DOE/ER-0388

ENERGY MATERIALS COORDINATING COMMITTEE (EMaCC)

Fiscal Year 1987

September 1988

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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Division of Materials Sciences
Washington, D.C. 20545

TABLE OF CONTENTS

	Page
Introduction	1
Membership List	2
FY 1987 EMaCC Meeting Program	5
Organization of the Report	6
FY 1987 Budget Summary Table for DOE Materials Activities	7
Program Descriptions	
OFFICE OF CONSERVATION AND RENEWABLE ENERGY	10
Office of Energy Utilization Research	12, 182
Energy Conversion and Utilization Technologies Division	15, 182
Office of Buildings and Community Systems	28, 203
Building Systems Division	29, 203
Office of Industrial Programs	33, 209
Improved Energy Productivity Division	34, 209
Waste Energy Reduction Division	35, 211
Office of Transportation Systems	37, 213
Office of Energy Storage and Distribution	50, 236
Energy Storage	51, 236
Office of Solar Heat Technologies	54, 242
Solar Buildings Technology Division	56, 242
Solar Thermal Technology Division	60, 250

TABLE OF CONTENTS (Continued)

	Page
Office of Solar Electric Technologies	62, 254
Photovoltaic Energy Technology Division	63, 254
Office of Renewable Technology	65, 257
Geothermal Technology Division (GTD)	66, 257
OFFICE OF ENERGY RESEARCH	68, 261
Office of Basic Energy Sciences	74, 261
Division of Engineering and Geosciences	76, 262
Division of Advanced Energy Projects	81, 278
Office of Health and Environmental Research	81, 278
Division of Physical and Technological Research	81, 279
Small Business Innovation Research Program	82, 280
OFFICE OF NUCLEAR ENERGY	89, 281
Office of Advanced Reactor Programs	92, 281
Office of Remedial Action and Waste Technology	94, 284
Office of Uranium Enrichment	95, 286
Office of Civilian Reactor Development	98, 288
Office of Space and Defense Power Systems	102, 296
Office of Naval Reactors	103, 299
OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT	105, 300
Office of Storage and Transportation Systems	107, 300

TABLE OF CONTENTS (Continued)

	Page
OFFICE OF DEFENSE PROGRAMS	112, 307
Office of Waste Research and Development	123, 307
Office of Weapons Research, Development and Testing	124, 308
OFFICE OF FOSSIL ENERGY	168, 389
Office of Technical Coordination	171, 389
Office of Surface Coal Gasification	181, 413
Directory	415
Keyword Index	453

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. Five topical subcommittees are established and are continuing their own programs: Structural Ceramics, Batteries and Fuel Cells, Radioactive Waste Containment, Steel, and Superconductivity (established in FY 1987). The FY 1987 meeting program is given on Page 5. In addition, the EMaCC aids in obtaining materials-related inputs for both intra- and inter-agency compilations.

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

The EMaCC reports to the Director of the Office of Energy Research in his capacity as overseer of the technical programs of the Department. This annual technical report is mandated by the EMaCC terms of reference. This report summarizes EMaCC activities for FY 1987 and describes the materials research programs of various offices and divisions within the Department.

The Chairman of EMaCC for FY 1987 was Iran L. Thomas; the Executive Secretary was Henry F. Walter. On behalf of the EMaCC, I thank the subcommittee chairmen Alan Landgrebe, Bob Schulz, Iran Thomas, and Henry Walter for their contributions to our program in FY 1987. The compilation of this report was assisted by Quest Research Corporation.

Henry F. Walter
Office of Remedial Action and Waste Technology
Division of Waste Treatment Projects
Chairman of EMaCC, FY 1988

MEMBERSHIP LIST
DEPARTMENT OF ENERGY
ENERGY MATERIALS COORDINATING COMMITTEE

Organization	Representative	Phone No.
CONSERVATION AND RENEWABLE ENERGY		
Energy Utilization Research	James J. Eberhardt, CE-12	586-5377
	David Mello, CE-12	586-9345
Buildings and Community Systems		
Building Systems	Sam Tagore, CE-131	586-9210
Building Equipment	John Ryan, CE-132	586-9130
	Ronald Fiskum, CE-132	586-9130
	Danny C. Lim, CE-132	586-9130
Industrial Programs		
Waste Energy Reduction	Scott Richlen, CE-141	586-2078
Improved Energy Productivity	Matthew McMonigle, CE-142	586-2082
Transportation Systems		
Heat Engine Propulsion	Robert B. Schulz, CE-151	586-8032
	Charles H. Craig, CE-151	586-1506
Energy Storage and Dist.		
Electric Energy Systems	Russell Eaton, CE-32	586-1506
Energy Storage	Michael Gurevich, CE-32	586-1495
	Eberhart Reimers, CE-32	586-4563
Solar Heat Technologies		
Solar Thermal Technology	Frank Wilkins, CE-331	586-1684
Solar Buildings Technology	John Goldsmith, CE-332	586-8779
	David Pellish, CE-332	586-6436
Solar Electric Technologies		
Wind/Ocean Technologies	William Richards, CE-351	586-5540
Photovoltaic Technology	Morton B. Prince, CE-352	586-1725

MEMBERSHIP LIST (Continued)

Organization	Representative	Phone No.
Renewable Energy		
Biofuels and Municipal Waste	Donald Walter, CE-341	586-6104
Geothermal Technology	Raymond LaSala, CE-342	586-4198
ENERGY RESEARCH		
Basic Energy Sciences		
Materials Sciences	Iran L. Thomas, ER-132	353-3426
Metallurgy and Ceramics	Robert J. Gottschall, ER-131	353-3428
Solid State Physics and Materials Chemistry	B. Chalmers Frazer, ER-132	353-3426
Engineering and Geosciences	Oscar P. Manley, ER-15	353-5822
Advanced Energy Projects	Ryszard Gajewski, ER-16	353-5995
Health and Environmental Research		
Physical and Technological Research	Gerald Goldstein, ER-74	353-5348
Fusion Energy		
Reactor Technologies	Theodore C. Reuther, ER-533	353-4963
NUCLEAR ENERGY		
Program Support		
Safety QA and Safeguards	Benjamin C. Wei, NE-46	353-3927
Remedial Action and Waste Technology		
Waste Treatment Projects	Henry F. Walter, NE-24	353-5510
Uranium Enrichment		
Technology Deployment and Strategic Planning	Arnold Litman, NE-34	353-5777

MEMBERSHIP LIST (Continued)

Organization	Representative	Phone No.
Reactor Systems Development and Technology		
Defense Energy Projects and Special Applications	William Barnett, NE-522	353-3097
Advanced Reactor Programs	Andrew Van Echo, NE-542	353-3930
	J. Edward Fox, NE-531	353-3985
	Arthur S. Mehner, NE-531	353-4474
Naval Reactors	Robert H. Steele, NE-60	557-5561
CIVILIAN RADIOACTIVE WASTE MANAGEMENT		
Facilities Siting Development		
Engineering Licensing	Mark Frei, RW-23	586-3217
Transportation and Waste	Tien Nguyen, RW-33	586-4970
DEFENSE PROGRAMS		
Defense Waste and Byproducts		
R&D and Byproducts	Ken Chacey, DP-123	353-4970
Weapons Research Development and Testing		
Weapons Research	A. E. Evans, DP-242.1	353-3098
	Robert A. Jones, DP-225.2	353-5492
Inertial Fusion		
Fusion Research	Carl B. Hilland, DP-232	353-3687
FOSSIL ENERGY		
Management, Planning, and Technical Coordination		
Technical Coordination	E. E. Hoffman, ORNL	(615) 576-0735
Coal Utilization, Advanced Conversion and Gasification		
Surface Coal Gasification	James P. Carr, FE-24	353-5985

FY 1987 EMaCC MEETING PROGRAM

Date/Place	Special Meeting Subjects and Guest Speakers	Subcommittee Chairman
10/10/86 Germantown	Structural Ceramics Subcommittee Bob Gottschall: Summary of Zirconia Symposium in Japan	Bob Schulz
1/8/87 Germantown	Radioactive Containment Subcommittee Status of RW, NE, and DP programs	Henry Walter
3/18/87 Forrestal	Batteries and Fuel Cells Subcommittee Status of DP, CE, FE, and ER programs	Alan Landgrebe
5/20/87 Germantown	Superconductivity Subcommittee Status of superconductivity in DOE and establishment of this subcommittee	Iran Thomas
6/11/87 Forrestal	"Japanese Superconductivity Materials Research" Dr. Shinroku Saito, Professor Emeritus Tokyo Institute of Technology	Iran Thomas

NOTE: For FY 1987, the EMaCC Chairman was Iran L. Thomas (ER-132) and the Executive Secretary was Henry F. Walter (NE-24).

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.

Each project is numbered in both parts of the Program Descriptions. These numbers facilitate cross referencing and comparison between the two parts.

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 1987 Budget Summary Table for materials activities in each of the programs within the DOE is presented on page 7.

FY 1987 BUDGET SUMMARY TABLE FOR DOE MATERIALS ACTIVITIES

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

	FY 1987
Energy Conservation	$ 32,056,500
Office of Energy Utilization Research	7,432,500
Office of Buildings and Community Systems	875,000
Office of Industrial Programs	3,258,000
Office of Transportation Systems	20,491,000
Renewable Energy	$ 28,070,800
Office of Energy Storage and Distribution	2,763,800
Office of Solar Heat Technologies	3,807,000
Office of Solar Electric Technologies	20,900,000
Office of Renewable Technology	600,000
Office of Energy Research	$173,245,522
Office of Basic Energy Sciences	158,747,026
Office of Health and Environmental Research	658,000
Office of Fusion Energy	--[1]
Small Business Innovation Research Program	13,840,496
Office of Nuclear Energy	$123,058,000
Office of Advanced Reactor Programs	3,400,000
Office of Remedial Action and Waste Technology	6,590,000
Office of Uranium Enrichment	17,570,000
Office of Civilian Reactor Development	28,188,000
Office of Space and Defense Power Systems	2,310,000
Office of Naval Reactors	65,000,000[2]

[1]Funding was not submitted for FY 1987.

[2]Approximate

FY 1987 BUDGET SUMMARY TABLE FOR DOE MATERIALS ACTIVITIES (continued)

	FY 1987
Office of Civilian Radioactive Waste Management	$ 10,563,000
Office of Storage and Transportation Systems	819,000
Office of Civilian Radioactive Waste Management/ Nevada Nuclear Waste Storage Investigations Project (OCRWM/NNWSI)	9,419,000
Sandia National Laboratories: Brittle Fracture Technology Program	325,000
Office of Defense Programs	$ 48,806,500
Office of Waste Research and Development	8,500
Office of Weapons Research, Development and Testing	48,798,000
Office of Fossil Energy	$ 6,850,000
Office of Technical Coordination	6,165,000
Office of Surface Coal Gasification	685,000
TOTAL	**$422,650,322**

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 1987 budgets for each. More details on the individual projects within the divisions and the specific tasks or subcontracts within the various projects are given in the paragraph descriptions.

OFFICE OF CONSERVATION AND RENEWABLE ENERGY

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

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

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

	FY 1987
1. Energy Conservation	$32,056,500
a. Office of Energy Utilization Research	$ 7,432,500
(1) Energy Conversion and Utilization Technologies Division	7,432,500
b. Office of Buildings and Community Systems	$ 875,000
(1) Building Systems Division	875,000
c. Office of Industrial Programs	$ 3,258,000
(1) Improved Energy Productivity Division	1,346,000
(2) Waste Energy Reduction Division	1,912,000
d. Office of Transportation Systems	$20,491,000
2. Renewable Energy	$28,070,000
a. Office of Energy Storage and Distribution	$ 2,763,800
(1) Energy Storage	2,763,800
(2) Electric Energy Systems	--[1]
b. Office of Solar Heat Technologies	$ 3,807,000
(1) Solar Buildings Technology Division	1,822,000
(2) Solar Thermal Technology Division	1,985,000
c. Office of Solar Electric Technologies	$20,900,000
(1) Photovoltaic Energy Technology Division	20,900,000
d. Office of Renewable Technology	600,000
(1) Geothermal Technologies Division	600,000

[1]Funding was not submitted for FY 1987.

