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 (ORNL); (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 various 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 Facilities572. Management of the AR&TD Fossil Energy Materials Program FY 1988
\$350,000

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: R. R. Judkins, P. T. Carlson and D. N. Braski,
(615) 574-4572/FTS 624-4572

The overall objective of the Advanced Research and Technology Development (AR&TD) Fossil Energy 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 AR&TD Fossil Energy 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 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

573. Coal Conversion and Utilization Plant Support Services FY 1988
\$43,000

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 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. This task will also provide failure analyses and on-site examinations for the Wilsonville, Alabama, Advanced Coal Liquefaction Research and Development Facility and other coal conversion plants as needed.

Keywords: Corrosion, Liquefaction, Failure Analysis

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

574. Materials Technical Support for the Great Plains Coal Gasification Plant

FY 1988
\$101,000

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 is to provide materials technical support services to the Great Plains Coal Gasification Project. The scope of the project will include assistance to the ANG Coal Gasification Company (Administrator of the Great Plains Coal Gasification Project) on any technical issues related to materials performance in that plant. Activities will include 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

575. Materials Technical Support for the Clean Coal Program FY 1988

\$25,000

DOE Contacts: R. Santore, FTS 723-6131 and E. E. Hoffman, (615) 576-0735/
FTS 626-0735

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

DIRECTORY

J. D. Achenbach
Department of Civil Engineering
Northwestern University
Evanston, IL 60201
(312) 491-5527

R. H. Adler
LLNL
University of California
P.O. Box 808
Livermore, CA 94550
(415) 423-4417

Ilhan Aksay
Dept. of Mat. Science & Eng.
University of Washington
Seattle, WA 98195
(206) 543-2625

L. F. Allard
ORNL
P.O. Box 2008
Bldg. 4515, MS 064
Oak Ridge, TN 37831
(615) 574-4981

R. E. Allred
Division 1812
Sandia National Laboratories
Albuquerque, NM 87185
(505) 844-5538

P. Angelini
ORNL
P.O. Box 2008
Bldg. 4515
Oak Ridge, TN 37830-6065
(615) 574-4565

C. Arnold, Jr.
Division 1811
Sandia National Laboratories
Albuquerque, NM 87185
(505) 844-8728

T. W. Arrigoni
U.S. Dept. of Energy
P.O. Box 10940
Pittsburgh, PA 15236
(312) 972-4450

J. S. Arzigian
Division 1815
Sandia National Laboratories
Albuquerque, NM 87185
(505) 844-2465

R. A. Assink
Division 1811
Sandia National Laboratories
Abuquerque, NM 87185
(505) 844-6372

V. Saimasarma Avva
N. Carolina State Univ.
Grahm Hall #8
Greensboro, NC 27411
(919) 379-7620

M. Murray Bailey
NASA Lewis Research Center
MS 77-6
21000 Brookpark Road
Cleveland, OH 44135
(216) 433-3416

Charles D. Baker
 Technical Res. Assoc., Inc.
 410 Chipeta Way, Suite 222
 Salt Lake City, UT 84108
 (801) 582-8080

L. Ballou
 LLNL
 University of California
 Livermore, CA 94550
 (213) 422-4911

Samuel J. Barish
 ER-16/GTN
 U.S. Dept. of Energy
 Washington, DC 20545
 (301) 353-4174

W. Barnett
 NE-55/GTN
 U.S. Dept. of Energy
 Washington, DC 20545
 (301) 353-3097

Harold N. Barr
 Hittman Mat. & Med. Components, Inc.
 9190 Red Branch Road
 Columbia, MD 21045
 (301) 730-7800

J. L. Bates
 Pacific Northwest Laboratories
 P.O. Box 999
 Richland, WA 99352
 (509) 375-2579

S. Bauer, Division G314
 Sandia National Laboratory
 P.O. Box 5800
 Albuquerque, NM 87185
 (505) 846-9645

D. J. Baxter
 Material Science & Tech. Div.
 Argonne National Laboratories
 9700 South Cass Ave
 Argonne, IL 60439
 (312) 972-5117

M. B. Beardsley
 Caterpillar, Inc.
 100 N.E. Adams Street
 Peoria, IL 61629
 (309) 578-8514

R. L. Beatty
 ORNL
 P.O. Box 2008
 Bldg. 4508, MS 088
 Oak Ridge, TN 37831
 (615) 574-4536

B. Beaudry
 Ames Laboratory
 Iowa State University
 Ames, Iowa 50011
 (515) 294-1366

P. F. Becher
 ORNL
 P.O. Box 2008
 Bldg. 4515, 068, Room 275
 Oak Ridge, TN 37831-6088
 (615) 574-5157

T. R. Beck
 Electrochemical Tech. Corp.
 3935 Leary Way, NW
 Seattle, WA 98107
 (206) 632-5965

R. G. Behrens
 LANL
 Los Alamos, NM 87545
 (505) 667-8327

K. W. Benn
Garrett Corporation
2739 E. Washington Street
Phoenix, AZ 85010
(602) 231-4373

John Benner
Solar Electric Conversion Div.
SERI
1617 Cole Blvd.
Golden, CO 80401
(303) 231-1396

Dave Benson
SERI
1617 Cole Blvd
Golden, CO 80401
(303) 231-1162

Clifton G. Bergeron
University of Illinois
Department of Ceramic Eng.
105 South Goodwin Avenue
204 Ceramics Building
Urbana, IL 61801
(217) 333-1770

Sam Berman
Bldg. 90, Rm. 3111
Lawrence Berkeley Laboratory
University of California
Berkeley, CA 94720
(415) 486-5682

R.M. Biefeld
Division 1150
Sandia National Laboratories
Albuquerque, NM 87185
(505) 844-1556

L. Blair
Los Alamos National Lab
P.O. Box 1663
Los Alamos, NM 87545
(505) 667-6250

J. Bockris
Texas A&M University
College Station, TX 77843-3255
(713) 845-5335

Robert Boettner
CE-112/FORS
U.S. Dept. of Energy
Washington, DC 20585
(202) 252-9136

W. D. Bond
Oak Ridge National Laboratory
P.O. Box 2008
Bldg. 7920, 384, Room 0014
Oak Ridge, TN 37831-6088
(615) 574-7071

M. K. Booker
ORNL
P.O. Box 2008
Oak Ridge, TN 37831-6088
(615) 574-5113

J. A. Borders
Division 1823
Sandia National Laboratories
Albuquerque, NM 87185
(505) 844-8855

J. A. M. Boulet
University of Tennessee
310 Perkins Hall
Knoxville, TN 37996
(615) 974-8376

R. J. Bourcier
Division 1832
Sandia National Laboratories
Albuquerque, NM 87185
(505) 844-6638

H. K. Bowen
Dept. of Mat. Science & Eng.
MIT
77 Massachusetts Avenue
Cambridge, MA 02139
(617) 253-6892

D. J. Bradley
Pacific Northwest Laboratory
Richland, WA 99352
(509) 375-2587

R. A. Bradley
ORNL
P.O. Box 2008
Bldg. 4515
Oak Ridge, TN 37831-6067
(615) 574-6094

C. R. Brinkman
ORNL
P.O. Box 2008
Bldg. 4500-S, MS 154
Oak Ridge, TN 37831
(615) 574-5106

S. E. Bronisz
LANL
Los Alamos, NM 87545
(505) 667-4665

J. A. Brooks
Division 8312
Sandia National Laboratories
Livermore, CA 94550
(415) 422-2051

K. L. Brower
Division 1110
Sandia National Laboratories
Albuquerque, NM 87185
(505) 844-6131

J. J. Brown, Jr.
Materials Engineering
Virginia Polytechnic Inst.
Blacksburg, VA 24061
(703) 961-6777

N. E. Brown
Division 1821
Sandia National Laboratories
Albuquerque, NM 87185
(505) 844-2747

S. T. Buljan
GTE Laboratories, Inc.
40 Sylvan Road
Waltham, MA 02254
(617) 890-8460

R. F. Bunshah
Mat. Science & Eng. Dept.
Univ. of CA, Los Angeles
6532 Boelter Hall
Los Angeles, CA 90024
(213) 825-2210

Richard Burrows
NASA Lewis Research Center
21000 Brookpark Road
MS 77-6
Cleveland, OH 44135
(216) 433-3388

R. J. Buss
Division 1812
Sandia National Laboratories
Albuquerque, NM 87185
(505) 844-7494

Oral Buyukozturk
MIT
77 Massachusetts Avenue
Cambridge, MA 02139
(617) 253-7186

E. Buzzeli
Westinghouse R&D Center
1310 Beulah Rd
Pittsburgh, PA 15235
(412) 256-1952

Elton Cairns
Lawrence Berkeley Laboratory
University of California
Berkeley, CA 94720
(415) 486-5028

A. J. Caputo
ORNL
P.O. Box 2008
Bldg. 9202, 002
Oak Ridge, TN 37831
(615) 574-4566

Juan Carbajo
ORNL
P.O. Box Y
Oak Ridge, TN 37831
(615) 574-3784

R. W. Carling, Div. 8313
Sandia National Laboratories
Livermore, CA 94550
(415) 422-2206

P. T. Carlson
Oak Ridge National Laboratory
P.O. Box 2008
Oak Ridge, TN 37831
(615) 574-6094

J. P. Carr
FE-14/GTN
U.S. Dept. of Energy
Washington, DC 20545
(301) 353-6519

D. W. Carroll
LANL
Los Alamos, NM 87545
(505) 667-2145

D. H. W. Carstens
LANL
Los Alamos, NM 87545
(505) 667-5849

Lawrence A. Casper
2630 Zanzibar Lane
Plymouth, MN 55447
(612) 541-2508

G. M. Caton
ORNL
P.O. Box 2008
Bldg. 4515
Oak Ridge, TN 37831-6065
(615) 574-7782

Ken Chacey
DP-123/GTN
U.S. Dept. of Energy
Washington, DC 20545
(301) 353-4970

W. F. Chambers
Division 1822
Sandia National Laboratories
Albuquerque, NM 87185
(505) 844-6163

A. T. Chapman
Georgia Institute of Technology
Georgia Tech Research Institute
Atlanta, GA 30332-0420
(404) 894-4815

Russell Chou
Materials Research Center
Lehigh University
Bethlehem, PA 18015
(215) 861-4235