OFFICE OF ENERGY UTILIZATION RESEARCH

	FY 1987
Office of Energy Utilization Research - Grand Total	$7,432,500
Energy Conversion and Utilization Technologies Division	$7,432,500
Materials Preparation, Synthesis, Deposition, Growth or Forming	$2,800,000
Solid Lubricants Deposited From the Gas Phase	50,000
Tribological Surface Modifications and Coatings	635,000
Modeling of Hard Coatings for Tribological Systems Operating Under Extreme Conditions	0
Tribological Studies on Coated High Speed Steel Cutting Tools	0
Abrasion and Impact Resistant Coatings	125,000
Mechanical Interactions of Rough Surfaces	0
Coordination of ECUT Plastics Recycling and Reuse Efforts	35,000
Ceramic Wear Microcontact Modeling	100,000
Assessment of the Economic Potential of Plastics Reuse	10,000
Laser Surface Modifications of Ceramics	75,000
Plasma-Assisted Sintering of Ceramics	110,000
Ion Implantation of Ceramics	345,000
Compositionally Modified Ceramics	225,000
Injection Molding of Electrosterically-Stabilized Oxide Suspensions in an Aqueous Medium	65,000
Assessment of the State of the Art in Machining and Surface Preparation of Ceramics	20,000
Microporous Ceramics	160,000
Chemical Vapor Deposition of Ceramic Composites	160,000
Thin-Wall Hollow Ceramic Spheres from Slurries	240,000
Strain Tolerant Ceramic Fibers from Liquid Crystal Polymer Precursors	50,000
Synthesis of SiC Whisker - $MoSi_2$ Matrix Composites for Elevated Temperature Applications	50,000
Ordered Metallic Alloys for Lightweight Applications	200,000
Assessment of Curing and Joining of Polymers	10,000
Separation of Impurities from Molten Metals Using MHD Forces	135,000
Materials Structures and Composition	$2,200,000
Mechanisms of Adherence at Ceramic Joints	160,000
Modeling of Boron-Effect in Ni_3Al	860,000
Predictions of Ordered Intermetallics	175,000
Predictions of Super-Strong Liquid Crystal Polymers	100,000

OFFICE OF ENERGY UTILIZATION RESEARCH (Continued)

	FY 1987
Materials Structures and Composition (continued)	
Predictions of Polymer Decompositions	140,000
Influence of Electronic Structure on Ordered Intermetallics	20,000
Reactive Polymer Processing Assessment	0
	(15,000 in FY 1986)
Liquid Crystalline Polymers Assessment	0
	(25,000 in FY 1985)
Inorganic Polymers Assessment	0
	(60,000 from FY 1985 and FY 1986)
Thermosetting Resins with Reversible Crosslinks	75,000
Biobased Polymers	150,000
Assessment of DoD/NASA Thermal Insulation Technology	20,000
The Role of Inert Gas Entrapped in Rapidly Solidified Materials	400,000
Novel Technique for Particulate Removal from Molten Metals	100,000
Materials Properties, Characterization, Behavior or Testing	$805,000
Ordered Metallic Alloys for High Temperature Applications	690,000
Measurements of Grain Boundary and Surface Energies of Metals and Ceramics	50,000
Effects of Laser Machining of Silicon Nitride	50,000
Assessment of Energy Conservation Implications of Corrosion	15,000
Device or Component Fabrication, Behavior or Testing	$1,490,000
Friction and Wear Research and Development	350,000
Development of a Wear Theory of Ceramics	100,000
Lubricant Research and Development	650,000
Energy Efficient Gears	50,000
Modeling of Solid Ceramic Joints	0
	(175,000 in FY 1986)
Electromagnetic Joining of Ceramics - Laboratory Proof of Concept	100,000
Development of Tests for Ceramic-Ceramic and Ceramic-Metal Joints	120,000
Nondestructive Evaluation (NDE) of Ceramic Joints	120,000
NMR of Green State Ceramics	0
	(75,000 in FY 1986)
Assessment of Energy Conservation Implications of High Temperature Superconductors	20,000

OFFICE OF ENERGY UTILIZATION RESEARCH (Continued)

	FY 1987
Instrumentation and Facilities	$137,500
Assessment of X-Ray Methods for Investigations of Ceramic Wear Surfaces	37,500
Thin Film Thermocouples for Heat Engines	100,000

OFFICE OF ENERGY UTILIZATION RESEARCH

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

Energy Conversion and Utilization Technologies Division

The mission of ECUT is to support generic, long-term, high-risk directed basic and applied research and exploratory development of new or improved concepts to produce a technology base which private industry can use in producing products that use energy more efficiently. Materials related research in the ECUT 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) 586-5377 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.

2. Tribological Surface Modifications and Coatings - DOE Contact D. Mello, (202) 586-9345; ANL Contact Fred Nichols, (312) 972-8292

   - Emphasis in FY 1987 is on the preparation of low friction surfaces for high temperature applications, by means of ion-beam-enhanced deposition of coatings.

- The hard coatings for cutting tool wear resistance project is concluding in FY 1987.

3. Modeling of Hard Coatings for Tribological Systems Operating Under Extreme Conditions - 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.

   - 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. Tribological Studies on Coated High Speed Steel Cutting Tools - DOE Contact D. Mello, (202) 586-9345; University of California in Los Angeles Contact Rointan Bunshah, (213) 825-2210

   - Prepared coatings by a patented Activated Reactive Evaporation Process, for characterization and evaluation at ANL, as part of the program to confirm and exploit Professor Kramer's theory.

5. Abrasion and Impact Resistant Coatings - 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.

   - 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, Al_2O_3, 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.

6. Mechanical Interactions of Rough Surfaces - DOE Contact D. Mello, (202) 586-9345; SKF Industries, Incorporated Contact John McCool, (215) 265-1900, ext. 267

- o Joint effort with Office of Basic Energy Sciences.
- o Developing guidelines and techniques for the processing of surface roughness data generated in analog form.
- o This project is concluding in FY 1987.

7. Coordination of ECUT Plastics Recycling and Reuse Efforts - DOE Contact Stanley M. Wolf, (202) 586-5377; Plastics Institute of America Contact Mike Curry or Al Spaak, (201) 420-5552

   - o Study of various methods for recycling or recovering value from post-consumer plastic wastes.
   - o Transfer of technology.

8. Ceramic Wear Microcontact Modeling - DOE Contact D. Mello, (202) 586-9345, SKF Industries, Incorporated Contact John McCool, (215) 265-1900, ext. 267.

   - o Investigation of comparative tribological performance of ceramics and surface modified materials based on microgeometrical effects, and utilizing a microcontact model of friction and wear.

9. Assessment of the Economic Potential of Plastics Reuse - DOE Contact Stanley M. Wolf, (202) 586-5377; ORNL Contact Randall Curlee, (615) 576-4864

   - o Study of the economic viability of plastics reuse and the institutional incentives and barriers impacting market acceptance of recycle technologies.

10. Laser Surface Modifications of Ceramics - DOE Contact Stanley M. Wolf, (202) 586-5377; North Carolina State University Contact Jagdish Narayan, (919) 737-7874

    - o Investigation of the effects induced by pulsed laser irradiation of thin films of metals deposited onto surfaces of ceramics.
    - o Work has expanded from silicon carbide to silicon nitride materials.

11. Plasma-Assisted Sintering of Ceramics - DOE Contact Stanley M. Wolf, (202) 586-5377; Northwestern University Contact D. Lynn Johnson, (312) 492-3537

    - o Investigation of the acceleration of sintering of ceramics via plasmas.
    - o Equipment building stage complete, tests in progress.

12. Ion Implantation of Ceramics - DOE Contact Stanley M. Wolf, (202) 586-5377; 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.

13. Compositionally Modified Ceramics - DOE Contact Stanley M. Wolf, (202) 586-5377; 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
    - Measurement of electrical and optical properties.

14. Injection Molding of Electrosterically-Stabilized Oxide Suspensions in an Aqueous Medium - DOE Contact Stanley M. Wolf, (202) 586-5377; University of Washington Contact Ilhan Aksay, (206) 543-2625

    - Attempts to produce a ceramic oxide suspension suitable for higher speed injection modeling but using an aqueous solvent and minimum organic additives.
    - Approach is to adsorb polymer onto surface of submicron particle in suspension.
    - Concentrating on alpha-Al_2O_3.

15. Assessment of the State of the Art in Machining and Surface Preparation of Ceramics - DOE Contact Stanley M. Wolf, (202) 586-5377; 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.

16. Microporous Ceramics - DOE Contact Stanley M. Wolf, (202) 586-5377; LBL Contact Arlon Hunt, (415) 486-5370

- o Development of process to produce controlled porosity materials with tailored thermal, optical, and physical characteristics.

- o Determination of the properties of the finished material as related to the preparation technique.

17. Chemical Vapor Deposition of Ceramic Composites - DOE Contact Stanley M. Wolf, (202) 586-5377; ORNL Contact Ted Besmann, (615) 574-6852

    - o Production of toughened ceramic matrix coatings via simultaneous chemical vapor deposition of dispersoid and matrix phases.

    - o Development of silicon nitride-boron nitride coatings prepared from dichlorosilane, boron trichloride, and ammonia.

18. Thin-Wall Hollow Ceramic Spheres from Slurries - DOE Contact Stanley M. Wolf, (202) 586-5377; Georgia Institute of Technology Contact A. T. Chapman, (404) 894-4815; ORNL Contact David McElroy, (615) 574-5976

    - o 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).

    - o Initial work on Al_2O_3 and Al_2O_3-Cr_2O_3 with emphasis on materials as potential thermal insulations.

    - o Measurement of thermal properties of beds of above materials for potential use as thermal insulations.

19. Strain Tolerant Ceramic Fibers from Liquid Crystal Polymer Precursors -DOE Contact Stanley M. Wolf, (202) 586-5377; University of Tennessee Contact Jack Fellers, (615) 974-5345; Collaborating ORNL Contact Mark Janney, (615) 574-4281

    - o Attempt to demonstrate the feasibility of a ceramic reinforcing fiber with some amount of plastic strain tolerance.

    - o 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.

20. Synthesis of SiC Whisker - $MoSi_2$ Matrix Composites for Elevated Temperature Applications - DOE Contact Stanley M. Wolf, (202) 586-5377; LANL Contact Frank Gac, (505) 667-5452

    - o Examination of SiC whisker-$MoSi_2$ matrix composites for potential elevated temperature structural applications in oxidizing environments.

21. Ordered Metallic Alloys for Lightweight Applications - DOE Contact Stanley M. Wolf, (202) 586-5377; ORNL Contact Wally Porter, (615) 574-5143; Dartmouth Contact Erland Schulson, (603) 646-2888

- o Identification and development of ordered metallic alloys as potential lightweight structural materials.
- o Mg-Si, Mg-Si-Li, and Mg-Al systems investigated.

22. Assessment of Curing and Joining of Polymers - DOE Contact Stanley M. Wolf, (202) 586-5377; ORNL Contacts Thomas Kollie, (615) 574-4571 and Paul Phillips, (615) 974-5304

- o Assessment aimed at identifying ECUT role, if any, in support of base technologies of curing and joining of polymers.
- o Concentration on technologies that would help US auto makers deploy lighter weight polymeric components in future vehicles.
- o Work to date limited to literature searches and site visits.

23. Separation of Impurities from Molten Metals Using MHD Forces - DOE Contact Stanley M. Wolf, (202) 586-5377; ORNL Contact David O. Hobson, (615) 574-5109

- o Theoretical and experimental proof-of-concepts.
- o W, pyrex beads removal from Hg.
- o SiC, Al_2O_3 removal from molten Al.
- o Computer modeling of MHD forces for optimization.

Materials Structures and Composition

24. Mechanisms of Adherence at Ceramic Joints - DOE Contact Stanley M. Wolf, (202) 586-5377; ORNL Contact Mike Santella, (615) 574-4805; Carnegie-Mellon University Contact Dick Fruehan, (412) 268-2677

- o Investigations of the mechanisms of adherence at ceramic-metal joints.
- o Developed novel thinning procedure for TEM analysis of joints which led to realization of sub-micron scale of features.
- o Develop thermodynamic models to predict reaction of ceramics with liquid metal alloys.

25. Modeling of Boron-Effect in Ni_3Al - DOE Contact Stanley M. Wolf, (202) 586-5377; 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 Ni_3Al 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.

26. Predictions of Ordered Intermetallics - DOE Contact Stanley M. Wolf, (202) 586-5377; 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.

27. Predictions of Super-Strong Liquid Crystal Polymers - DOE Contact Stanley M. Wolf, (202) 586-5377; 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.

28. Predictions of Polymer Decompositions - DOE Contact Stanley M. Wolf, (202) 586-5377; 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.

29. Influence of Electronic Structure on Ordered Intermetallics - DOE Contact Stanley M. Wolf, (202) 586-5377; 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.

- o 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.

30. Reactive Polymer Processing Assessment - DOE Contact Stanley M. Wolf, (202) 586-5377; ORNL Contact Thomas Kollie, (615) 574-4571; University of Pittsburgh Contact Tom Lindt, (412) 624-5308

    - o Assessment of base technology research in the area of reactive polymer processing in order to facilitate the greater use of lightweight polymer-based structural components.
    - o Assessment completed in late FY 1987.

31. Liquid Crystalline Polymers Assessment - DOE Contact Stanley M. Wolf, (202) 586-377; University of Tennessee Contact Paul Phillips, (615) 974-5304

    - o Identification of research activities currently underway in the area of liquid crystalline polymers.
    - o Define research program to augment knowledge base.

32. Inorganic Polymers Assessment - DOE Contact Stanley M. Wolf, (202) 586-5377; Pennsylvania State University Contact Harry Allcock, (814) 865-3527; ORNL Contact Randy Curlee, (615) 576-4864

    - o Assessment of research and development support of inorganic polymers.

33. Thermosetting Resins with Reversible Crosslinks - DOE Contact Stanley M. Wolf, (202) 586-5377; Polytechnic of New York Contact Giuliana Tesoro (718) 643-5244

    - o Development of thermosetting resins with "reversible crosslinks."
    - o Feasibility shown in FY 1986 in epoxy with disulfide crosslink.
    - o 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.

34. Biobased Polymers - DOE Stanley M. Wolf, (202) 586-5377; SERI Contact Helena Chum, (303) 231-7249

    - o 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.

- o Formulation of a research program for the development of biobased materials: biomass-derived plastics, innovative bioprocessing, and biotechnology-produced lightweight materials.

35. Assessment of DoD/NASA Thermal Insulation Technology - DOE Contact Stanley M. Wolf, (202) 586-5377; University of Kentucky Contact Alan Fine, (606) 257-3713

    - o Assessment of the possibilities of technology transfer of specialized concepts from aerospace and other government programs to energy conservation applications in the civilian sector.

36. The Role of Inert Gas Entrapped in Rapidly Solidified Materials - DOE Contact Stanley M. Wolf, (202) 586-5377; 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

    - o 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.

    - o Significant strengthening of several RSM's containing He.

37. Novel Technique for Particulate Removal from Molten Metals - DOE Contact Stanley M. Wolf, (202) 586-5377; ORNL Contact D. O. Hobson, (615) 574-5109

    - o Development of a device to remove particulates from a flowing molten metal stream just before it solidifies.

    - o Work focusing on molten aluminum with Al_2O_3 particles.

Materials Properties, Characterization, Behavior, or Testing

38. Ordered Metallic Alloys for High Temperature Applications -DOE Contact Stanley M. Wolf, (202) 586-5377; 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

    - o Development and determination of properties of ductile long-range ordered alloys mainly based on aluminides and silicides.

    - o Main applications in high temperature service in steam turbines, heat engines, and heat exchangers.

39. Measurements of Grain Boundary and Surface Energies of Metals and Ceramics - DOE Contact Stanley M. Wolf, (202) 586-5377; ORNL Contact Thomas Kollie, (615) 574-4571

- 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.

40. Effects of Laser Machining of Silicon Nitride - DOE Contact Stanley M. Wolf, (202) 586-5377; 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.

41. Assessment of Energy Conservation Implications of Corrosion - DOE Contact Stanley M. Wolf, (202) 586-5377; ORNL Contact Randy Curlee, (615) 576-4864; Battelle Columbus Laboratories Contact W. Halder Fisher, (614) 424-6424

  - Battelle database as part of 1978 NBS study on Economic Effects of Metallic Corrosion in the United States examined with regard to energy costs of corrosion.

  - Energy costs of metallic corrosion within the United States about 7 quads/year with about 2 quads/year preventable with current technology.

Device or Component Fabrication, Behavior, or Testing

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

  - Measurements of the friction coefficient and wear rates under unidirectional sliding and investigations of the wear mechanisms of ceramics during tests of ceramics run against themselves and other ceramics up to 800°F.

  - A high-temperature tribometor has been developed and is under evaluation.

  - Experimental measurements of the wear rate (vs. tungsten carbide) of ion-implanted titanium diboride are underway.

43. Development of a Wear Theory of Ceramics - DOE Contact D. Mello, (202) 586-9345; Georgia Institute of Technology Contact Ward Winer, (404) 894-3270

- The wearing surfaces of the ends of ceramic pins are observed through a rotating transparent sapphire (Al_2O_3) disk to observe and measure the temperature of the "hot spots" (i.e., extremely hot surface asperities).

- A theory of unlubricated wear of ceramics based on plastic deformation and shear of the "hot spot" asperities is under development.

44. Lubricant Research and Development - DOE Contact D. Mello, (202) 586-9345; NBS-Gaithersburg Contact Stephen Hsu, (301) 921-2113

- Commercial base stock (without additives) oils were separated into molecular fractions and the fractions were tested for friction and wear qualities and oxidation stability.

- Measurements indicated that there are significant differences in the lubricant qualities of the various molecular constituents of base stock oils. The most lubricious molecular constituent has been identified and its structure is being investigated.

- An in situ micro-Raman spectroscope for tribochemical film analysis has been developed.

45. Energy Efficient Gears - DOE Contact D. Mello, (202) 586-9345; Northwestern University Contact Herbert Cheng, (312) 491-7062

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

- A dynamic time-dependent wear model for partial-elasto-hydrodynamic contacts is under development.

46. Modeling of Solid Ceramic Joints - DOE Contact Stanley M. Wolf, (202) 586-5377; 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.

47. Electromagnetic Joining of Ceramics - Laboratory Proof of Concept - DOE Contact Stanley M. Wolf, (202) 586-5377; Quest Research Corporation, Inc.

Contact Richard Silberglitt, (703) 893-6401; NRL Contact Dave Lewis, (202) 767-2131

- o Develop methods for joining ceramic materials to one another by microwave-induced heating of the joint interface.

- o Work to date on alumina, mullite, and silicon nitride to themselves.

48. Development of Tests for Ceramic-Ceramic and Ceramic-Metal Joints - DOE Contact Stanley M. Wolf, (202) 586-5377; ORNL Contact Artie Moorhead, (615) 574-5153

- o Development test specimens for measurement of strength and fracture toughness of ceramic-ceramic and ceramic-metal joints.

- o Fabricate and test brazed fracture toughness specimens for comparison with theoretical data generated by finite models.

49. Nondestructive Evaluation (NDE) of Ceramic Joints - DOE Contact Stanley M. Wolf, (202) 586-5377; ORNL Contact Bob McClung, (615) 574-4466

- o 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.

- o Most work to date on acoustic techniques.

50. NMR of Green State Ceramics - DOE Contact Stanley M. Wolf, (202) 586-5377; ANL Contact Bill Ellingson, (312) 972-5068

- o Exploration of the use of advanced nuclear magnetic resonance (NMR) imaging methods to characterize green-state ceramic materials.

51. Assessment of Energy Conservation Implications of High Temperature Superconductors - DOE Contact Stanley M. Wolf, (202) 586-5377; ORNL Contact Thomas Kollie, (615) 574-4571

- o Object was to determine if DOE ECUT had any reason to consider support of R&D aimed at future applications of recently discovered high temperature ($T_c \approx 100K$) superconductors in energy conserving systems.

- o ORNL completed assessment in May 1987 with positive assertion of possible ECUT role but called for more in-depth assessment to properly define.

- o Larger follow-on assessment (to be jointly funded by ECUT, DOE Fossil Energy, and Electric Power Research Institute) organized for start in early FY 1988.

Instrumentation and Facilities

52. Assessment of X-ray Methods for Investigations of Ceramic Wear Surfaces - DOE Contact Stanley M. Wolf, (202) 586-5377; 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.

53. Thin Film Thermocouples for Heat Engines - DOE Contact Stanley M. Wolf, (202) 586-5377; NBS-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.

OFFICE OF BUILDINGS AND COMMUNITY SYSTEMS

	FY 1987
Office of Buildings and Community Systems - Grand Total	$875,000
Building Systems Division	$875,000
Materials Properties, Behavior, Characterization, or Testing	$875,000
Unguarded Thin Heater Tester	100,000
Studies of Loose-fill Insulation	90,000
Heat Flow Modeling	50,000
Heat Flux Transducer Calibration Design	30,000
Variable R/Switchable Surface Analysis	40,000
Building Materials Research Plan and Moisture Studies	140,000
Analysis of Metal Building Behavior	70,000
Assessment of Properties of Wood	20,000
Recommended R-Levels - ZIP Program	45,000
Impact of CFC Restrictions	40,000
Gas Diffusion and Effective Conductivity of Foam Insulation Versus Age	95,000
Improved Standard Reference Materials	50,000
High Temperature Insulation Standard Reference Materials	75,000
Assessment of Low Density Concretes and Cement Insulation	30,000

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 Sam Tagore, (202) 586-9210.

Materials Properties, Behavior, Characterization, or Testing

54. Unguarded Thin Heater Tester - DOE Contact Sam Tagore, (202) 586-9210; ORNL Contact David McElroy, (615) 574-5976

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

55. Studies of Loose-Fill Insulation - DOE Contact Sam Tagore, (202) 586-9210; ORNL Contact David McElroy, (615) 574-5976

- o Laboratory and field studies of loose fill insulation materials to determine the effects of settling on density and R-value in attics.
- o Testing involves manufactured housing and vibration of these materials in a simulated wall cavity.

56. Heat Flow Modeling - DOE Contact Sam Tagore, (202) 586-9210; ORNL Contact David McElroy, (615) 574-5976

- o Mathematical modeling of heat transfer along longitudinal and radial coordinates of thin heater tester.
- o Elucidation of "apparent" thermal conductivity in materials.

57. Heat Flux Transducer Calibration Design - DOE Contact Sam Tagore, (202) 586-9210; ORNL Contact David McElroy, (615) 574-5976

- o 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.

58. Variable R/Switchable Surface Analysis - DOE Contact Sam Tagore, (202) 586-9210; ORNL Contact David McElroy, (615) 574-5976

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

59. Building Materials Research Plan and Moisture Studies - DOE Contact Sam Tagore, (202) 586-9210; NJIT Contact Erv Bales, (201) 596-3010

- o Chapter presenting the national need for research on building materials by the Building Thermal Envelope Coordinating Council a current research agenda.
- o Study on the physics of moisture interactions with building materials.

60. Analysis of Metal Building Behavior - DOE Contact Sam Tagore, (202) 586-9210; BNL Contact W. Loss, (516) 666-2052

- o Analysis of heat transfer losses of a metal building at BNL to include influence of fasteners, compressed insulation infiltration, and slab losses.

61. Assessment of Properties of Wood - DOE Contact Sam Tagore, (202) 586-9210; Forest Products Laboratory Contact A. Ten Wolde, (608) 264-5629

- o Assessment of currently available information on the thermal conductivity and specific heat of wood and wood products.

62. Recommended R-Levels - ZIP Program - DOE Contact Sam Tagore, (202) 586-9210; NBS Contact Steve Petersen, (301) 975-6136

- o Provide recommendations for R-values in residences for insulation zones in the USA.
- o Document the computer program, ZIP, that was used to select the recommended R-value levels.

63. Impact of CFC Restrictions - DOE Contact Sam Tagore, (202) 586-9210; NBS Contact H. Fanney, (301) 975-5864

- o This work evaluates the thermal performance and economics of alternative insulations that contain smaller or zero levels of CFC on walls and roof applications.

64. Gas Diffusion and Effective Conductivity of Foam Insulation Versus Age - DOE Contact Sam Tagore, (202) 586-9210; MIT Contact Dr. Leon Glicksman, (617) 253-2233

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

65. Improved Standard Reference Materials - DOE Contact Sam Tagore, (202) 586-9210; NBS Contact Hunter Fanney, (301) 975-5864

- o Candidates for improved standard reference materials are being investigated using a one meter diameter line-heat-source guarded hot plate.

66. High Temperature Insulation Standard Reference Materials - DOE Contact Sam Tagore, (202) 586-9210; NBS Contact D. R. Smith, (303) 497-3733

- o Ceraboard and a high temperature loose-fill insulation are candidates to be investigated for use as new Standard Reference Materials, using a new 800°K guarded hot plate.

67. Assessment of Low Density Concretes and Cement Insulation -DOE Contact Sam Tagore, (202) 586-9210; NBS Contact Walter Rossiter, (301) 975-6719

- Review of existing information and building practices concerning the use of lightweight concrete and foamed cement insulation.

- Properties and composition of the materials, test methods used for evaluating the materials, the effect of the materials on other building components, types of applications and constructions for which they are used, and installation techniques.