D. C. Christensen
LANL
Los Alamos, NM 87545
(505) 667-2556

Richard Christensen
LLNL
University of California
P.O. Box 808
Livermore, CA 94550
(415) 422-7136

L. Christophorou
ORNL
P.O. Box 2008
Bldg. 4500S, 122, Rm. H156
Oak Ridge, TN 37831
(615) 574-6199

Russel J. Churchill
American Research Corp. of Va.
642 First Street
P.O. Box 3406
Radford, VA 24143-3406
(703) 731-0836

M. J. Cieslak
Division 1833
Sandia National Laboratories
Albuquerque, NM 87185
(505) 846-7500

D. E. Clark
Materials Technology Div
Idaho National Eng. Laboratory
Idaho Falls, ID 83415
FTS 583-2627

Robert Clark
Sandia National Laboratory
Albuquerque, NM 87185
(505) 844-6332

S. K. Clark
Dept. of Mech. Eng. & App. Mech.
University of Michigan
Ann Arbor, MI 48109
(313) 764-4256

A. H. Claver
Battelle-Columbus Labs
505 King Avenue
Columbus, OH 43201
(614) 424-4377

Michael O. Cloninger
Yucca Mountain Project
DOE Nevada Operations Office
P.O. Box 98518
Las Vegas, NV 89195-8518
(702) 794-7847

R. L. Clough
Sandia National Laboratories
Albuquerque, NM 87185
(505) 844-3492

Joe K. Cochran, Jr.
School of Ceramic Eng.
Georgia Inst. of Technology
Atlanta, GA 30332
(404) 894-2851

Marvin M. Cohen
ER-533/GTN
U.S. Dept. of Energy
Washington, DC 20545
(301) 353-4253

Robert Cook
LLNL
University of California
P.O. Box 808
Livermore, CA 94550
(415) 422-6993

J. E. Costa
Division 8314
Sandia National Laboratories
Livermore, CA 94550
(415) 422-2352

Frederick A. Creswick
ORNL
P.O. Box 2009
Oak Ridge, TN 37831
(615) 574-2009

Gary M. Crosbie
Ceramics Research
Ford Motor Company
P.O. Box 2053
Dearborn, MI 48121-2053
(313) 327-1208

Randy Curlee
ORNL
P.O. Box 2008
Oak Ridge, TN 37831
(615) 576-4864

M. J. Curry
Plastics Inst. of America
Stevens Inst. of Tech.
Castle Point Station
Hoboken, NJ 07030
(201) 420-5552

Raymond A. Cutler
Ceramatec, Inc.
163 West 1700 South
Salt Lake City, UT 84115
(801) 486-5071

Steinar Dale
ORNL
P.O. Box 2008
Bldg. 5500, 366, Room A217
Oak Ridge, TN 37831
(615) 574-4829

S. J. Dapkunas
National Institute of Standards
and Technology
Gaithersburg, MD 20899
(301) 975-6119

John Davis
McDonnell Douglas Astro. Co.
Fusion Energy Program
P.O. Box 516, Bldg 278
St. Louis, MO 63166
(314) 234-4826

Robert F. Davis
Dept. of Materials Eng.
North Carolina State University
232 Riddick Lab, Box 7907
Raleigh, NC 27695
(919) 737-3272

Bob Delannoy
DOE - Richland Oper. Office
P.O. Box 550
Richland, WA 99352
(509) 376-2247

Victor Der
ER-531/GTN
U.S. Dept. of Energy
Washington DC 20545
(301) 353-5736

Francis de Winter
Altas Corporation
308 Encinal Street
Santa Cruz, CA 95060
(408) 425-1211

J. M. Dickinson
LANL
Los Alamos, NM 87545
(505) 667-4325

R. Diegle
Division 1841
Sandia National Labs
Albuquerque, NM 87185
(505) 846-3450

D. R. Diercks
Mat. Science & Tech. Div.
Argonne National Labs
9700 South Cass Ave
Argonne, Illinois 60439
(312) 972-5032

A. D. Donaldson
Materials Technology Div.
Idaho National Eng. Lab
Idaho Falls, ID 83415
FTS 583-2627

Donald G. Doran
Sanford Eng. Dev. Lab
P.O. Box 1970
Richland, WA 99352
(509) 444-3187

Allen Dragoo
National Institute of Standards
and Technology
Bldg. 223, #A258
564 - Fracture and Deformation
Gaithersburg, MD 20899
(301) 975-5785/FTS 879-5785

W. D. Drotning
Division 1824
Sandia National Laboratories
Albuquerque, NM 87185
(505) 844-7934

T. J. Drummond
Division 1150
Sandia National Laboratories
Albuquerque, NM 87185
(505) 844-9677

C. Michael Dube
Dynamics Technology, Inc.
22939 Hawthorne Blvd., #200
Torrance, CA 90505
(213) 373-0666

George Duda
ER-72/GTN
U.S. Dept. of Energy
Washington, DC 20545
(301) 353-3651

C. Duffy
LANL P.O. Box 1663
Los Alamos, NM 87545
(505) 843-5154

Keith F. Dufrane
Battelle-Columbus Labs
505 King Avenue
Columbus, OH 43201
(614) 424-4618

E. M. Dunn
GTE Laboratories, Inc.
40 Sylvan Road
Waltham, MA 02254
(617) 466-2312

Sunil Dutta
NASA Lewis Research Center
21000 Brookpark Road, MS 49-3
Cleveland, OH 44135
(216) 433-3282

T. E. Easler
Material Science & Tech. Div.
Argonne National Laboratories
9700 South Cass Avenue
Building 212
Argonne, Illinois 60439
(312) 972-5084

W. P. Eatherly
ORNL
P.O. Box 2008
Oak Ridge, TN 37831-6088
(615) 574-5220

Russell Eaton
CE-143/FORS
U.S. Dept. of Energy
Washington, DC 20585
(202) 252-4844

Christopher A. Ebel
Norton Company
Goddard Road
Northboro, MA 01532-1545
(617) 393-5950

James J. Eberhardt
CE-12/FORS
U.S. Dept. of Energy
Washington, DC 20585
(202) 586-5377

K. H. Eckelmeyer
Division 1822
Sandia National Laboratories
Albuquerque, NM 87185
(505) 844-7775

G. R. Edwards
Colorado School of Mines
Golden, CO 80401
(303) 273-3773

V. K. Eggert
LLNL
University of California
Livermore, CA 94550
(213) 422-4911

W. A. Ellingson
Argonne National Laboratories
Mat. Science Div., Bldg. 212
9700 South Cass
Argonne, Illinois 60439
(312) 972-5068

J. W. Elmer
MIT
77 Massachusetts Avenue
Cambridge, MA 02139
(617) 253-2233

James Ely
Thermophysical Properties Div.
Ctr. for Chemical Engineering
National Eng. Laboratory
National Institute of Standards
of Technology
Boulder, CO 80303
(303) 320-5467

D. Emerson
LLNL
University of California
Livermore, CA 94550
(213) 422-6504

Gerald Entine
Rad. Monitoring Devices, Inc.
44 Hunt Street
Watertown, MA 02172
(617) 926-1167

Mike Epstein
Battelle-Columbus Labs
505 King Avenue
Columbus, OH 43201
(614) 424-6424

R. H. Ericksen
Division 1813
Sandia National Laboratories
Albuquerque, NM 87185
(505) 844-8333

A. E. Evans
DP-242.1./GTN
U.S. Dept. of Energy
Washington, DC 20545
(301) 353-3098

Bob Evans
NASA Lewis Research Center
21000 Brookpark Road, MS 77-6
Cleveland, OH 44135
(216) 433-3400

Deane Evans
Steven Winter Associates
350 5th Avenue
New York, NY 10001
(212) 564-5800

John Fairbanks
CE-151/FORS
U.S. Dept. of Energy
Washington, DC 20585
(202) 586-8012

P. D. Fairchild
ORNL
P.O. Box Y
Bldg. 9102-2, 001, Room 0210
Oak Ridge, TN 37831
(615) 574-2009

D. A. Farkas
Virginia Polytechnic Institute
and University
Blacksburg, VA 24061
(703) 961-4742

J. E. Farmer
Division 8313
Sandia National Laboratories
Livermore, CA 94550
(415) 422-3418

G. C. Farrington
University of Pennsylvania
Philadelphia, PA 19104
(215) 898-8337

D. C. Fee
ANL
9700 South Cass Avenue
Argonne, IL 60439
(312) 972-8931

W. Feduska
Westinghouse Electric Corp.
R&D Center
1310 Beulah Road
Pittsburgh, PA 15235
(412) 256-1951

Mattison K. Ferber
ORNL
P.O. Box 2008
Building 4515
Oak Ridge, TN 37831-6064
(615) 576-0818

Stephen Fisher
Memory Metals, Inc.
652 Glenbrook Road
P.O. Box 2518
Stanford, CT 06906
(203) 358-0437

Ronald J. Fiskum
CE-132/FORS
U.S. Dept. of Energy
Washington, DC 20585
(202) 252-9130