OFFICE OF INDUSTRIAL PROGRAMS

	FY 1987
Office of Industrial Programs - Grand Total	$3,258,000
Improved Energy Productivity Division	$1,346,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 546,000
Composite Cathode Materiel Development	150,000
Cerox Inert Anode Material	150,000
Corrosion Resistant Amorphous Metallic Films	246,000
Investigation of Material for Inert Electrodes in Aluminum Electrodeposition Cells	0
Materials Properties, Behavior, Characterization or Testing	$ 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
Waste Energy Reduction Division	$ 1,912,000
Materials Properties, Behavior, Characterization or Testing	$ 1,312,000
Advanced Heat Exchanger Material Technology Development	800,000
Assessment of Strength Limiting Flaws in Ceramic Heat Exchanger Components	344,000
National Laboratory Support to Assessment of Strength Limiting Flaws in Ceramic Heat Exchanger Components	168,000
Device or Component Fabrication, Behavior or Testing	$ 600,000
HiPHES System Design Studies	400,000
Fiber Architecture Design Studies	200,000

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

68. 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.

69. 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.

70. 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.

71. Investigation of Material for Inert Electrodes in Aluminum Electro-Deposition 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

72. 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.

73. Expand and Control Inert Electrode Cell Operating Conditions - DOE Contact M. J. McMonigle, (202) 586-2087; PNL Contact Pat Hart, (509) 375-2906; MIT Contact John Haggarty, (617) 253-3487

    - 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 Properties, Behavior, Characterization, or Testing

74. Advanced Heat Exchanger Material Technology Development - DOE Contact S. Richlen, (202) 586-2078; ORNL Contact E. Long, (615) 574-5172

    - 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.

75. Assessment of Strength Limiting Flaws in Ceramic Heat Exchanger Components - DOE Contact S. Richlen, (202) 586-2078; Babcock & Wilcox Contact T. Powers, (804) 522-5038

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

76. 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

- o 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

77. HiPHES System Design Studies - DOE Contact S. Richlen, (202) 586-2078

- o Development of preliminary designs for high pressure heat exchange systems (HiPHES).

78. Fiber Architecture Design Studies - DOE Contact S. Richlen, (202) 586-2078; ORNL Contact J. Blass, (615) 574-0721

- o Studies of fiber architecture to support design base development for ceramic composite HiPHES components.

OFFICE OF TRANSPORTATION SYSTEMS

	FY 1987
Office Of Transportation Systems - Grand Total	$20,491,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 4,157,000
Silicon Carbide Powder Synthesis	0
Turbomilling of SiC	124,000
Sintered Silicon Nitride	200,000
Si_3N_4 Powder Synthesis	478,000
Processing of Monolithics	1,000,000
Dispersion Toughened Si_3N_4	0
Dispersion Toughened Si_3N_4	0
Dispersion Toughened Si_3N_4	200,000
Composite Development	560,000
Advanced Composites	168,000
Dispersion Toughened Oxide Composites	322,000
Transformation Toughened Ceramic Processing	362,000
Development of Toughened Ceramics	107,000
Sol-Gel Oxide Powder	100,000
Advanced Transformation Toughened Oxides	0
Injection Molded Composites	186,000
Low Expansion Ceramics	150,000
Active Metal Brazing PSZ-Iron	200,000
Materials Properties, Behavior, Characterization or Testing	$ 2,851,000
Ceramic Component Design Technology	100,000
Microstructural Modeling of Cracks	69,000
Adherence of Coatings	18,000
Dynamic Interfaces	175,000
Advanced Statistical Calculations	60,000
Advanced Statistic Calculations	0
Physical Properties	75,000
Translucence Effects	3,000
Project Data Base	103,000
Characterization of Transformation-Toughened Ceramics	100,000
Fracture Behavior of Toughened Ceramics	207,000
Cyclic Fatigue of Toughened Ceramics	215,000
Rotor Materials Data Base	250,000
Static Behavior of Toughened Ceramics	15,000
Ceramic Durability Evaluation AGT	75,000
Ceramic Corrosion Evaluation AGT	100,000

OFFICE OF TRANSPORTATION SYSTEMS (Continued)

	FY 1987
Materials Properties, Behavior, Characterization or Testing (Continued)	
Corrosion/Erosion Effects	50,000
Environmental Effects In Toughened Ceramics	500,000
High Temperature Fracture Toughness Measurement	0
High Temperature Tensile Testing	200,000
Standard Tensile Test Development	120,000
Fracture Toughness Determination of Thin Coatings	55,000
Non-Destructive Evaluation	141,000
Ceramic Component NDE Technology	90,000
Computed X-Ray Tomography	120,000
Technology Transfer and Management Coordination	$ 1,277,000
Standard Reference Materials	270,000
Technology Transfer Assessment, Support Contracts, IEA	255,000
Management and Coordination	752,000
Device or Component Fabrication or Testing	$12,206,000
Metal-Ceramic Joints	499,000
Metal-Oxide Ceramic Joints	625,000
Ceramic-Ceramic Joints	639,000
Advanced Coating Technology AGT	351,000
Advanced Coating Technology	75,000
Wear-Resistant Coatings	248,000
Wear-Resistant Coatings	244,000
Sliding Seal Materials for Diesel Engines	75,000
High Temperature Solid Lubricant Coatings	50,000
Thick Thermal Barrier Coatings	200,000
Thick Thermal Barrier Coatings	200,000
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 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. Project management responsibility for heat engine technology has been delegated to the NASA Lewis Research Center.

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. 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) is operated at the 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

79. Silicon Carbide Powder Synthesis - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact E. L. Long, Jr., (615) 574-5172; Standard Oil Engineered Materials 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).

80. 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. Whittmer, (618) 536-2396

- o Perform a feasibility study to determine the potential of turbomilling as a means of reducing particulate impurities in SiC whiskers.
- o 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.

81. 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

- o Determine optimum sintering aid and time-temperature- pressure for sintered Si_3N_4.
- o Includes technical support for sintering of silicon nitride (AMTL) via on-site personnel assignments to conduct high nitrogen pressure sintering experiments.

82. Si_3N_4 Powder Synthesis - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact D. Ray Johnson, (615) 576-6832; Ford Contact G. M. Crosbie, (313) 574-1208

- o 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.

83. Processing Of Monolithics - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact D. Ray Johnson, (615) 576-6832 and R. L. Beatty, (615) 574-4536; Contractor Contact New procurement in 1987

- o Develop 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, resulting in a high-temperature ceramic with the strength and toughness required of an AGT rotor, and with a Weibull modulus of approximately 20.

84. Dispersion Toughened Si_3N_4 - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact T. N. Tiegs, (615) 574-5173; Garrett Processing Company Contact H. C. Yeh, (213) 618-7449

- o 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.

85. Dispersion Toughened Si_3N_4 - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact T. N. Tiegs, (615) 574-5173; Rockwell International Corp./ Rocketdyne Div. Contact G. D. Schnittgrund, (818) 710-5972

- o Develop Si_3N_4 composite with high toughness, high strength, and high temperature capability amendable to a low-cost near-net-shape forming process for heat engine applications based on a commercially available silicon nitride powder and a proprietary hafnia-rich mixed oxide toughened agent.

86. Dispersion Toughened Si_3N_4 - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact M. A. Janney, (615) 574-4281; GTE Labs Inc. Contact S. T. Buljan, (617) 890-8460

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

87. Composite Development - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact D. Ray Johnson, (615) 576-6832; Norton Company Contact C. A. Ebel, (617) 393-5950

- o Develop fully dense Si_3N_4 matrix SiC whisker composites utilizing the ASEA HIP (hot isostatic pressure) process.

88. 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

- o Study feasibility of the formation of Si_3N_4 matrix composites containing Si_3N_4 whiskers by transient liquid phase sintering.

89. Dispersion Toughened Oxide Composites - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact D. Ray Johnson, (615) 576-6832 and T. N. Tiegs, (615) 574-5173

- o Develop whisker-toughened alumina and mullite matrix composites with improved strength and toughness over monolithic oxide ceramics.

90. Transformation Toughened Ceramics Processing - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact P. F. Becher, (615) 574-5157; Norton Company Contact Giulio A. Rossi, (617) 393-6600

- o 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.

91. Development of Toughened Ceramics - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact D. Ray Johnson, (615) 576-6832; Ceramatec Contact R. A. Cutler, (801) 486-5071

   - Develop layered ceramic composites which incorporate zirconia as a second phase to achieve improved strength and toughness at temperatures of up to 1000°C.

   - Study processing methods for fabricating these layered composites via sintering.

92. Sol-Gel Oxide Powder - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact D. Ray Johnson, (615) 576-6832 and W. D. Bond, (615) 574-7071

   - Determine processing requirements to provide homogeneous submicron dispersion of zirconia (yttria) and zirconia (hafnia-yttria) in alumina powders and provide coatings for silicon carbide whiskers.

93. Advanced Transformation Toughened Oxides - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact D. Ray Johnson, (615) 576-6832; AMTL/University Of Michigan Contact T. Y. Tien, (313) 764-9449

   - Development of low thermal conductivity transformation- toughened alumina and mullite ceramics.

94. Injection Molded Composites - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact 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 fire parts.

95. 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.

96. Active Metal Brazing PSZ-Iron - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact 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.

Materials, Properties, Behavior, Characterization, or Testing

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

    o Develop probabilistic computer codes for ceramic component design.

98. Microstructural Modeling of Cracks - 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

    o Investigate and develop models for fracture of cracks with realistic geometry under arbitrary stress states.

99. Adherence of Coatings - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact C. J. McHargue, (615) 574-4344; University of Tennessee Contact J. E. Stoneking, (615) 974-2171

    o Conduct studies on adherence of coatings deposited on substrates subjected to ion beam mixing.

100. Dynamic Interfaces - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact E. L. Long, Jr., (615) 574-5172; Battelle Columbus Labs Contact K. F. Dufrane, (614) 424-4618

    o 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.

101. Advanced Statistical Calculations - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact D. Ray Johnson, (615) 576-6832 and W. P. Eatherly, (615) 574-5220

    o Develop advanced statistical tools for characterizing the strength of structural ceramics in a meaningful and realistic way for use in design codes.

102. Advanced Statistics Calculations - DOE Contact Robert B. Schulz, 202-586-8051; ORNL Contact W. P. Eatherly, (615) 574-5220; GE Labs Contact C. A. Johnson, (518) 387-6421

    o Develop advanced statistical techniques for describing and characterizing frequency distributions of strength in realistic cases of multiple and time-dependent distributions.

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

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

104. Translucence Effects - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact D. L. McElroy, (615) 574-5976; Integral Technologies Inc. (ITI) Contact Thomas Morel, (312) 789-0003

- o Evaluate effects of translucence on diesel engines where ceramics are being considered for heat barrier applications.

105. Project Data Base - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contacts D. Ray Johnson, (615) 576-6832 and M. K. Booker, (615) 574-5113

- o Develop a comprehensive computer data base containing the experimental data on properties of ceramic materials generated in the overall program effort.

106. Characterization of Transformation-Toughened Ceramics - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact D. Ray Johnson, (615) 576-6832; U.S. Army Materials Technology Laboratory (AMTL) Contact Jeffrey J. Swab, (617) 923-5410

- o Determine the effect of time-at-temperature on toughened oxide ceramics especially zirconia and alumina zirconia materials.
- o Screen advanced and experimental toughened oxide ceramics.

107. Fracture Behavior of Toughened Ceramics - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact D. Ray Johnson, (615) 576-6832 and P. F. Becher, (615) 574-5157

- o Characterize the high-temperature strength and toughness of state-of-the-art structural ceramics for heat engine applications.

108. Cyclic Fatigue of Toughened Ceramics - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact D. Ray Johnson, (615-) 76-6832 and K. C. Liu, (615) 574-5116

- o Develop and demonstrate the capability of performing uniaxial tension-tension dynamic fatigue testing of structural ceramics at elevated temperatures.
- o Establish a data base for design and analysis applications.

109. Rotor Materials Data Base - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contacts D. Ray Johnson, (615) 576-6832; K. C. Liu, (615) 574-5116; and M. K. Ferber, (615) 576-0818

- o Generate high temperature mechanical properties data for candidate ceramic rotor materials.

110. Static Behavior Of Toughened Ceramics - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact Victor J. Tennery, (615) 574-5123

- o Study the long-term mechanical stability of toughened ceramics for diesel engine applications.

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

- o Assess the capability of ceramic materials to perform satisfactorily at temperatures up to 2500°C for as long as 3500 hours.

112. Ceramic Corrosion Evaluation AGT - Doe Contact Saunders B. Kramer, (202) 586-8012; NASA Contact Carl A. Stearns, (216) 433-5504

- o Determine the effects of fuel and ingested impurities on candidate turbine engine ceramic materials.

113. Corrosion/Erosion Effects - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact D. Ray Johnson, (615) 576-6832; NBS Contact S. M. Wiederhorn, (301) 975-2000

- o Characterize the behavior of AGT materials subjected to corrosion by salts in combustion air and/or alternate fuels combined with erosion by combustion.

114. Environmental Effects In Toughened Ceramics - 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

- o Investigate effects of water vapor (in combustion gas from adiabatic diesel) on time-dependent strength of transformation-toughened ceramics.

115. High Temperature Fracture Toughness Measurement - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact Victor J. Tennery, (615) 574-5123; University of Washington Contact R. C. Bradt, (206) 543-2600

- o Develop and demonstrate improved fracture toughness test(s).

116. 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. Sarma Avva, (919) 334-7620

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

117. Standard Tensile Test Development - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact D. Ray Johnson, (615) 576-6832; NBS Contact S. M. Wiederhorn, (301) 975-5222

- o Development of tensile test standards for characterizing strength and creep behavior of ceramic specimens at elevated temperature.

118. 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

- o 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).

119. Non-Destructive Evaluation - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact D. Ray Johnson, (615) 576-6832 and R. W. McClung, (615) 574-4466

- o Conduct non-destructive evaluation (NDE) development to identify approaches for quantitative determination of conditions (including both properties and flaws) in ceramics that affect the structural performance.

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

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

121. Computed X-Ray 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

- o Develop X-ray beam hardening corrections for polychromatic X-ray sources when used with computed tomography machines to inspect structural ceramics, and develop appropriate test phantoms for calibration of polychromatic X-ray source CT scanners when used to inspect ceramic materials.

Technology Transfer and Management Coordination

122. Standard Reference Materials - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact D. Ray Johnson, (615) 576-6832; NBS Contact A. L. Dragoo, (301) 975-5785

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

123. Technology Transfer Assessment, Support Contracts, IEA - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact D. Ray Johnson, (615) 576-6832

- o Facilitate the transfer of technology to private industry.

124. Management and Coordination - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact D. Ray Johnson, (615) 576-6832

- o Assess the ceramic technology needs for advanced automotive heat engines, formulate technical plans to meet these needs, and prioritize and implement a long-range research and development program.

Device or Component Fabrication or Testing

125. Metal-Ceramic Joints - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact D. Ray Johnson, (615) 576-6832; GTE Contact E. M. Dunn, (617) 466-2312

- o Develop analytical and experimental methods for designing and evaluating reliable silicon carbide to metal and silicon nitride to metal joints.

126. Metal-Oxide Ceramic Joints - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact D. Ray Johnson, (615) 576-6832; Battelle Columbus Laboratories Contact R. A. Schmidt, (614) 424-4396

- o Perform an analytical and experimental evaluation of joining ceramic oxides to ceramic oxides and ceramic oxides to metals.

127. Ceramic-Ceramic Joints - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact D. Ray Johnson, (615) 576-6832; Norton Contact Donald O. Patten, Jr., (617) 393-5963

- o 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.

128. Advanced Coating Technology AGT - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact D. Ray Johnson, (615) 576-6832; GTE Labs Contact V. K. Sarin, (617) 890-8460

- o Development of coating compositions and procedures that will yield long-term adherence and reduce or eliminate contact-stress damage to silicon nitride, silicon carbide, and other ceramic materials when utilized in advanced gas turbine engines. Multiple/graded coatings will be applied by computer controlled CVD process.

129. Advanced Coating Technology - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact D. Ray Johnson, (615) 576-6832, and D. P. Stinton, (615) 574-4556

- o Develop an adherent coating that will reduce or eliminate contact-stress damage to silicon nitride, silicon carbide, or other ceramics used as static components in gas turbine engines.

130. Wear-Resistant Coatings - 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

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

131. Wear-Resistant Coatings - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact D. P. Stinton, (615) 574-4556; Cummins Contact Malcolm Naylor, (812) 377-5000

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

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

- o Develop improved sliding seal materials for low-heat rejection diesel engines.

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

- o Develop high temperature wear-resistant coating systems for use in diesel engines.

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

- o Develop zirconia-based coating systems for diesel engine components.

135. Thick Thermal Barrier Coatings - DOE Contact John Fairbanks, (202) 586-8066; NASA LeRC Contact M. Murray Bailey, (216) 433-3416; Caterpillar, Inc. Contact H. J. Larson, (309) 578-6549

- o Develop zirconia-based thermal barrier coatings for use in diesel engines.

136. Advanced Turbine Technology Applications Project (ATTAP, AGT-100) - DOE Contact Saunders B. Kramer (202) 586-8012; NASA LeRC Contact Paul Kerwin, (216) 433-3409; General Motors Allison Gas Turbine Division Co. Contact Phil Haley, (317) 230-2272

- o Develop and demonstrate ceramic component technology applicable to a high temperature automotive turbine engine.

137. Advanced Turbine Technology Applications Project (ATTAP, AGT-101) - DOE Contact Saunders B. Kramer, (202) 586-8012; NASA LeRC Contact Thomas Strom, (216) 433-3408; Garrett Turbine Engine Contact Dan Kreiner, (602) 220-3465

- o Develop and demonstrate ceramic component technology applicable to a high temperature automotive turbine engine.

OFFICE OF ENERGY STORAGE AND DISTRIBUTION

	FY 1987
Office of Energy Storage and Distribution - Grand Total	$2,763,800[1]
Energy Storage	$2,763,800[1]
Materials Preparation, Synthesis, Deposition, Growth or Forming	$2,190,000
Medium Temperature Solid Electrolytes: Proton Conductors	125,000
Hydrogen Production with Photoactive Semiconductor Catalysts	125,000
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
Materials Properties, Behavior, Characterization or Testing	$573,800[1]
High Temperature Steam Electrolysis	50,000
Cold Storage of Hydrogen on Activated Carbon	100,000
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

[1]Includes the following projects which are listed under the Office of Solar Heat Technologies but funded by the Office of Energy Storage and Distribution:

- Thermal Energy Storage Materials R&D
- Advanced Phase-Change Materials and Systems for Solar Passive Heating and Cooling of Residential Buildings

OFFICE OF ENERGY STORAGE AND DISTRIBUTION

The mission of the Office of Energy Storage and Distribution is to provide overall direction, interpret policy objectives and establish management procedures for a balanced program of technology planning, research and development, and test and evaluation, which will foster the establishment of a reasonable cross section of Electric Energy Distribution and Energy Storage Systems technology options.

The Office manages the electric energy distribution and storage systems groups of technologies in the formulation, and execution of appropriate national energy policies and programs and the verification of program balance and priorities among the technologies. 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.

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 research is divided into three subprograms: Electrochemical Energy Storage, Thermal Energy Storage and Chemical/Hydrogen Energy Storage.

Materials Preparation, Synthesis, Deposition, Growth or Forming

138. Medium Temperature Solid Electrolytes: Proton Conductors - DOE Contact M. Gurevich, (202) 586-1495; 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.

139. Hydrogen Production with Photoactive Semiconductor Catalysts - DOE Contact M. Gurevich, (202) 586-1495; 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.

140. Ceramics Research - DOE Contact A. Landgrebe, (202) 586-1483; LBL Contact E. Cairns, (415) 486-5028; SNL Contact R. Clark, (505) 844-6332

- o Develop superconducting ionic materials.
- o 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

- o Evaluate aluminum alloys for use as negative electrodes in aluminum-air batteries.
- o 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

- o 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

- o 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

- o 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

- o 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. High Temperature Steam Electrolysis - DOE Contact M. Gurevich, (202) 586-1495; Westinghouse R&D Center Contact W. Feduska, (412) 256-1951

   - Development of solid oxide electrolyte cells operated in the high temperature electrolysis mode at 1000°C for hydrogen production.

147. Cold Storage of Hydrogen on Activated Carbon - DOE Contact M. Gurevich, (202) 586-1495; Syracuse University Contact J. Schwartz, (315) 423-2807

   - Operation of macrobalance apparatus at cryogenic temperatures to permit verification of enhanced hydrogen storage on catalyzed activated carbons.

   - Identify optimum carbon/catalyst system useful in the operating temperature-pressure ranges appropriate to vehicle applications.

148. 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 SO_3 SO_2 + 1/2 0_2 when concentrated sunlight is absorbed by a gas/particle mixture.

149. 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.

150. 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.

OFFICE OF SOLAR HEAT TECHNOLOGIES

	FY 1987
Office of Solar Heat Technologies - Grand Total	$3,807,000
Solar Buildings Technology Division	$1,822,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 810,000
Thermochromic Materials Research for Optical Switching Films	125,000
Electrochromic Coatings R&D	175,000
Optical Switching Materials	150,000
Solid State Electrochromic "Smart" Windows	127,000
Optics and Materials for Controlled Radiant Energy in Buildings	187,000
Holographic Diffractive Structures for Enhanced Daylighting	46,000
Materials Properties, Behavior, Characterization or Testing	$1,012,000[1]
Generic Aperture Materials	150,000
Exposure Testing	30,000
Thermal Energy Storage Materials R&D	175,000[2]
Advanced Phase-Change Materials and Systems for Solar Passive Heating and Cooling of Residential Buildings	75,000[2]
Desiccant Materials/Dehumidifier Geometries Research	311,000
Advanced Desiccant Materials Research	150,000
Open Cycle Absorption Solar Cooling	209,000
Solar Cooling Research Facility	0
Materials with Enhanced Transport Properties for High Performance Desiccant Systems	15,000
Evaluation of Photochromic Plastics	47,000
Daylighting Enhancement	100,000
Solar Thermal Technology Division	$1,985,000
Materials Preparation, Synthesis, Deposition Growth or Forming	$ 808,000
Silver/Polymer Reflector Research	808,000

[1]Does not include projects funded by the Office of Energy Storage.

[2]Funded by the Office of Energy Storage.

OFFICE OF SOLAR HEAT TECHNOLOGIES (continued)

	FY 1987
Solar Thermal Technology Division (continued)	
Materials Properties, Behavior, Characterization or Testing	$1,777,000
High Temperature Materials	185,000
High Flux Effects on Materials	645,000
Composite Materials for Concentrators	182,000
Radiant Transport and Optical Properties of Materials	165,000

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 supplies. The objectives of the program are to: (1) develop solar energy technologies that can be practically used to supply 70-80 percent of building space heating, hot water, cooling, and lighting requirements at costs competitive with conventional technologies; and (2) provide industry with the information and techniques required to improve component and system reliability and durability to achieve acceptable system performance and equipment service life. 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

151. 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 surfaces to control insolation through building envelopes.

    - Development of undoped crystalline VO_2 pigments that switch and doped pigments produced by mixing VO_2 pigments with tungsten or tungsten oxide.

152. Electrochromic Coatings R&D - DOE Contact M. M. Jenior, (202) 586-2998; SERI Contact D. Benson, (303) 231-1162

    - Develop a laboratory-scale plasma-enhanced chemical vapor deposition (PE-CVD) process for producing practical, cost-effective electrochromic coatings for architectural glass.

- o Experimentally determine the optimum deposition parameters and improve the understanding of electrochromic response in metal oxide films.

153. Optical Switching Materials - DOE Contact M. M. Jenior, (202) 586-2998; LBL Contact Steven Selkowitz, (415) 486-5064

- o Research and synthesize new electrochromic materials that have a broadband or selective optical response different than that of existing materials using low-cost deposition techniques.
- o Develop device designs for new electrochromic materials.
- o Provide scientific coordination for all DOE contractors in the area of switching devices.

154. Solid State Electrochromic "Smart" Windows - DOE Contact M. M. Jenior, (202) 586-2998, EIC Contact R. D. Rauch, (617) 769-9450

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

155. Optics and Materials for Controlled Radiant Energy in Buildings - DOE Contact M. M. Jenior, (202) 586-2998; Tufts University Contact R. B. Goldner, (617) 628-5000

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

156. 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

- o Develop a low-cost holographic diffractive structure (HDS) system that maximizes the utilization of sunlight for daylighting.
- o Develop a working prototype capable of achieving a 47° acceptance angle, full azimuth range, and optimal efficiency.

Materials Properties, Behavior, Characterization, or Testing

157. Generic Aperture Materials - DOE Contact M. M. Jenior, (202) 586-2998; LBL Contact Steven Selkowitz, (415) 486-5064

- o Perform research and development necessary to overcome present obstacles to commercial development of transparent insulating glazings such as silica aerogel.

158. Exposure Testing - DOE Contact R. Hassett, (202) 586-8163; LANL Contact S. Moore, (505) 667-2228

- o Conduct solar radiation, elevated temperature and moisture exposure testing.
- o Collect and analyze information on insolation, temperature, humidity, and ultraviolet radiation.
- o Correlate short-term and accelerated tests and develop degradation prediction models.

159. Thermal Energy Storage Materials R&D - DOE Contact R. Hassett, (202) 586-8163; SERI Contact D. Benson, (303) 231-1162

- o Complete analyses and laboratory-scale research and testing on new TES materials concept in order to provide their practical potential well enough for private industry to adopt the concept and develop products based upon it.