Dennis Fitzgerald
Jet Propulsion Laboratory
California Inst. of Technology
4800 Oak Grove Dr.
Bldg. 512, Room 103
Pasadena, CA 91109
(818) 577-9079

J. E. Flinn
Materials Technology Div.
Idaho National Eng. Laboratory
Idaho Falls, ID 83415
FTS 583-8127

E. Flower
Lawrence Livermore Nat. Lab
University of California
P.O. Box 808
Livermore, CA 94550
(415) 423-0740

P. S. Follansbee
LANL
Los Alamos, NM 87545
(505) 667-8021

D. M. Follstaedt
Division 1110
Sandia National Laboratories
Albuquerque, NM 87185
(505) 844-2102

F. Forsyth
Brookhaven National Lab
Upton, NY 11973
(516) 282-4676

Earle Fowler
ER-226/GTN
U.S. Dept. of Energy
Washington, DC 20545
(301) 353-4801

J. E. Fox, NE-15
HTR Development Division
19901 Germantown Road
Germantown, MD 20274
(301) 353-4162

Anthony Fraioli
Argonne National Laboratory
9700 South Cass Ave.
Argonne, IL 60439
(303) 972-7550

P. W. Fuerschbach
Division 1833
Sandia National Laboratories
Albuquerque, NM 87185
(505) 846-2464

E. R. Fuller
National Institute of Standards
and Technology
Gaithersburg, MD 20899
(301) 921-2942

J. C. Fulton
CE-122/FORS
U.S. Dept. of Energy
Washington, DC 20585
(202) 252-8668

M. J. Furnam
Federal Building
Richland, WA 99352
(509) 376-7062

F. D. Gac
LANL
Los Alamos, NM 87545
(505) 667-5126

G. F. Gallegos
LLNL
University of California
P.O. Box 808
Livermore, CA 94550
(415) 422-7002

Yogendra S. Garud
S. Levy, Inc.
3425 South Bascom Avenue
Campbell, CA 95008
(408) 377-4870

George E. Gazza
U.S. Army Materials Tech. Lab
405 Arsenal Street
Watertown, MA 02172
(617) 923-5408

W. Gerken
CE-111/FORS
U.S. Dept. of Energy
Washington, DC 20585
(202) 586-9187

F. P. Gerstle, Jr.
Sandia National Laboratories
Albuquerque, NM 87185
(505) 844-4304

C. P. Gertz
Yucca Mountain Project Mgr.
U.S. Dept. of Energy
P.O. Box 98518
Las Vegas, NV 89193
(702) 794-7920

Larry Gestaut
Eltech Systems Corp.
Painsville, OH 44077
(216) 357-4041

E. R. Gilbert
Pacific Northwest Laboratory
Richland, WA 99352
(509) 375-2533

D. S. Ginley
Division 1150
Sandia National Laboratories
Albuquerque, NM 87185
(505) 844-8863

A. Glass
KMS Fusion
3621 South State Road
Ann Harbor, MI 48106
(313) 769-8500

R. Glass
LLNL
University of California
P.O. Box 808
Livermore, CA 94550
(415) 423-7140

Leon Glicksman
MIT
77 Massachusetts Avenue
Cambridge, MA 02139
(617) 253-2233

F. D. Gmeindl
METC
P.O. Box 880
Morgantown, WV 26505
(304) 291-4751

John Goldsmith
CE-332/FORS
U.S. Dept. of Energy
Washington, DC 20585
(202) 586-8171

Gerald Goldstein
ER-74/GTN
U.S. Dept. of Energy
Washington, DC 20545
(301) 353-5348

B. Goodman
SERI
1617 Cole Blvd
Golden, CO 80401
(303) 231-1005

S. H. Goods
Divison 8314
Sandia National Laboratories
Livermore, CA 94550
(415) 422-3274

Paul D. Gorsuch
Space Systems Division
General Electric Company
P.O. Box 8555
Philadelphia, PA 19101
(215) 354-5047

R. J. Gottschall
ER-131/GTN
U.S. Dept. of Energy
Washington, DC 20545
(301) 353-3428/FTS 353-3428

Fred S. Goulding
Instrumentation Division
Lawerence Berkeley Laboratory
Berkeley, California 94720
(415) 486-6432

R. A. Graham
Division 1130
Sandia National Laboratories
Albuquerque, NM 87185
(505) 844-1931

Allen R. Grahn
Bonneville Scientific
918 East 900 South
Salt Lake City, UT 84105
(801) 359-0402

Eric Gregory
Supercon, Inc.
830 Boston Turnpike
Shrewsbury, MA 01545
(617) 842-0174

Gordon Gross
SERI
1617 Cole Blvd.
Golden, CO 80401
(303) 231-1222

N. Grossman
NE-53/GTN
U.S. Dept. of Energy
Washington, DC 20545
(301) 353-3745

T. R. Guess
Division 1812
Sandia National Laboratories
Albuquerque, NM 87185
(505) 844-5604

M. Gurevich
CE-141/FORS
U.S. Dept. of Energy
Washington, DC 20585
(202) 586-1507

Wilhelm Gusster
Sandia Laboratories
P.O. Box 5800
Albuquerque, NM 87185
(415) 422-1648

John P. Gyeknyesi
NASA Lewis Research Center
2100 Brookpark Road
MS 49-7
Cleveland, OH 44135
(216) 433-3210

J. S. Haggarty
MIT
77 Massachusetts Avenue
Cambridge, MA 02139
(617) 253-2129

Phil Haley
Allison Turbine Operations
P.O. Box 420
Indianapolis, IN 46206-0420
(317) 230-2272

John M. Halstead
SOHIO Engineered Materials
P.O. Box 1054
Niagara Falls, NY 14302
(716) 278-2330

L. A. Harrah
Division 1811
Sandia National Labs
Albuquerque, NM 87185
(505) 844-6847

Pat Hart
Pacific Northwest Labs
P.O. Box 999
Richland, WA 99352
(504) 375-2906

R. W. Haskell
GE Research Laboratory
P.O. Box 8
Schenectady, NY 12301
(518) 385-4226

Jeff Hay
Chem.-Mat. Science Div.
Los Alamos National Lab
Los Alamos, NM 87545
(505) 843-2097

A. K. Hays
Division 1831
Sandia National Labs
Albuquerque, NM 87185
(505) 844-9996

Norman L. Hecht
University of Dayton
300 College Park, KL165
Dayton, OH 45469-0001
(513) 229-4343

Richard L. Heestand
Metals and Ceramics Div.
ORNL
P.O. Box 2008
Bldg. 4508, 083, Room 128
Oak Ridge, TN 37831
(615) 574-4352

Walter Heldt
Helix Associates, Inc.
835 Dawson Drive
Newark, DE 19713
(302) 738-6581

H. E. Helms
General Motors Corp.
T-18
P.O. Box 420
Indianapolis, IN 46206-0420
(317) 242-5355

Kamithi Hemachalam
Intermagnetics General Corp.
1875 Thomaston Avenue
Waterbury, CT 06704
(203) 753-5215

Timothy Henderson
KMS Fusion, Inc.
Ann Arbor, MI 48106
(313) 769-8500

Carl Henning
Lawrence Livermore Nat. Lab
P.O. Box 5511
Livermore, CA 94550
(415) 532-0235

Thomas P. Herbell
NASA Lewis Research Center
21000 Brookpark Road, 105-1
Cleveland, OH 44135
(216) 433-3246

B. P. Hildebrand
Sigma Research, Inc.
565 Industry Drive
Seattle, WA 98188
(206) 575-9324

Carl B. Hilland
DP-232/GTN
U.S. Dept. of Energy
Washington, DC 20545
(301) 353-3687

J. M. Hobday
METC
P.O. Box 880
Morgantown, WV 26505
(304) 291-4347/FTS 923-4347

D. M. Hoffman
Lawrence Livermore Nat. Lab
University of California
P.O. Box 808
Livermore, CA 94550
(415) 422-7759

E. E. Hoffman
U.S. Dept. of Energy
P.O. Box 2001
Oak Ridge, TN 37831-8600
(615) 576-0735

John Holbrook
Battelle-Columbus Laboratories
505 King Ave.
Columbus, OH 43201-2693
(614) 424-4347

G. J. Hooper
CE-324/FORS
U.S. Dept. of Energy
Washington, DC 20585
(202) 586-4153

F. M. Hosking
Division 1833
Sandia National Laboratories
Albuquerque, NM 87185
(505) 844-8401

Charles R. Houska
Dept. of Materials Eng.
Holden Hall
Virginia Polytechnic Institute
Blacksburg, VA 24061
(703) 961-5652

Stephen M. Hsu, Group Leader
Chem. Stability & Corr. Div.
Center for Materials Science
National Measurements Lab
National Institute of Standards
and Technology
Gaithersburg, MD 20899
(301) 975-6119/FTS 879-6119

W. J. Huber
METC
P.O. Box 880
Morgantown, WV 26505
(304) 291-4663

Robert A. Huggins
Dept. of Mat. Science & Eng.
Peterson 550I
Stanford University
Stanford, CA 94305
(415) 497-4110

Arlon Hunt
Lawrence Berkeley Laboratory
University of California
Berkeley, CA 94720
(415) 486-5370

George F. Hurley
Chemistry-Materials Sci. Div.
Los Alamos National Laboratory
Los Alamos, NM 87545
(505) 667-9498

Jerome Hust
Chemical Eng. Sciences Div.
Center for Bldg. Technology
National Institute of Standards
and Technology
Gaithersburg, MD 20899
(303) 497-3733

Gerald C. Huth
Univ. of Southern California
Inst. for Phys. & Imag. Sci.
4676 Admiralty Way
Marina del Rey, CA 90292
(213) 822-9184

Louis C. Ianniello
ER-13/GTN
U.S. Dept. of Energy
Washington, DC 20545
(301) 353-3427/FTS 353-3427

D. David Ingram
Universal Energy Systems, Inc.
4401 Dayton-Xenia Road
Dayton, OH 45432
(513) 426-6900

L. K. Ives
National Institute of Standards
and Technology
Gaithersburg, MD 20899
(301) 921-2843

D. D. Jackson
LLNL
University of California
P.O. Box 808
Livermore, CA 94550
(415) 422-8054

N. S. Jacobson
NASA Lewis Research Center
21000 Brookpark Road
Cleveland, OH 44135
(216) 433-5498

Mark A. Janney
ORNL
P.O. Box 2008
Bldg. 4515, 069, Room 228
Oak Ridge, TN 37831-6088
(615) 574-4281

Joseph E. Japka
Procedyne Corporation
221 Somerset Street
New Brunswick, NJ 08903
(201) 249-8347

C. E. Jaske
Physical Metallurgy Section
Battelle-Columbus Labs
505 King Avenue
Columbus, OH 43201
(614) 424-4417

J. L. Jellison
Division 1833
Sandia National Laboratories
Albuquerque, NM 87185
(505) 844-6397

M. M. Jenior
CE-332/FORS
U.S. Dept. of Energy
Washington, DC 20585
(202) 586-2998

J. E. Jensen
CVI Inc.
P.O. Box 2138
Columbus, OH 43216
(614) 876-7381

N. R. Johanson
University of Tennessee
Knoxville, TN 37996
(615) 455-0631

Carl E. Johnson
Chemical Technology Division
Argonne National Laboratory
9700 Cass Ave, Bldg. 205
Argonne, IL 60439
(312) 972-7533

Curtis A. Johnson
GE Research Laboratory
P.O. Box 8
Bldg. 31 #3C7
Schenectady, NY 12301
(518) 387-6421

D. L. Johnson, Chairman
 Dept. of Mat. Science & Eng.
 Room 1034
 2145 Sheridan Road
 Northwestern University
 Evanston, IL 60201
 (312) 492-3537

D. Ray Johnson
 ORNL
 Metals & Ceramics Div.
 P.O. Box 2008
 Bldg. 4515, 066, Room 206
 Oak Ridge, TN 37831-6088
 (615) 576-6832

H. R. Johnson
 Division 8313
 Sandia National Laboratories
 Livermore, CA 94550
 (415) 422-2822

Q. C. Johnson
 LLNL
 University of California
 P.O. Box 808
 Livermore, CA 94550
 (415) 422-6669

R. J. Johnson
 Hanford Eng. Dev. Lab.
 P.O. Box 1970
 Richland, WA 99352
 (509) 376-0715

T. Johnson
 Bldg. 205
 9700 South Cass Avenue
 Argonne, IL 60439
 (312) 972-5964

H. Jones
 GA Technologies
 P.O. Box 81608
 San Diego, CA 92138
 (615) 455-2360

Robert Jones
 Los Alamos National Lab.
 P.O. Box 1663, M/S J577
 Los Alamos, NM 87545
 (505) 667-6441

W. B. Jones
 Division 1832
 Sandia National Laboratories
 Albuquerque, NM 87185
 (505) 844-4026

Ram Kachare
 M/S 238-343
 Flat Plate Solar Array Project
 Jet Propulsion Laboratory
 Pasadena, CA 91109
 (213) 354-4583

M. J. Kania
 ORNL
 P.O. Box 2008
 Bldg. 3525, 390, Room 109
 Oak Ridge, TN 37831
 (615) 576-4856

Landis Kannberg
 Pacific Northwest Lab
 Battelle Blvd.
 P.O. Box 999
 Richland, WA 99352
 (509) 375-3919

M. E. Kassner
LLNL
University of California
P.O. Box 808
Livermore, CA 94550
(415) 422-7002

Carlos Katz
Cable Technology Lab
P.O. Box 707
New Brunswick, NJ 08903
(201) 846-3220

Robert N. Katz
Chief, Ceramics Res. Division
Army Mat. & Mech. Res. Ctr.
405 Arsenal Street
Watertown, MA 02172
(617) 923-5415

E. N. Kauffman
Lawrence Livermore Nat. Lab
University of California
P.O. Box 808
Livermore, CA 94550
(415) 423-2640

Larry Kazmerski
Solar Electric Conv. Div.
SERI
1617 Cole Blvd.
Golden, CO 80401
FTS 327-1115

M. R. Keenan
Division 1813
Sandia National Laboratories
Albuquerque, NM 87185
(505) 844-6631

J. R. Keiser
ORNL
P.O. Box 2008
Bldg. 4500-S, 156, Room 0734
Oak Ridge, TN 37830
(615) 574-4453

J. A. Kelber
Division 1812
Sandia National Laboratories
Albuquerque, NM 87185
(505) 844-3408

R. G. Kepler
Sandia National Laboratories
Albuquerque, NM 87185
(505) 844-7520

Paul T. Kerwin
NASA Lewis Research Center
21000 Brookpark Road, MS 77-6
Cleveland, OH 44135
(216) 433-3409

Lawrence W. Kessler
Sonoscan, Inc.
530 East Green Street
Bensenville, IL 60106
(213) 766-7088

Han Kim
GTE Labs
40 Sylvan Road
Waltham, MA 02254
(617) 466-2742

O. F. Kimball
General Electric Co.
1 River Road
Schenectady, NY 12345
(518) 385-1427

J. H. Kinney
 LLNL
 University of California
 P.O. Box 808
 Livermore, CA 94550
 (415) 422-6669

G. S. Kino
 Edward Ginzton Laboratory
 Stanford University
 Stanford, CA 94305
 (415) 497-0205

Thomas Kitchens
 ER-132/GTN
 U.S. Dept. of Energy
 Washington, DC 20545
 (301) 353-3426

E. E. Klaus
 Penn State
 Room 108, Fenske Laboratory
 Univ Park, PA 16802
 (814) 865-2574

Paul Klemmens
 University of Connecticut
 Box U-46
 Storrs, CT 06268
 (203) 486-3134

S. J. Klima
 NASA Lewis Research Center
 MS 106-1
 21000 Brookpark Road
 Cleveland, OH 44135
 (216) 433-6020

J. A. Knapp
 Division 1110
 Sandia National Laboratories
 Albuquerque, NM 87185
 (505) 844-2305

G. A. Knorovsky
 Division 1833
 Sandia National Laboratories
 Albuquerque, NM 87185
 (505) 844-1109

C. C. Koch
 Materials Eng. Department
 North Carolina State University
 Raliegh, NC 27650
 (919) 737-2377

George Kolstad
 ER-15/GTN
 U.S. Dept. of Energy
 Washington, DC 20545
 (301) 353-5822

D. Krajcinovic
 Dept. of Civil Eng.,
 Mechanics & Metallurgy
 University of Illinois
 Chicago, IL 60680
 (312) 996-7000

Saunders B. Kramer
 CE-151/FORS
 U.S. Dept. of Energy
 Wasington DC 20585
 (202) 586-8012

K. G. Kreider
 National Institute of Standards
 and Technology
 Washington, DC 20234
 (301) 921-3281

D. M. Kreiner
 Garrett Auxiliary Power Div.
 P.O. Box 5217
 Phoenix, AZ 85034
 (602) 220-3465

L. E. Kukacka
Brookhaven National Laboratory
Upton, NY 11973
(516) 282-3065

S. R. Kurtz
Division 1811
Sandia National Laboratories
Albuquerque, NM 87185
(505) 844-5436

C. M. Lampert
Lawrence Berkeley Laboratory
University of California
Berkeley, CA 94720
(415) 486-6093

P. E. Lamont
Federal Building
Richland, WA 99352
(509) 376-6117

A. Landgrebe
CE-32/FORS
U.S. Dept. of Energy
Washington, DC 20585
(202) 586-1483

P. M. Lang
NE-42/GTN
U.S. Dept. of Energy
Washington, DC 20545
(301) 353-3313

James Lankford
Southwest Research Inst.
Materials & Science
6220 Culebra Road
P.O. Drawer 28510
San Antonio, TX 78284
(512) 684-5111

Herbert J. Larson
Caterpillar, Inc.
Building F
100 N.E. Adams
Peoria, IL 61629
(309) 578-6549

R. LaSala
CE-324/FORS
U.S. Dept. of Energy
Washington, DC 20585
(202) 586-8077

H. A. Lawler
Standard Oil Eng. Mat. Co.
Structural Ceramics Div.
P.O. Box 1054, Bldg. 91-2
Niagara Falls, NY 14302
(716) 278-6345

W. N. Lawless
CeramPhysics, Inc.
921 Eastwind Drive, Suite 110
Westerville, OH 43081
(614) 882-2231

Robert LeChevalier
U.S. Dept. of Energy
San Francisco Oper. Office
1333 Broadway
Oakland, CA 94612
(415) 273-6362

S. R. Lee
U.S. Dept. of Energy
P.O. Box 10940
Pittsburgh, PA 15236
(412) 675-6137

Franklin D. Lemkey
United Tech. Research Ctr.
Silver Lane
East Hartford, CT 06108
(203) 727-7318

Douglas Lemon
Pacific Northwest Labs
P.O. Box 999
Richland, WA 99352
(509) 375-2306

Edward M. Lenoe
Office of Naval Research
Air Force Off. of Scien. Res.
Liaison Office, Far East
APO San Francisco, CA 96503
(03) 401-8968/(03) 401-8924