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

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

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

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

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

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

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

- o Identify a suitable mixture of absorbent-refrigerant pairs for use in a high performance open-cycle absorption system.
- o Perform experiments to determine crystallization concentration as a function of temperature.
- o Develop equations for calculating the thermophysical properties of various solutions.

164. Solar Cooling Research Facility - DOE Contact J. Goldsmith, (202) 586-8779; Florida Solar Energy Center Contact S. Chandra, (305) 783-0300

- o Identify the utility and application of desiccant materials.
- o Develop innovative materials and systems.

165. Materials with Enhanced Transport Properties for High Performance Desiccant Systems - DOE Contact J. Goldsmith, (202) 586-8779; Illinois Institute of Technology Contact Z. Lavan, (312) 567-3189

- o Conduct desiccant analysis and materials research in enhanced heat and mass diffusion rates.
- o Develop improved understanding of the limited heat and mass transfer rates.

166. Evaluation of Photochromic Plastics - DOE Contact M. M. Jenior, (202) 586-2998; American Optical Corporation Contact N. Chu, (617) 765-9711

- o Evaluate photochromic plastic materials for their potential application to architectural glazing in buildings designed to use or control solar energy.

167. Daylighting Enhancement - DOE Contact M. M. Jenior, (202) 586-2998; LBL Contact Steven Selkowitz, (415) 486-5064

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

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

168. Silver/Polymer Reflector Research - DOE Contact Frank Wilkins, (202) 586-1684; SERI Contact Paul Schissel, (303) 231-1226

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

Materials Properties, Behavior, Characterization, or Testing

169. High Temperature Materials - DOE Contact Frank Wilkins, (202) 586-1684; SERI Contact Daniel M. Blake, (303) 231-1202

- o Establish the stability limits of suspensions of metal oxide powders in molten nitrate salt mixtures.
- o Identify and define failure modes of metal tubes that have been subjected to high flux, high temperature, and thermal cycling.
- o Investigate durability of ceramic and metallic parts under cyclic heating typical of solar thermal systems.

170. High Flux Effects on Materials - DOE Contact Frank Wilkins, (202) 586-1684; SERI Contact Daniel M. Blake, (303) 231-1222

- o Investigate surface transformations under high solar flux.
- o Prepare wear resistant and corrosion resistant coatings on metals using high solar flux.
- o Produce high temperature ceramics with solar flux.
- o Investigate high flux photo-enhanced degradation of materials, and identify possible changes in coatings to reduce these effects.
- o Characterize the effects of high solar flux on carbon fibers and carbon-carbon composites.
- o Compare the effects on materials caused by heat only with those produced by high solar flux.

171. Composite Materials for Concentrators - DOE Contact Frank Wilkins, (202) 586-1684; SERI Contact L. Marty Murphy, (303) 231-1050

- o Determine feasibility of using advanced composite materials and wood laminates for low cost heliostats.

172. Radiant Transport and Optical Properties of Materials - DOE Contact Frank Wilkins, (202) 586-1684; SERI Contact John Webb, (303) 231-1430

- o Determine radiant transport properties of molten salts and molten salt blackeners.
- o Characterize radiative and optical properties of materials for new receiver designs.

OFFICE OF SOLAR ELECTRIC TECHNOLOGIES

	FY 1987
Office of Solar Electric Technologies - Grand Total	$20,900,000
Photovoltaic Energy Technology Division	$20,900,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$16,000,000
Amorphous Silicon for Solar Cells	10,500,000
Polycrystalline Thin Film Materials for Solar Cells	3,500,000
Deposition of III-V Semiconductors for High-Efficiency Solar Cells	2,000,000
Materials Properties, Behavior, Characterization or Testing	$ 2,900,000
Materials and Device Characterization	2,900,000
Device or Component Fabrication, Behavior or Testing	$ 2,000,000
High-Efficiency Crystal Silicon Solar Cells	2,000,000

OFFICE OF SOLAR ELECTRIC TECHNOLOGIES

Photovoltaic Energy Technology Division

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

Materials Preparation, Synthesis, Deposition, Growth or Forming

173. Amorphous Silicon for Solar Cells - DOE Contact Morton B. Prince, (202) 586-1725; SERI Contact Ed Sabisky, (303) 231-1483

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

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

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

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

175. 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 Dan Arvizu, (505) 846-0387

    - 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 concentrator cells and 20 percent and 100 cm^2 flat plate cells.

Materials Properties, Behavior, Characterization or Testing

176. 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

177. High-Efficiency Crystal Silicon Solar Cells - DOE Contact Morton B. Prince, (202) 586-1725; SERI Contact John Benner, (303) 231-1396; SNLA Contact Dan Arvizu, (505) 846-0387

    - 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 TECHNOLOGY

	FY 1987
Office of Renewable Technology - Grand Total	$600,000
Geothermal Technologies Division	$600,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$365,000
High Temperature Elastomers for Dynamic Sealing Applications	100,000
Geothermal Waste Utilization and Disposal	25,000
Materials for Non-Metallic Heat Exchangers	75,000
Biochemical Concentration and Removal of Toxic Components from Geothermal Wastes	165,000
Materials Properties, Behavior, Characterization or Testing	$235,000
Corrosion Resistant Elastomeric Liners for Well Casing	52,000
Advanced High Temperature Geothermal Well Cements	125,000
Corrosion in Binary Geothermal Systems	48,000
Metallic Liners for Well Casing	10,000

OFFICE OF RENEWABLE TECHNOLOGY

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

178. High Temperature Elastomers for Dynamic Sealing Applications - DOE Contact R. LaSala, (202) 896-4198; BNL Contact L. E. Kukacka, (516) 282-3065

    - o Chemical modification of previously developed and tested Y-267 EPDM 260°C static seal material for use in dynamic sealing applications.
    - o Optimization of EPDM formulations for use in critical high cost applications such as in drill pipe protectors, rotating head seals and blow-out preventors.

179. Geothermal Waste Utilization and Disposal - DOE Contact G. J. Hooper, (202) 896-1146; BNL Contact L. E. Kukacka, (516) 282-3065

    - o Studies of methods for stabilizing toxic geothermal residues in composites so that they can be used for general construction purposes.

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

    - o Development of corrosion resistant metallic and silicon carbide-filled composites that have thermal conductivities in the range of stainless steels.

181. 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

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

Materials Properties, Behavior, Characterization or Testing

182. Corrosion Resistant Elastomeric Liners for Well Casing - DOE Contact R. LaSala, (202) 896-4198; BNL Contact L. E. Kukacka, (516) 282-3065

- o Development of corrosion resistant metallic and silicon carbide-filled composites that have thermal conductivities in the range of stainless steels.

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

- o Characterization of promising lightweight, high temperature well cements under placement and downhole environmental conditions.
- o Mechanisms of cement deterioration in high CO_2-containing geothermal brines.

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

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

185. Metallic Liners for Well Casing - DOE Contact R. LaSala, (202) 896-4198; BNL Contact D. van Rooyen, (516) 282-4050

- o Quantitative corrosion data from laboratory tests of metals being considered for use as liners on geothermal well casings.

OFFICE OF ENERGY RESEARCH

	FY 1987
Office of Energy Research - Grand Total	$173,245,522
Office of Basic Energy Sciences	$158,757,026
Division of Materials Sciences	$155,000,000
Division of Engineering and Geosciences	$ 3,674,000
Materials Properties, Behavior, Characterization or Testing	$ 3,674,000
Bounds on Dynamic Plastic Deformation	123,000
Diffusion, Fluid Flow and Sound Propagation in Disordered Media	65,000
In-Flight Measurement of the Temperature of Small, High Velocity Particles	90,000
Experimental Measurement of the Plasma/Particle Interaction	328,000
Integrated Sensor/Model Development for Automated Welding	496,000
Nondestructive Characterization of Fracture Dynamics and Crack Growth	193,000
Boiling of Aqueous Polymer Solutions	67,000
Plasma Reduction of Metallic Oxide Particles	76,000
High-Temperature Gas-Particle Reactions	230,000
Mathematical Modeling of Transport Phenomena in Plasma Systems	102,000
In-Process Control of Residual Stresses and Distortion in Automatic Welding	87,000
Multivariable Control of the Gas-Metal Arc Welding Processes	102,000
Modeling of GMA Weld Pool Geometry and Metal Transfer	88,000
Modeling and Analysis of Surface Cracks	200,000
Thermal Plasma Processing of Materials	142,000
Transport Properties of Disordered Porous Media from the Microstructure	90,000
Effects of Crack Geometry and Near-Crack Materials Behavior on Scattering of Ultrasonic Waves for QNDE Applications	65,000
Inelastic Deformation and Damage at High Temperature	120,000
Energy Changes in Transforming Solids	0
Nondestructive Testing	115,000
Effective Elastic Properties of Cracked Solids	107,000
Elastic-Plastic Fracture Analysis Emphasis on Surface Flaws	365,000
Continuous Damage Theory	44,000

OFFICE OF ENERGY RESEARCH (Continued)

	FY 1987
Office of Basic Energy Sciences (Continued)	
Division of Engineering and Geosciences (Continued)	
Materials Properties, Behavior, Characterization or Testing (Continued)	
Loss Characteristics of Cord-Rubber Composites	73,000
Effects of Crack Geometry and Near-Crack Material Behavior on Scattering of Ultrasonic Waves for QNDE Applications	65,000
Multiviewing Transducer System	241,000
Division of Advanced Energy Projects	$ 73,026
Aerodynamic Focusing of Particles and Heavy Molecules	73,026
Office of Health and Environmental Research	$ 658,000
Division of Physical and Technological Research	$ 658,000
Materials Properties, Behavior, Characterization or Testing	$ 658,000
Semiconductor Radiation Detector Technology	398,000
Development of Silicon Avalanche Internal Gain Radiation Detection Structures	260,000
Small Business Innovation Research Program	$ 13,840,496
Materials Preparation, Synthesis, Deposition, Growth, or Forming	5,494,384[1]
Phase I Projects:	
The Preparation of High Temperature Intermetallic Compounds at Low Temperatures	49,913
High-Flux, High-Selectivity Cyclodextrin Membranes	49,821
Novel High-Flux Antifouling Membrane Coatings	49,821
Design, Fabrication, and Interface Characterization of Ceramic Fiber-Ceramic Matrix Composites	48,870
New Low Thermal Expansion Structural Ceramics	49,994

[1]Totals reflect the fact that Phase II funding levels are spread over a two-year period.

	FY 1987
Materials Preparation, Synthesis, Deposition, Growth, or Forming (continued)	
Synthesis of High-Strength Alumina Whiskers for Reinforcing Ceramic and Metallic Matrices	49,885
Cost-Effective Techniques for Development of Radiation-Resistant Organic Insulators for Superconducting Magnets	49,916
Composite Materials with Low Z, Self-Regenerating Coatings for Fusion First Walls and Limiters	49,917
Coatings for High Temperature Ceramic Filters	49,880
A Tritium Permeation Resistant Polymer Coating	48,844
The Development of NbN-Coated Graphite Superconducting Materials	48,588
The Rapid Growth and Harvesting of SiC Whiskers from Composite Particles	50,000
High Density Silicon Nitride Ceramic Materials	49,782
Continuous Extrusion of Nb_3Sn Superconductors	49,835
Advanced Insulating Coatings for Plasma Confinement Systems	49,901
Deposition of Metastable Thin Film Materials by Light-Assisted Metalorganic Chemical Vapor Deposition	49,821
Electrically Conductive Polymers by Ion Implantation	49,936
Process Development for Producing Nb_3Sn Multifilament Superconductors of High Current Density	49,983
The Development of a Process for Making Multifilamentary NbN	50,000
Graphite Reinforced Copper Alloys for Fusion Reactor Applications	50,000
Synthesis of Inorganic Films by Ion Beam Irradiation of Organosilicon Polymer Films	49,904
Amorphous Ferromagnetic Material with Ultra-Low Eddy Current Losses	50,000
Phase II Projects: (First Year)	
The Development of Nb_3Sn 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 EnergyMagnet Applications	499,918
An Internal-External Bronze Process for the Manufacture of Large Filament Nb_3Sn	499,981

OFFICE OF ENERGY RESEARCH (Continued)

	FY 1987
Materials Preparation, Synthesis, Deposition, Growth, or Forming (continued)	
Phase II Projects: (Second Year)	
Fabrication and Characterization of Ceramic-Matrix-Ceramic Whisker Composites with Random Orientation of the Whiskers	498,816
Development of a Continuous Process to Clad Superconductors with High-Purity Aluminum	499,859
The Direct Production of Intermetallic Compound Powder	500,000
The Investigation of an Improved Processing Method for High Current Density, Fine-Filamentary Superconductors	499,994
The Development of a Process for Producing Aluminum Stabilized, Fine-Filamentary Superconducting Composites	499,992
Materials Properties, Behavior, Characterization, or Testing	$849,518[2]
Phase I Projects:	
Laser-Based Ultrasonic Excitation and Speckle Interferometric Detection Systems for Nondestructive Evaluation of High Temperature Ceramics	49,898
High Thermal Conductivity Sintered AlN	49,950
Photovoltaic and Photoelectrochemical Properties of Polydiacetylenes	50,000
Ultrasonic Grinding of Zeolites for Radioactive Water Treatment	49,860
High-Speed, High-Resolution Ultrasonic NDT/E of Superconducting Magnet Mono- and Multifilamentary Wire	50,000
Monitoring Erosion in Coal Combustion Engines Using Surface Layer Activation	49,830
Optimization of Properties of Ductile Superconducting Alloys for Operation up to 10T	50,000
Phase II Projects: (First Year)	
Investigation of Fatigue Failure Initiation and Propagation in Wind-Turbine-Grade Wood/Epoxy Laminate Containing Several Veneer Joint Styles	$ 499,980

[2]Totals reflect the fact that Phase II funding levels are spread over a two-year period.