S. R. Levine
NASA Lewis Research Center
21000 Brookpart Road
Cleveland, OH 44135
(216) 433-3276

Terry Levinson
CE-12/FORS
U.S. Dept. of Energy
Washington, DC 20585
(202) 586-5377

A. V. Levy
Lawerence Berkley Lab
University of California
One Cyclotron Road
Berkley, CA 94720
(415) 486-5822

John Lewellen
NE-53/GTN
U.S. Dept. of Energy
Washington, DC 20545
(301) 353-2899

Danny C. Lim
CE-112/FORS
U.S. Dept. of Energy
Washington, DC 20585
(202) 586-9130

L. J. Lindberg
Garrett Turbine Engine Co.
111 South 34th Street
P.O. Box 5217
Phoenix, AZ 85010
(602) 231-4002

J. Lipkin
Sandia National Laboratories
Livermore, CA 94550
(415) 422-2417

A. Litman
NE-35/GTN
U.S. Dept. of Energy
Washington, DC 20545
(301) 353-5777

C. T. Liu
Metals Ceramics Division
ORNL
P.O. Box 2008
Bldg. 4500-S, 115, Rm. S280
Oak Ridge, TN 37831
(615) 574-5516

K. C. Liu
ORNL
P.O. Box 2008
Bldg. 4500-S, MS 155
Oak Ridge, TN 37831
(615) 574-5116

Earl L. Long, Jr.
ORNL
Metals & Ceramics Div.
P.O. Box 2008
Bldg. 4515, 069, Room 229
Oak Ridge, TN 37831
(615) 574-5127

Michael Lopez
U.S. Dept. of Energy
San Francisco Oper. Office
1333 Broadway
Oakland, CA 94612
(415) 273-4264

T. C. Lowe
Divison 8316
Sandia National Laboratories
Livermore, CA 9450
(415) 422-3187

C. D. Lundin
307 Dougherty Eng. Bldg.
University of Tennessee
Knoxville, TN 37996
(615) 974-5310

MAJ Ross E. Lushbough
DP-225.2/GTN
U.S. Dept. of Energy
Washington, DC 20545
(301) 353-3912

E. A. Maestas
West Valley Project Office
U.S. Dept. of Energy
P.O. Box 191
West Valley, NY 14171-0191
(716) 942-4314

Richard Mah
Los Alamos National Lab
P.O. Box 1663
Los Alamos, NM 87545
(505) 607-3238

W. Mahin
Lawrence Livermore Nat. Lab
University of California
P.O. Box 808
Livermore, CA 94550
(415) 423-0740

Arturo Maimoni
Lawrence Livermore Nat. Lab
P.O. Box 808
Livermore, CA 94450
(415) 422-8575

Mokhtas S. Maklad
EOTEC Corporation
420 Frontage Road
West Haven, CT 06516
(203) 934-7961

Mark K. Malmros
MKM Research/Ohmicron
P.O. Box I
Washington Crossing, PA 18977
(609) 737-9050

Oscar P. Manley
ER-15/GTN
U.S. Dept. of Energy
Washington, DC 20545
(301) 353-5822

D. L. Marriott
University of Illinois
1206 West Green Street
RM 350 MEB
Urbana, IL 61801
(217) 333-7237

Mathew Marrocco
Maxdem, Inc.
267 S. Fair Oaks Avenue
Pasadena, CA 91105
(818) 793-5224

R. G. Martin
Analysis Consultants
21831 Zuni Drive
El Toro, CA 92630
(714) 380-1204

H. Maru
Energy Research Corporation
3 Great Pasture Road
Danbury, CT 06810
(412) 578-2700

Tadeusz Massalski
69 MI
Naval Postgraduate School
Monterey, CA 93943
(412) 578-2700

K. Masubuchi
Lab for Manuf. and Prod.
MIT
Cambridge, MA 02139
(617) 255-6820

W. A. May, Jr.
LANL
Los Alamos, NM 87545
(505) 667-6362

Jacob Maya
GTE Products Corp
Silvania Lighting Center
Danvers, MA 01923
(617) 777-1900

T. B. McCall
Rockwell Hanford Operations
P.O. Box 800
Richland, WA 99352
(509) 376-7114

James W. McCauley
Army Materials Tech. Lab
SLCMT-OMM
Arsenal Street
Watertown, MA 02172-0001
(617) 923-5238

M. R. McClellan, Division 8315
Sandia National Laboratories
Livermore, CA 94550
(415) 422-2598

Robert W. McClung
ORNL
P.O. Box 2008
Bldg. 4500-S, 151, Rm. D63
Oak Ridge, TN 37831-6088
(615) 574-4466

J. I. McCool
SKF Industries, Inc.
1100 First Avenue
King of Prussia, PA 19406
(215) 265-1900

D. McCright
LLNL
University of California
Livermore, CA 94550
(213) 423-7051

R. McCrory
University of Rochester
Lab for Laser Energetics
250 E River Road
Rochester NY 14623

James C. McCue
Technology Prod. & Services, Inc.
P.O. Box 1230
West Palm Beach, FL 33420
(305) 686-5949

J. M. McDonald
Sandia National Laboratories
Albuquerque, NM 87185
(505) 846-7735

Roger J. McDonald
Brookhaven National Laboratory
Bldg. 475
Upton, NY 11973
(515) 282-4197

H. K. McDowell
LANL
Los Alamos, NM 87545
(505) 667-4686

David L. McElroy
ORNL
P.O. Box 2008
Bldg. 4508, 092, Rm. 239
Oak Ridge, TN 37831-6088
(615) 574-5976

A. J. McEvily
Metallurgy Dept., U-136
University of Connecticut
Storrs, CT 06268
(203) 486-2941

T. D. McGee
Mat. Science & Engineering
110 Engineering Annex
Iowa State University
Ames, IA 50011
(515) 294-9619

R. R. McGuire
Lawrence Livermore Nat. Lab
University of California
P.O. Box 808
Livermore, CA 94550
(415) 422-7792

Carl McHargue
ORNL
P.O. Box 2008
Bldg. 4500-S, 118, Rm. A274
Oak Ridge, TN 37831
(615) 574-4344

M. J. McMonigle
CE-122/FORS
U.S. Dept. of Energy
Washington, DC 20585
(202) 586-2087

G. H. Meier
848 Benevum Hall
University of Pittsburgh
Pittsburgh, PA 15261
(412) 624-5316

J. E. Mendel
Pacific Northwest Lab.
P.O. Box 999
Richland, WA 99352
(509) 375-2905

P. D. Metz
Brookhaven National Lab.
Upton, NY 11973
(516) 282-3123

A. Meyer
International Fuel Cells
P.O. Box 739
195 Governors Hwy
South Windsor, CT 06074
(203) 727-2214

B. E. Mills
Sandia National Laboratories
Livermore, CA 94550
(415) 422-3230

Joseph B. Milstein
Energy Materials Corporation
P.O. Box 1143
Sterling Road
South Lancaster, MA 01561
(617) 456-8707

M. V. Mitchell
AiResearch Casting Co.
19800 Van Ness
Torrance, CA 90509
(213) 618-7411

Artie Moorhead
ORNL
P.O. Box 2008
Bldg. 4515
Oak Ridge, TN 37830-6069
(615) 574-5153

Thomas Morel
Integral Technologies
415 E. Plaza Drive
Westmont, IL 60559
(312) 789-0003

G. Morris
LLNL
University of California
P.O. Box 808
Livermore, CA 94550
(415) 423-1770

Andrew Morrison
M/S 238-343
Flat Plate Solar Array Project
Jet Propulsion Laboratory
Pasadena, CA 91109
(213) 354-7200

Craig Mortenson
BPA/FORS
U.S. Dept. of Energy
Washington, DC 20585
(202) 586-5656

J. Moteff
University of Cincinnati
Department of Material Science
Metallurgical Engineering
498 Rhodes Hall
Cincinnati, OH 45221-0012
(513) 475-3096

Arnulf Muan
Pennsylvania State University
EMS Experiment Station
415 Walker Bldg.
University Park, PA 16802
(814) 865-7659

A. W. Mullendore
Division 1831
Sandia National Laboratories
Albuquerque, NM 87185
(505) 844-6833

L. Marty Murphy
SERI
1617 Cole Blvd
Golden, CO 80401
(303) 231-1050

Jagdish Narayan
Dept. of Materials Eng.
N. Carolina State University
Raleigh, NC 27650
(919) 767-2933

J. E. Nasise
LANL
Los Alamos, NM 87545
(505) 667-1459

K. Natesan
Argonne National Lab.
Materials Science Division
9700 South Cass
Argonne, IL 60439
(312) 972-5068

M. Naylor
Cummins Engine Co., Inc.
Box 3005
Mail Code 50183
Columbus, IN 47202-3005
(812) 377-5000

Fred Nichols
Argonne National Laboratory
9700 South Cass
Argonne, IL 60439
(312) 972-8292

M. C. Nichols
Sandia National Laboratories
Livermore, CA 94550
(415) 422-2906

R. M. Nielson
Materials Technology Div.
Idaho National Eng. Laboratory
Idaho Falls, ID 83415
(208) 526-8274

P. J. Nigrey
Division 1150
Sandia National Laboratories
Albuquerque, NM 87185
(505) 844-8985

F. B. Nimick, Division G313
Sandia National Laboratory
P.O. Box 5800
Albuquerque, NM 87185
(505) 844-6696

D. A. Nissen
Sandia National Laboratories
Livermore, CA 94550
(415) 422-2767

R. Gerald Nix
SERI
1617 Cole Blvd
Golden, CO 80401
(303) 231-1757

T. A. Nolan
ORNL
P.O. Box 2008
Bldg. 4515, MS 064
Oak Ridge, TN 37831
(615) 574-0811

Donald Nutt
Comp. Tech. and Imagery, Inc.
215 Center Park Drive, #1500
Knoxville, TN 37422
(615) 966-7539

P. C. Odegard
Divison 8216
Sandia National Laboratories
Livermore, CA 94550
(415) 422-2789

G. R. Odette
Dept. of Chem. & Nuclear Eng.
University of California
Santa Barbara, CA 93106
(805) 961-3525

Thomas Ohlemiller
Center for Bldg. Technology
National Institute of Standards
and Technology
Gaithersburg, MD 20899
(301) 921-3771

Ben Oliver
Materials Science & Eng.
421 Dougherty Hall
Knoxville, TN 37996
(615) 974-5326

Randall B. Olsen
Chronos Research Labs, Inc.
3025 Via de Caballo
Olivenhaim, CA 92024
(619) 756-1447

Mark J. O'Neill
ENTECH, Inc.
P.O. Box 612246
DFW Airport, TX 75261
(214) 456-0900

G. C. Osbourn
Division 1130
Sandia National Laboratories
Albuquerque, NM 87185
(505) 844-8850

Roland Otto
Lawrence Berkeley Lab.
Bldg 73, 106A
Berkeley, CA 94720
(415) 486-5289

V. Oversby
LLNL
University of California
Livermore, CA 94550
(213) 423-2228

Gennody Ozeryansky
Intermagnetics General Corp.
1875 Thomaston Avenue
Waterbury, CT 06704
(203) 753-5215

J. K. G. Panitz
Division 1834 SNL
Albuquerque, NM 87185
(505) 844-8604

E. R. Parker
456 Hearst
Univ. of Ca., Berkeley
Berkeley, CA 24720
(415) 642-0863

Jack Parks
Argonne National Laboratory
9700 South Cass Avenue
Argonne, IL 60439
(312) 972-4334

W. Patrick
LLNL
University of California
Livermore, CA 94550
(213) 422-6495

D. O. Patten
Norton Company
High Performance Ceramics
Goddard Road
Northboro, MA 01532
(617) 393-5963

Directory

H. C. Peebles
Division 1831
Sandia National Laboratories
Albuquerque, NM 87185
(505) 844-1647

David Pellish
CE-312/FORS
U.S. Dept. of Energy
Washington, DC 20585
(202) 586-8110

Ahmad Pesaran
SERI
1617 Cole Blvd.
Golden, CO 80401
(303) 231-7636

Randy Petri
IGT
3424 S. Stale St.
Chicago, IL 60616
(312) 567-3985

John Petrovic
Chemistry-Mat. Science Div.
Los Alamos National Laboratory
Los Alamos, NM 87545
(505) 667-5452

Paul Phillips
Oak Ridge National Laboratory
P.O. Box 2008
Oak Ridge, TN 37831
(615) 574-5114

S. T. Picraux
Division 1110
Sandia National Laboratories
Albuquerque, NM 87185
(505) 844-7681

R. D. Pierce
Argonne National Laboratories
Chemical Tech Division
Bldg. 205, Room W-125
Argonne, IL 60439
(312) 972-4450

Melvin A. Piestrup
Adelphi Technology
13800 Skyline Blvd.
Woodside, CA 94062
(415) 851-0633

E. Pinkhasov
Vapor Technologies, Inc.
1 Bradford Road
Mt. Vernon, NY 10553
(914) 664-1495

L. E. Pope
Division 1834
Sandia National Laboratories
Albuquerque, NM 87185
(505) 844-5041

Joseph Prael
Case Western Reserve Univ.
Cleveland, OH 44106
(216) 368-2000

Morton B. Prince
CE-352/FORS
U.S. Dept. of Energy
Washington, DC 20585
(202) 586-1725

Donald Priestly
ER-542/GTN
U.S. Dept. of Energy
Washington, DC 20545
(301) 353-3421

G. T. Privon
ORNL
P.O. Box 2009
Building 9102-2, Rm. 209
Oak Ridge, TN 37831
(615) 574-1013

Peter Pronko
Universal Energy Systems
4401 Dayton-Xenia Road
Dayton, OH 45432
(513) 426-6900

Michael Pulscak
CE-352/FORS
U.S. Dept. of Energy
Washington, DC 20585
(202) 586-1726

Herbert Pummel
Altex Corporation
P.O. Box 10084
Chicago, IL 60610
(312) 372-3440

R. Quinn
Division 1846
Sandia National Labs
Albuquerque, NM 87185
(505) 844-1933

P. B. Rand
Division 1813
Sandia National Labs
Albuquerque, NM 87185
(505) 844-7953

Robert Rapp
Dept. of Metal. Eng.
Ohio State University
Columbus, OH 43210
(614) 422-2491

Richard Razgaitis
Battelle-Columbus Labs
505 King Avenue
Columbus, OH 43201
(614) 424-4212

Eberhardt Reimers
CE-32/FORS
U.S. Dept. of Energy
Washington, DC 20585
(202) 586-4563

Brian Rennex
Natl. Institute of Standards
and Technology
Center of Bldg. Technology
Gaithersburg, MD 20899
(301) 921-3195

W. G. Reuter
Materials Technology Div.
Idaho National Eng. Lab
Idaho Falls, ID 83415
(205) 526-0111

Theodore C. Reuther
ER-533/GTN
U.S. Dept. of Energy
Washington, DC 20545
(301) 353-4963

S. Richlen
CE-141/FORS
U.S. Dept. of Energy
Washington, DC 20585
(202) 586-2078

R. O. Ritchie
456 Hearst
University of Cal., Berkeley
Berkeley, CA 24720
(415) 642-0863

P. L. Rittenhouse
ORNL
P.O. Box 2008
Bldg. 45005, 138, Rm. A158
Oak Ridge, TN 37831
(615) 574-5103

H. F. Rizzo
Lawrence Livermore Nat. Lab
University of California
P.O. Box 808
Livermore, CA 94550
(415) 422-6369

D. I. Roberts
GA Technologies
P.O. Box 81608
San Diego, CA 92138
(619) 455-2560

S. L. Robinson
Division 8314
Sandia National Laboratories
Livermore, CA 94550
(415) 422-2209

Allan Roger
EG&E Idaho, Inc.
P.O. Box 1625
Idaho Falls, ID 83415
(208) 526-1756

Arthur H. Rogers
Synergistic Detector Designs
2438 Wyandotte Street
Building A
Mountain View, CA 94943
(415) 964-4756

A. D. Romig
Division 1832
Sandia National Laboratories
Albuquerque, NM 87185
(505) 844-8358

Timothy L. Rose
EIC Laboratories, Inc.
111 Downing Street
Norwood, MA 02062
(617) 764-9450

R. S. Rosen
LLNL
University of California
P.O. Box 808
Livermore, CA 94550
(415) 422-9559

P. N. Ross
Mat. & Metal. Research Div.
Lawrence Berkeley Labs
University of Berkeley
Berkeley, CA 94720
(415) 486-4000

Giulio A. Rossi
Norton Company
Goddard Road
Northboro, MA 01532-1545
(617) 393-5829

Walter Rossiter
Center for Bldg. Technology
National Institute of Standards
and Technology
Gaithersburg, MD 20899
(301) 921-3109

Arthur Rowcliffe
Metals and Ceramics Division
ORNL
P.O. Box 2008
Bldg. 5500, 376, Rm. A111
Oak Ridge, TN 37831
(615) 576-4864

M. Rubin
Lawrence Berkeley Laboratory
University of California
Berkeley, CA 94720
(415) 486-7124

E. Russell
LLNL
University of California
Livermore, CA 94550
(213) 423-6398

C. O. Ruud
159 MRL
University Park, PA 16802
(814) 863-2843

Ed Sabisky
Solar Electric Conv. Div.
SERI
1617 Cole Blvd.
Golden, CO 80401
(303) 231-1483

J. R. Sadoway
MIT
77 Massachusetts Avenue
Cambridge, MA 02139
(617) 253-3300

Djordjiji R. Sain
Nuclear Con. Services, Inc.
P.O. Box 29151
Columbus, OH 43229
(614) 846-5710

F. Salzano
Brookhaven National Laboratory
Upton, NY 11973
(516) 282-4458

R. J. Salzbrenner
Division 1832
Sandia National Laboratories
Albuquerque, NM 87185
(505) 844-5041

J. Sankar
Dept of Mechanical Engineering
North Carolina A&T University
Greensboro, NC 27411
(919) 379-7620

Mike L. Santella
ORNL
P.O. Box 2008
Oak Ridge, TN 37831-6088
(615) 574-4805

V. K. Sarin
GTE
40 Sylvan Road
Waltham, MA 02254
(617) 890-8460

C. M. Scheuerman
NASA Lewis Research Center
21000 Brookpark Road, MS 49-1
Cleveland, OH 44135
(216) 433-3205

Y. Schienle
Garrett Turbine Engine Co.
111 South 34th Street
P.O. Box 5217
Phoenix, AZ 85034
(602) 231-4666

Paul Schissel
SERI
1617 Cole Blvd.
Golden, CO 80401
(303) 231-1226

R. A. Schmidt
Battelle Columbus Labs
Mechanics Section
505 King Avenue
Columbus, OH 43201-2693
(614) 424-4396

S. J. Schneider
National Institute of Standards
and Technology
Gaithersburg, MD 20899
(301) 921-2901

G. D. Schnittgrund
Rockwell International
Rocketdyne Division
6633 Canoga Avenue
Canoga Park, CA 91304
(818) 710-5972

W. K. Schubert
Division 1815, SNL
Albuquerque, NM 87185
(505) 846-2466

Erland M. Schulson
33 Haskins Road
Hanover, NH 03755
(603) 646-2888

Robert B. Schulz
CE-151/FORS
U.S. Dept. of Energy
Washington, DC 20585
(202) 586-8051