	FY 1987
Device or Component Fabrication, Behavior or Testing	$ 5,469,269[3]
Phase I Projects:	
Research and Development of Multisegment Ceramic Ring Cryogenic Seals	50,000
Gate Valves for Fusion Applications - Radial-Directed, Fluid-Pressure-Loaded, All-Metal-Sealed Double Gates	50,000
Interfacial Condensation Polymers for Analyte-Specific Sensor Coatings	49,367
Continuous Casting of Metallic Nuclear Fuel without Containment Contact	49,658
Miniature Electromagnetic Bearings for Cryogenic Applications	49,902
Advanced Abrasive-Waterjet Techniques for the Decontamination and Decommissioning of Nuclear Facilities	49,514
Non-Noble Metal Catalysts for Metal-Air or Fuel Cell Cathodes	50,000
High Energy Density Composite Flywheels for Space-Based Energy Storage Systems	48,685
Using Porous Metals for Vapor-Liquid Separation in Liquid Metal Rankine Cycle Space Power Systems	50,000
A Boron Phosphide Semiconductor Neutron Detector	49,721
The Development of Shielded X-Ray Plasma Diagnostic Detectors for High Radiation Backgrounds	49,993
The Development of Optimum Structural Supports for Large Aperture Stretched Membrane Heliostats	48,662
Optical Optimization of Multijunction Thin Film Silicon: Hydrogen Solar Cells	48,000
The Effect of Different Levels of Manganese on Mechanical Properties and Coupling	49,995
Advanced Heat Pipes for AVLIS Collector Plate Cooling	49,803
Phase II Projects: (First 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	445,062

[3]Totals reflect the fact that Phase II funding levels are spread over a two-year period.

OFFICE OF ENERGY RESEARCH (Continued)

	FY 1987
Device or Component Fabrication, Behavior or Testing	$ 5,469,269[4]
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
Phase II Projects: (Second Year)	
The Design and Fabrication of Flat Panels with High Acoustic Transmissivity	$ 500,000
Highly Versatile Multilayer Tactile Sensor Arrays	500,000
Direct Energy Conversion with Pyroelectric Polymer	499,749
Reduction of Low-Level Radwaste Disposal in Water Clean-Up Systems by Use of Magnetite	499,667
Instrumentation and Facilities	$ 2,027,325[4]
Phase I Projects:	
Premonochromator X-Ray Optic Substrate Development for New Generation Synchrotron Source Beamlines	$ 49,124
Phase II Projects: (Second Year)	
The Construction of a Soft X-Ray Source Using Transition Radiation for Lithography	$ 478,564
A New Two-Dimensional Position Encoder for Positron Emission Tomography (PET)	500,000
A High Efficiency Helium-3 Neutron Detector	499,667
An InP Semiconductor Neutrino Detector	499,970

[4]Totals reflect the fact that Phase II funding levels are spread over a two-year period.

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 1987 for the Division of Materials Sciences were $155,000,000. This was allocated to 432 projects. Many projects cross the traditional categories and, for example, involve property-structure relationships. Nevertheless, the approximate funding distribution for FY 1987 was:

	$ (Millions)
Materials Preparation, Synthesis, Deposition, Growth or Forming	19.0
Materials Structure and Composition	25.4
Materials Properties, Behavior, Characterization or Testing	76.1
Device or Component Fabrication, Behavior or Testing	--
Facilities	34.5

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 1987 (DOE/ER-0348 dated September 1987). 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

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

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

187. 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.

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

   - Measure particle temperatures and sensitivities while electrodynamically suspended.

   - Develop analog and digital signal processing techniques for in-flight property evaluation.

   - Application of developed techniques to measure particle temperatures in a high-temperature plasma.

189. 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.

190. 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, J. A. Johnson, 208-526-9021, J. O. Bolstad, (208) 526-1753

- o Develop model of gas metal arc welding process suitable for real-time process control.
- o Develop optical sensing capability to provide weld-bead geometry data.
- o Develop ultrasonic sensing capability to directly sense weld bead site wall penetration and fusion.

191. 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

- o Develop instrumentation and models to measure and predict interaction between ultrasound and gorwing cracks in engineering materials.
- o Investigate methods of sensing properties of growing cracks.

192. Boiling of Aqueous Polymer Solutions - DOE Contact Oscar P. Manley, (301) 353-5822; University of Illinois at Chicago Contact J. P. Hartnett, (312) 996-4490

- o Study pool boiling behavior of aqueous polymer solutions.

193. Plasma Reduction of Metallic Oxide Particles - DOE Contact Oscar P. Manley, (301) 353-5822; MIT Contacts J. F. Eliott, (617) 253-3305, J. Szekely, (617) 253-3305, R. E. Spjut, (617) 253-0252

- o Characterize the reduction to metal of oxide particles into the tail flame of an arc plasma.

194. High-Temperature Gas-Particle Reactions - DOE Contact Oscar P. Manley, (301) 353-5822; MIT Contacts J. F. Eliott, (617) 253-3305, R. E. Spjut, (617) 253-0252

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

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

- o 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.

196. 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

- o Develop technology of in-process control of residual stress and distortion in automatic welding.

197. 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

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

198. Modeling of GMA Weld Pool Geometry and Metal Transfer - DOE Contact Oscar P. Manley, (301) 353-5822; MIT Contact William Unkel, (617) 253-2193

- o Develop physically-based, computationally-simple models of GMAW processes.
- o Use models to identify process modifications for more effective multivariable control.

199. Modeling and Analysis of Surface Cracks - DOE Contact Oscar P. Manley, (301) 353-5822; MIT Contacts David M. Parks, (617) 253-1630

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

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

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

201. 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

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

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

- o Apply the scattered field approach to the characterization and detection of cracklike flaws.

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

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

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

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

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

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

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

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

207. 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

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

- o 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.

208. Continuous Damage Theory - DOE Contact Oscar P. Manley, (301) 353-5822; University of Illinois Contact D. Krajcinovic, (312) 996-7000

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

209. Loss Characteristics of Cord-Rubber Composites - DOE Contact Oscar P. Manley, (301) 353-5822; University of Michigan Contact S. K. Clark, (313) 764-4256

- o Data acquisition on the loss characteristics of cord-rubber composites under both uniaxial and multiaxial stress states, including the effects of prestrain, frequency, strain amplitude and temperature in the assessment of the visco-elastic properties of the materials.
- o Analysis of the rolling loss of a pneumatic tire using the viscoelastic properties obtained in the first task, together with finite element codes suitable for the problem. Theoretical results will be compared against measured values.

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

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

211. Multiviewing Transducer System - DOE Contact Oscar P. Manley, (301) 353-5822; Iowa State University Contact D. O. Thompson, (515) 294-5320

- o Demonstration of a composite multiviewing NDE transducer.

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

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

Division of Advanced Energy Projects

212. 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

- o 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.

- o Accompanying theoretical studies using Brownian dynamics simulations.

Office of Health and Environmental Research

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

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

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

- o 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.

214. Development of Silicon Avalanche Internal Gain Radiation Detection Structures - DOE Contact G. Goldstein, (301) 353-5348; University of Southern California Contact G. Huth, (213) 822-9184

- Silicon avalanche radiation detectors are developed using single crystal neutron transmission doped silicon. Research focuses on studies of the avalanche process and development of specific devices.

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 6 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 2 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, 1986 (DOE/ER-0285), Abstracts of Phase II Awards, 1985 (DOE/ER-0209/1), and Abstracts of Phase II Awards, 1986 (DOE/ER-0286). 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:

High Thermal Conductivity Dispersion-Strengthened Silicon Nitride - DOE Contact Samuel J. Barish, (301) 353-3054; Ceramatec, Inc. Contact David W. Richerson, (801) 486-5071

Improved Silicon Germanium Thermoelectrics - DOE Contact Bill Barnett, (301) 353-3097; Electro Tech Corporation Contact Norbert B. Elsner, (619) 459-1016

Development of High-Temperature Amorphous Alloys - DOE Contact Samuel J. Barish, (301) 353-3054; Flow Research Company Contact Arthur C. Day, (206) 872-7080

Processing Science: Understanding and Control of the Whisker Matrix Interface in Ceramic-Ceramic Composites - DOE Contact Samuel J. Barish, (301) 353-3054; Flow Research Company Contact Birol Sonuparak, (206) 872-7080

The Development of Nb_3Sn Superconductor with Micron-Size Filaments, High-Current Densities, and Low Magnetization - DOE Contact Victor Der, (301) 353-5736; Intermagnetics General Corporation Contact Gennady Ozeryansky, (203) 753-5215

Mechanical Reliability of Superplastically Forged Silicon Nitride - DOE Contact Samuel J. Barish, (301) 353-3054; Jupiter Technologies, Inc. Contact Prakash C. Panda, (607) 257-4514

Improved Brazing Techniques for Machinable Glass Ceramics -DOE Contact Marvin Cohen, (301) 353-4253; Lintel Technology, Inc. Contact Dr. Chou H. Li, (516) 484-1719

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

Improvement of Copper/Epoxy Composites for Fusion Energy Magnet Applications -DOE Contact Marvin Cohen, (301) 353-4253; PDA Engineering Contact William H. Pfeifer, (714) 556-2800

An Internal-External Bronze Process for the Manufacture of Large Filament Nb_3Sn -DOE Contact Victor Der, (301) 353-5736; Supercon, Inc. Contact Eric Gregory, (617) 842-0174

High-Current Density Nb_3Sn Superconductors Made by Powder Metallurgy - DOE Contact Victor Der, (301) 353-5736; Supercon, Inc. Contact Eric Gregory, (617) 842-0174

A Search for Metal Oxide-Metal Nitride Eutectic Systems - DOE Contact Samuel J. Barish, (301) 353-3054; Syn Crys, Inc. Contact G. Wayne Clark, (615) 482-3411

Metallophilic Oxides in Copper for Fusion Reactors - DOE Contact Ted Reuther, (301) 353-4963; Technical Research Associates, Inc. Contact J. K. Weeks, (801) 582-8080

TiC Infiltrated Graphite Fiber Structures for Fusion Reactors - DOE Contact Marvin Cohen, (301) 353-4253; Ultramet Contact Richard B. Kaplan, (818) 899-0236

Surface Modification by Ion Beams for Improved Corrosion Resistance - DOE Contact Samuel J. Barish, (301) 353-3054; Universal Energy Systems Contact Dr. Rabi Bhattacharya, (513) 426-6900

Phase II Projects: (First Year)

Fabrication and Characterization of Ceramic Matrix-Ceramic Whisker Composites with Random Orientation of the Whiskers - DOE Contact Iran Thomas, (301) 353-3426; Ceramatec, Inc. Contact L. Viswanathan, (801) 486-5071

Development of a Continuous Process to Clad Superconductors With High-Purity Aluminum - DOE Contact Earle Fowler, (301) 353-4801; Intermagnetics General Corporation Contact Kanithi Hemachalam, (203) 753-5215

The Direct Production of Intermetallic Compound Powder - DOE Contact Iran Thomas, (301) 353-3426; Materials and Electrochemical Research Corporation Contact James C. Withers, (602) 749-3257

The Investigation of an Improved Processing Method for High Current Density, Fine-Filamentary Superconductors - DOE Contact Earle Fowler, (301) 353-4801; Supercon, Inc. Contact Eric Gregory, (617) 842-0174

The Development of a Process for Producing Aluminum Stabilized, Fine-Filamentary Superconducting Composites - DOE Contact Earle Fowler, (301) 353-4801; Supercon, Inc. Contact Eric Gregory, (617) 842-0174

Phase II Projects: (Second Year)