James Schwarz
Dept. of Chem. Eng. &
Material Science
Syracuse University
320 Hinds Hall
Syracuse, NY 13244
(315) 423-4575

R. Schwerzel
Battelle-Columbus Labs
505 King Avenue
Columbus, OH 43201
FTS 976-5637

Peter Scofield
CE-131/FORS
U.S. Dept. of Energy
Washington, DC 20585

James L. Scott
Metals and Ceramics Div.
ORNL
P.O. Box 2008
Bldg. 4508
Oak Ridge, TN 37831-6091
(615) 624-4834

R. E. Setchell
Division 1130
Sandia National Labs
Albuquerque, NM 87185
(505) 844-5459

J. A. Seydel
Materials Science Division
Idaho National Eng. Lab
Idaho Falls, ID 83415
(208) 526-0111

D. W. Shannon
Pacific Northwest Laboratory
Battelle Blvd.
P.O. Box 999
Richland, WA 99352
(509) 376-3139

D. J. Sharp
Division 1831
Sandia National Laboratories
Albuquerque, NM 87185
(505) 844-8604

B. J. Shaw
Westinghouse R&D Center
1310 Beulah Road
Pittsburgh, PA 15235
(412) 256-1201

D. E. Shelor
RW-3/FORS
U.S. Dept. of Energy
Washington, DC 20585
(202) 586-9433

M. W. Shupe
U.S. Dept. of Energy
785 DOE Place
Idaho Falls, ID 83402
(208) 526-9534

V. K. Sikka
ORNL
P.O. Box 2008
Bldg. 4508, 083, Rm. 129
Oak Ridge, TN 37831
(615) 574-5112

Richard Silbergliitt
QuesTech, Inc.
7600-A Leesburg Pike
Falls Church, VA 22043
(703) 760-1043

T. B. Simpson
FE-34/GTN
U.S. Dept. of Energy
Washington, DC 20545
(301) 353-3913

J. P. Singh
Argonne National Labs
9700 South Cass
Argonne, IL 60439
(312) 972-5068

Maurice J. Sinnott
Chemical and Metall. Eng.
University of Michigan
H Dow Building
Ann Arbor, MI 48109-2136
(313) 764-4314

Piran Sioshamsi
Spire Corporation
Patriots Park
Bedford, MA 02173
(617) 275-6000

Hal Sliney
NASA Lewis Research Center
21000 Brookpark Road
MS 23-2
Cleveland, OH 44135
(216) 433-6055

M. F. Smith
Division 1834
Sandia National Laboratories
Albuquerque, NM 87185
(505) 846-4270

Peter L. Smith
Newton Optical Technologies
167 Valentine Street
Newton, MA 02165
(617) 495-4984

J. E. Smugeresky
Division 8312
Sandia National Laboratories
Livermore, CA 94550
(415) 422-2910

N. R. Sorensen
Division 1841
Sandia National Laboratories
Albuquerque, NM 87185
(505) 844-1097

R. R. Sowell
Division 8131
Sandia National Laboratories
Albuquerque, NM 87185
(505) 844-1038

David B. Spencer
Waste Energy Technology Corp.
One DeAngelo Drive
Bedford, MA 01730
(617) 275-6400

R. F. Sperlein
U.S. Dept. of Energy
P.O. Box 10940
Pittsburgh, PA 15236
(312) 972-5985

J. R. Springarn
Division 8312, SNL
Livermore, CA 94550
(415) 422-3307

William Sproul
Borg-Warner Company
1200 South Wolf Road
Des Plaines, IL 60018
(312) 827-3131

Mark B. Spitzer
Spire Corporation
Patriots Park
Bedford, MA 01730
(617) 275-6000

O. M. Stansfield
GA Technologies
P.O. Box 81608
San Diego, CA 92138
(619) 455-2095

T. L. Starr
Georgia Tech Res. Inst.
Georgia Inst. of Technology
Atlanta, GA 30332
(404) 894-3678

Carl A. Stearns
NASA Lewis Research Center
MS 106-1
21000 Brookpark Road
Cleveland, OH 44135
(216) 433-5504

R. H. Steele
NE-60/NR
U.S. Dept. of Energy
Washington, DC 20545
(301) 557-5565

H. J. Stein
Division 1110
Sandia National Laboratories
Albuquerque, NM 87185
(505) 844-6279

Carl A. Stearns
NASA Lewis Research Center
21000 Brook River Road
Cleveland, OH 44135
(216) 433-5500

Joseph R. Stephens
NASA Lewis Research Center
21000 Brookpark Road
Cleveland, OH 44135
(216) 433-3195

George Stickford
Battelle-Columbus Labs
505 King Avenue
Columbus, OH 43201
(614) 424-4810

D. P. Stinton
ORNL
P.O. Box 2008
Bldg. 4515, 063, Rm. 111
Oak Ridge, TN 37831
(615) 574-4556

Thomas G. Stoebe
Chairman, Mat. Sci. & Eng.
University of Washington
Roberts Hall, FB-10
Seattle, WA 98195
(206) 543-2600

Norman Stoloff
Materials Engineering Dept.
Rensselaer Polytechnic Inst.
Troy, NY 12181
(518) 266-6436

J. E. Stoneking
Dept. of Eng. Science & Mech.
310 Perkins Hall
Knoxville, TN 37996
(615) 974-2171

G. Stoner
University of Virginia
Charlottesville, VA 22901
(804) 924-3277

Edwin E. Strain
Garrett Corporation
111 S. 34th Street
P.O. Box 5217
MS 301-2N
Phoenix, AZ 85010
(602) 231-2797

Reinhold N. W. Strnot
KJS Associates
1616 Hillrose Place
Fairborn, OH 45324
(513) 879-0114

Thomas N. Strom
NASA Lewis Research Center
21000 Brookpark Road, MS 77-6
Cleveland, OH 44135
(216) 433-3408

David Sutter
ER-224/GTN
U.S. Dept. of Energy
Washington, DC 20545
(301) 353-5228

Patrick Sutton
CE-151/FORS
U.S. Dept. of Energy
Washington, DC 20585
(202) 586-8012

Jeffrey J. Swab
U.S. Army Materials Tech. Lab
405 Arsenal Street
Watertown, MA 02172
(617) 923-5410

R. W. Swindeman
ORNL
P.O. Box 2008
Bldg. 4500-S, 155, Rm. 0040
Oak Ridge, TN 37831
(615) 574-5108

W. Tabakoff
Dept. of Aerospace Eng.
M/L 70
University of Cincinnati
Cincinnati, OH 45221
(513) 475-2849

L. E. Tanner
LLNL
University of California
P.O. Box 808
Livermore, CA 94550
(415) 423-2653

H. L. Tardy
Division 1824
Sandia National Laboratories
Albuquerque, NM 87185
(505) 846-6548

Victor J. Tennery
ORNL
High Temp. Materials Lab
P.O. Box 2008
Bldg. 4515, 062, Rm. 146
Oak Ridge, TN 37831-6088
(615) 574-5123

Giuliana Tesoro
Plastics Institute of America
Stevens Institutes of Tech.
Castle Point Station
Hoboken, NJ 07030
(201) 420-5552

C. A. Thomas
U.S. Dept. of Energy
P.O. box 10940
Pittsburgh, PA 15236
(312) 972-5731

Iran L. Thomas
ER-132/GTN
U.S. Dept. of Energy
Washington, DC 20545
(301) 353-3426

D. O. Thompson
Ames Laboratory
Iowa State University
Ames, IA 50011
(515) 294-5320

John K. Tien
Columbia University
1137 S.W. Mudd Building
New York, NY 10027
(212) 280-5192

T. Y. Tien
Mat. and Metal. Eng.
University of Michigan
Ann Arbor, MI 48109
(813) 764-9449

T. N. Tieg
ORNL
Bldg. 4515, 069, Rm. 230
P.O. Box 2008
Oak Ridge, TN 37831-6088
(615) 574-5173

Nancy J. Tighe
National Institute of Standards
and Technology
564 Fracture and Deformation
Washington, DC 20234
(301) 921-2901

R. H. Titran
 NASA Lewis Research Center
 21000 Brookpark Road, MS 49-1
 Cleveland, OH 44135
 (216) 433-3198

John J. Tomlinson
 ORNL
 Bldg. 9204-1, MS 8045
 P.O. Box 2009
 Oak Ridge, TN 37831-8045
 (615) 574-0768

Timothy Tong
 Dept. of Mechanical Eng.
 University of Kentucky
 Lexington, KY 40506
 (606) 257-3236

J. A. VanDenAvyle
 Division 1832
 Sandia National Laboratories
 Albuquerque, NM 87185
 (505) 844-1016

A. Van Echo
 NE-462/GTN
 U.S. Dept. of Energy
 Washington, DC 20545
 (301) 353-3930

D. van Rooyen
 Brookhaven National Lab.
 Upton, NY 11973
 (516) 282-4050

Alex Vary
 NASA Lewis Research Center
 21000 Brookpark Road
 Cleveland, OH 44135
 (216) 433-6019

Krishna Vedula
 Dept. of Metal. & Mat. Science
 Case Western Reserve University
 10900 Euclid Avenue
 Cleveland, OH 44115
 (216) 368-4211

Shannon Vinyard
 Southwest Research Institute
 P.O. Drawer 28510
 San Antonio, TX 78284
 (512) 684-5111

L. Viswanathan
 Ceramatec, Inc.
 163 West 1700 South
 Salt Lake City, UT 84115
 (801) 486-5071

David Waksman
 National Institute of Standards
 and Technology
 Building 226
 Gaithersburg, MD 20899
 (301) 921-3114

H. F. Walter
 NE-25/GTN
 U.S. Dept. of Energy
 Washington, DC 20545
 (301) 353-5510

J. B. Walter
 Materials Technology Div.
 Idaho National Eng. Lab
 Idaho Falls, ID 83415
 FTS 583-2627

Joseph K. Weeks, Jr.
 Technical Res. Assoc., Inc.
 410 Chipeta Way, Suite 222
 Salt Lake City, UT 84108
 (802) 582-8080

Rolf Weil
Dep. of Mat. & Metal. Eng.
Stevens Inst. of Technology
Castle Point Station
Hoboken, NJ 07030
(201) 420-5257

H. L. Weisberg
R&D Associates
4640 Admiral Way
Marina del Ray, CA 90290
(213) 822-1715

C. D. Weiss
Caterpillar, Inc.
100 N.E. Adams Street
Peoria, IL 61629
(309) 578-8672

Haskell Weiss
LLNL
University of California
P.O. Box 808
Livermore, CA 94550
(415) 422-6268

Joseph F. Wenkus
Areas Corporation
202 Boston Road
North Billerica, MA 01862
(617) 667-3000

James Wert
Dept. of Mat. Science & Eng.
Vanderbilt University
Station B, P.O. Box 1621
Nashville, TN 37235
(615) 322-3583

Stanley Whetstone
ER-23/GTN
U.S. Dept. of Energy
Washington, DC 20545

J. B. Whitley
Sandia National Laboratories
Albuquerque, NM 87185
(505) 844-5353

Sheldon M. Wiederhorn
National Institute of Standards
and Technology
Bldg. 223, #A329
Gaithersburg, MD 20899
(301) 975-2000

William Wilhelm
Brookhaven National Lab
Solar Technology Group
Building 701
Upton, NY 11973
(516) 282-4708

Frank Wilkins
CE-314/FORS
U.S. Dept. of Energy
Washington, DC 20585
(202) 586-1694

A. D. Wilks
Signal UOP Research Center
50 UOP Plaza
Des Plaines, IL 60016
(312) 492-3179

Robin Williams
ORNL
P.O. Box 2008
Bldg. 4508, 092, Rm. 243
Oak Ridge, TN 37831
(615) 576-2631

A. Wilson
LANL
Los Alamos, NM 87545
(505) 667-6404

Ward O. Winer
Mechanical Eng. Department
Georgia Inst. of Technology
Atlanta, GA 30332
(404) 894-3270

C. E. Witherell
LLNL
University of California
P.O. Box 808
Livermore, CA 94550
(415) 422-8341

James Withers
Mat. & Electro. Research Corp.
4660 North Via Madre
Tucson, AZ 85749
(602) 749-3257

D. E. Wittmer
S. Illinois Univ./Carbondale
Dept. of Mech. Eng. & Egy Pro.
Carbondale, IL 62901
(618) 536-2396, ext. 21

T. Wolery
LLNL
University of California
Livermore, CA 94550
(213) 423-5789

James C. Wood
NASA Lewis Research Center
MS 500-210
21000 Brookpark Road
Cleveland, OH 44135
(216) 433-4000

J. B. Woodard
Division 8316
Sandia National Laboratories
Livermore, CA 94550
(415) 422-3115

J. R. Wooten
Rocketdyne
6633 Canoga Avenue
Mail Code BA-26
Canoga Park, CA 91303
(818) 710-5972

I. G. Wright
Battelle-Columbus Labs
505 King Ave
Columbus, OH 43201-2693
(614) 424-4377

R. N. Wright
Materials Technology Div.
Idaho National Eng. Laboratory
Idaho Falls, ID 83415
FTS 583-2627

Geert Wyntjes
OPTRA, Inc.
1727 Revere Beach Parkway
Everett, MA 02149
(617) 389-7711

Howard Yacobucci
NASA Lewis Research Center
21000 Brookpark Road, MS 77-6
Cleveland, OH 44135
(216) 433-3415

David Yarbrough
Department of Chem. Eng.
Tennessee Tech. University
1155 N. Dixie Ave.
Cookville, TN 38505
(615) 528-3494

H. C. Yeh
Air Research Casting Co.
19800 VanNess Avenue
Torrance, CA 90509
(213) 618-7449

Thomas M. Yonushonis
Cummins Engine Co., Inc.
Box 3005
Mail Code 50183
Columbus, IN 47202-3005
(812) 377-7078

J. Yow
LLNL
University of California
Livermore, CA 94550
(213) 423-3521

Charlie Yust
ORNL
P.O. Box 2008
Bldg. 4515, 063, Rm. 106
Oak Ridge, TN 37830
(615) 574-4812

Frederica Zangrando
SERI
1617 Cole Blvd.
Golden, CO 80401
(303) 231-1716

F. J. Zanner
Division 1833
Sandia National Laboratories
Albuquerque, NM 87185
(505) 844-7073

C. M. Zeh
METC
P.O. Box 880
Morgantown, WV 26505
(304) 291-4265

M. Zeigler
Division 1811, SNL
Albuquerque, NM 87185
(505) 844-0324

A. M. Zerega
CE-151/FORS
U.S. Dept. of Energy
Washington, DC 20585
(202) 586-8053/FTS 896-8014

R. M. Zimmerman, Division 6313
Sandia National Laboratory
P.O. Box 5800
Albuquerque, NM 87185
(505) 846-0187

J. W. Zindel
Sandia National Laboratories
Livermore, CA 94550
(415) 422-2051

Kenneth Zwiebel
SERI
1617 Cole Blvd
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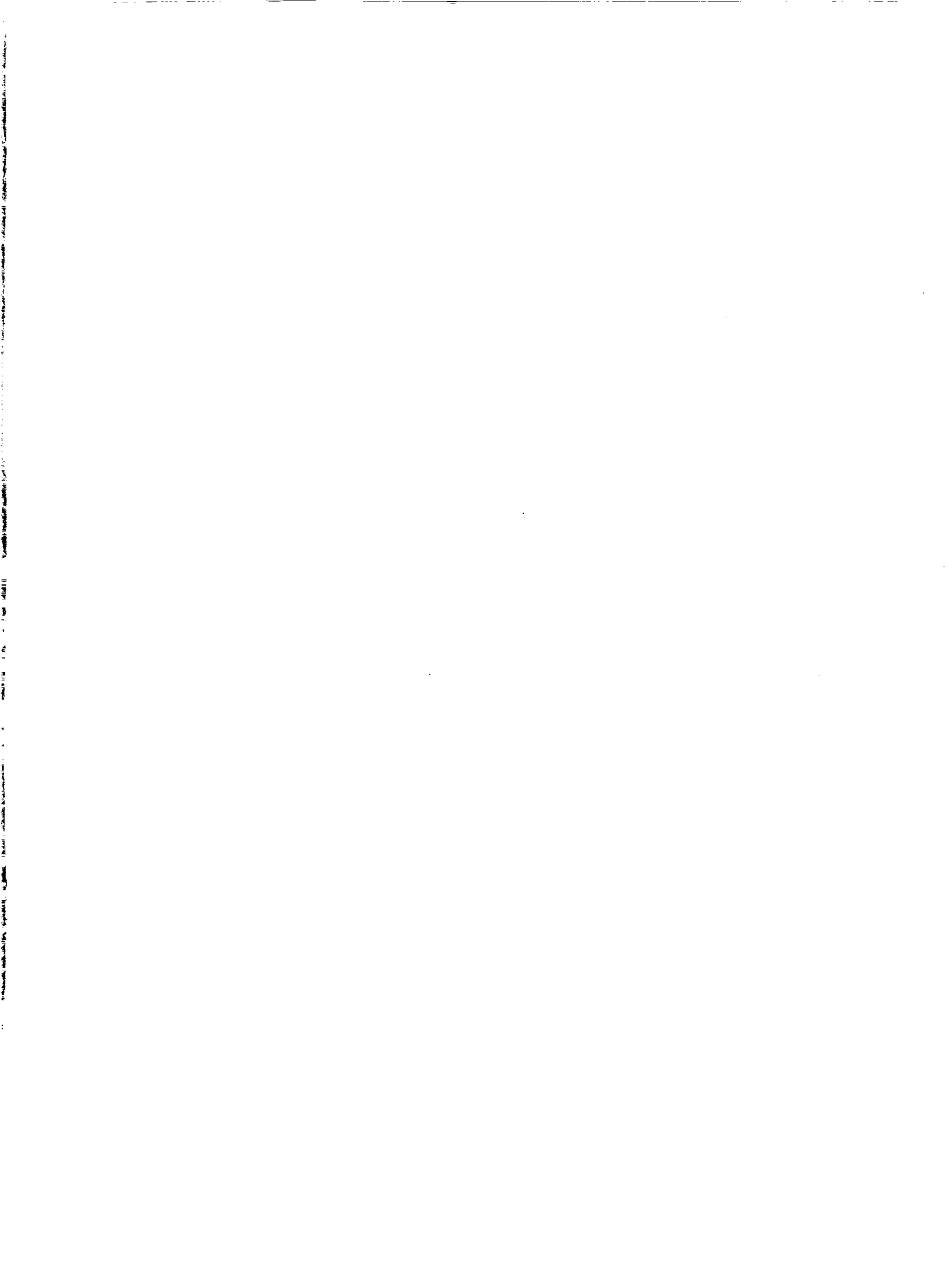
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