Growth of BaF_2 Crystals by the Heat-Exchanger Method (HEM) with Enhanced Fast Component for Scintillator Applications - DOE Contact Stanley Whetstone, (301) 353-3613; Crystal Systems, Inc. Contact Chandra P. Khattak, (617) 745-0088

Brazing of Machineable Glass Ceramics and Other Ceramic Materials - DOE Contact Marvin Cohen, (301) 353-4253; Hittman Materials & Medical Components, Inc. Contact Harold N. Barr, (301) 730-7800

Development of a New Process for the Production of Very Fine Filamentary Superconducting NbTi Composites - DOE Contact Earle Fowler, (301) 353-4801; Supercon, Inc. Contact Eric Gregory, (617) 842-0174

Materials Properties, Behavior, Characterization, or Testing

Phase I Projects:

An Investigation of Fatigue Failure Initiation and Propagation in Wind-Tubine-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

Applications of Direct Recoil Spectroscopy for Surface Analysis of Li, H, and D on Fusion Materials - DOE Contact Marvin Cohen, (301) 353-4253; Ionwerks Contact J. Albert Schultz, (713) 667-1691

Nonorganic, Low-Pressure Solid Lubricants by Ion Beam Enhanced Deposition - DOE Contact Marvin Cohen, (301) 353-4253; Spire Corporation Contact James Hirvonen, (617) 275-6000

A Novel Hybrid Lubrication Approach for Advanced Heat Engines - DOE Contact Terry Levinson, (202) 586-5377; Technology Assessment & Transfer, Inc. Contact Larry L. Fehrenbacher, (301) 858-0248

Phase II Projects: (Second Year)

Processing and Characterization of SiCALON Ceramics - DOE Contact Iran Thomas, (301) 353-3426; Ceramatec, Inc. Contact Raymond A. Cutler, (801) 487-5411

Reduction of Surface Recombination in Silicon Solar Cells -DOE Contact Richard King, (202) 586-1693; Spire Corporation Contact Mark B. Spitzer, (617) 275-6000

Device or Component Fabrication, Behavior, or Testing

Phase I Projects:

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

Development of High-Resolution Gratings Produced from Advanced Materials by Chemical Vapor Deposition Techniques - DOE Contact Donald Priester, (301) 353-3421; CVD, Inc. Contact Parul Purohit, (617) 933-9243

A Feasibility Assessment of the Thermotunnel Energy Converter - DOE Contact Bill Barnett, (301) 353-3097; Energetics, Inc. Contact Thomas S. Bustard, (301) 992-4000

Study of Filament Instability in Multifilamentary NbTi/Cu Composites - DOE Contact Earle Fowler, (301) 353-4801; Intermagnetics General Corporation Contact Kanithi Hamachalam, (203) 753-5215

A Differential Microcalorimetric Biosensor Based on Pyroelectric Thin Polymer Films - DOE Contact Janet Dorigan, (301) 353-5778; Ohmicron Corporation Contact Mark K. Malmros, (609) 737-9050

Surface Figure Measurements of X-Ray Optics - DOE Contact Samuel J. Barish, (301) 353-3054; Optel Systems/Optel Bar Code Systems, Inc. Contact Thomas C. Bristow, (716) 385-6760

A Real-Time, Noncontact Optical Surface Motion Monitor - DOE Contact Stan Sobczynski, 202-586-1878; Optra, Inc. Contact Geert Wyntjes, (617) 535-7670

A Fiber Optic Tactile Sensor for Robotics Applications - DOE Contact Oscar Manley, (301) 353-5822; Physical Optics Corporation Contact Joanna Jannson, (213) 371-3909

High-Temperature Thermionics for Burst Power Applications -DOE Contact Ira Helms, (301) 353-5845; Rasor Associates, Inc. Contact John McVey, (408) 734-1622

A Contactless Self-Scanning High-Temperature NDE Flaw Detector - DOE Contact Phillip Hemmig, (301) 353-3579; SONOQUEST/Advanced Ultrasonics Research Contact Jacques R. Chamuel, (617) 239-0554

An Improved Thermionic Conversion Device Using Oxide with Metallic or Metal Carbide Composites - DOE Contact Bill Barnett, (301) 353-3097; Technology for Energy Corporation Contact Francis E. LeVert, (615) 966-5856

Microlaminated Ferromagnetic Composites for Magnetic Switching - DOE Contact David Bailey, (301) 353-4078; Xi Magnetics, Inc. Contact John L. Wallace, (215) 347-1768

Phase II Projects: (First Year)

The Design and Fabrication of Flat Panels with High Acoustic Transmissivity - DOE Contact Iran Thomas, (301) 353-3426; Analysis Consultants Contact B. G. Martin, (714) 380-1204

Highly Versatile Multilayer Tactile Sensor Arrays - DOE Contact Oscar Manley, (301) 353-5822; Bonneville Scientific Contact Allen R. Grahn, (801) 359-0402

Direct Energy Conversion with a Pryoelectric Polymer - DOE Contact Bill Barnett, (301) 353-3097; Chronos Research Laboratories, Inc. Contact Randall B. Olsen, (619) 756-1447

Reduction of Low-Level Radwaste Disposal in Water Clean-up Systems by Use of Magnetite - DOE Contact Scott Hinschberger, (208) 526-1288; Nuclear Consulting Services, Inc. Contact Djordjiji R. Sain, (614) 846-5710

Phase II Projects: (Second Year)

Eddy-Current, Nondestructive Evaluation of Laser-Glazed Metallic Surfaces - DOE Contact Iran Thomas, (301) 353-3426; American Research Corporation of Virginia Contact Russell J. Churchill, (703) 731-0836

Fresnel-Lens Photovoltaic Concentrator Design Innovations -DOE Contact Michael Pulscak, (202) 586-6264; ENTECH, Inc. Contact Mark J. O'Neill, (214) 456-0900

Development of Fe-Nd-B Metal-Matrix Magnets - DOE Contact Iran Thomas, (301) 353-3426; KJS Associates Contact Reinhold M. W. Strnat, (513) 879-0114

Immuniodiagnostic Biosensor Device Based on Conductive Organic Polymers - DOE Contact George Duda, (301) 353-3651; MKM Research/Ohmicron Contact Mark K. Malmros, (609) 737-9050

Titanium Nitride Coating of High-Speed Steel and Carbide Metal Cutting Tools Using Fluid Bed Furnace Technology - DOE Contact Raymond LaSala, (202) 586-4198; Procedyne Corporation Contact Joseph E. Japka, (201) 249-8347

Method and Device for Nondestructive Inspection of Niobium to Improve Superconductivity - DOE Contact David Sutter, (301) 353-5228; Sonoscan, Inc. Contact Lawrence W. Kessler, (312) 766-7088

Wear Resistant Ferrous Metal Matrix Composites for Municipal Solid Waste Processors - DOE Contact Donald Walter, (202) 586-4679; Waste Energy Technology Corporation Contact David B. Spencer, (617) 275-6400

Instrumentation and Facilities

Phase I Projects:

UV Holographic Mirrors with High Diffraction Efficiency - DOE Contact Samuel J. Barish, (301) 353-3054; Physical Optics Corporation Contact Joanna Jannson, (213) 371-3909

Phase II Projects: (First Year)

The Construction of a Soft X-Ray Source Using Transition Radiation for Lithography - DOE Contact Iron Thomas, (301) 353-3426; Adelphi Technology Contact Melvin A. Piestrup, (415) 861-0633

A New Two-Dimensional Position Encoder for Position Emission Tomography (PET) - DOE Contact Gerald Goldstein, (301) 353-3426; Computer Technology and Imaging, Inc. Contact Ronald Nutt, (615) 966-7539

A High Efficiency Helium-3 Neutron Detector - DOE Contact Stanley Whetstone, (301) 353-3613; KMS Fusion, Inc. Contact Timothy M. Henderson, (313) 769-8500

An InP Semiconductor Neutrino Detector - DOE Contact Stanley Whetstone, (301) 353-3613; Radiation Monitoring Devices, Inc. Contact Gerald Entine, (617) 926-1167

Phase II Projects: (Second Year)

Fiber-Optic Track Detector - DOE Contact Stanley Whetstone, (301) 353-3613; Synergistic Detector Designs Contact Arthur H. Rogers, (415) 964-4756

OFFICE OF NUCLEAR ENERGY

	FY 1987
Office of Nuclear Energy - Grand Total	$123,058,000
Office of Advanced Reactor Programs	$ 3,400,000
Division of High Temperature Gas-Cooled Reactors	$ 3,400,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 790,000
Fuel Process Development	790,000
Materials Properties, Behavior, Characterization or Testing	$ 2,610,000
Fuel Materials Development	515,000
Fuel Development and Testing	1,065,000
Graphite Development	65,000
Graphite Development and Testing	390,000
Metals Technology Development	195,000
Structural Materials Development	380,000
Office of Remedial Action and Waste Technology	$ 6,590,000
Division of Waste Treatment Projects	$ 6,590,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 4,100,000
Technical Support to West Valley Demonstration Project	3,100,000
Materials Properties, Behavior, Characterization or Testing	$ 2,090,000
Materials Characterization Center	
Testing of West Valley Formulation Glass	525,000
Test Development and Testing of West Valley Reference Formulation Glass	1,100,000
Process and Product Quality Optimization for West Valley Waste Form	465,000
Device or Component Fabrication, Behavior or Testing	$ 400,000
Special Waste Form Lysimeter for Arid Regions	200,000
Special Waste Form Lysimeter for Humid Regions	200,000

OFFICE OF NUCLEAR ENERGY (Continued)

	FY 1987
Office of Uranium Enrichment	$ 17,570,000
Device or Component Fabrication, Behavior or Testing	$ 8,785,000
Gaseous Diffusion: Barrier Quality	2,150,000
Gaseous Diffusion: Materials and Chemistry Support	2,515,000
Atomic Vapor Laser Isotope Separation (AVLIS)	
AVLIS: Separator Materials	3,220,000
AVLIS: Uranium Processing	900,000
Office of Civilian Reactor Development	$ 28,188,000
Division of Technology Support Programs (LMRs)	$ 28,188,000
Fuels and Core Materials	$ 19,811,000
Materials Properties, Behavior, Characterization or Testing	$ 19,811,000
Fuel Performance Demonstration	4,846,000
Pyroprocess Development	3,000,000
Fuel Safety Experiments and Analysis	2,965,000
Core Design Studies	2,500,000
Fuel Cycle Studies (Metal Fuel)	2,000,000
Design Methodology Development and Applications	3,700,000
Innovative Design Key Features Test	0
Reactor Systems Component Development	800,000
Structural Materials and Design Methodology	$ 8,377,000
Materials Properties, Behavior, Characterization or Testing	$ 8,377,000
Structural Design/Life Assurance Technology	400,000
Modified 9 Cr-1 Mo Steel Design Properties	400,000
Nondestructive Testing Technology for Heat Exchangers	40,000
Nuclear Systems Materials Handbook	72,000
Materials Survey	0
Absorber and Reflector Procurement	0
MOTA Fabrication and Operation	0
Absorber Development	300,000

	FY 1987
Structural Materials and Design Methodology (continued)	
Materials Properties, Behavior, Characterization or Testing (continued)	
FFTF Metal Core	1,400,000
Core Demonstration Experiment (CDE)	2,000,000
FFTF Assembly Operations	3,765,000
Office of Space and Defense Power Systems	$ 2,310,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 1,800,000
Development of Improved Thermoelectric Materials for Space Nuclear Power Systems	550,000
Development of an Improved Process for the Manufacture of DOP-26 Iridium Alloy Blanks	750,000
Carbon Bonded Carbon Fiber Insulation Manufacturing Process Development and Product Characterization	500,000
Device of Component Fabrication, Behavior or Testing	$ 160,000
Nondestructive Testing Methods Development and Application to Thermoelectric Materials and Devices	160,000
Materials Properties, Behavior, Characterization or Testing	$ 350,000
Characterization of State-of-the-Art Thermoelectric Device/Materials and Exploratory Studied of Rare Earth Sulfide Thermoelectric Materials	350,000
Office of Naval Reactors	$ 65,000,000[1]

[1]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 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

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

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

Materials Properties, Behavior, Characterization or Testing

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

- o Development of technology base required to design, qualify, and license fuel systems for near-term steam cycle and advanced process heat HTGRs.
- o Preparation and evaluation of irradiation experiments.
- o Performance of post-irradiation fission product release tests.
- o Development and verification of fuel performance models.

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

- o Fabrication, testing, and evaluation of irradiation experiments; development of post-irradiation examination equipment and methods.
- o Evaluation of fuel performance and development of fission product release mechanism and models.

218. Graphite Development - DOE Contact J. E. Fox, (301) 353-3985; GA Technologies Contact R. Vollman, (619) 455-3310

- o Selection, characterization, and qualification of graphite materials for application in HTRs.
- o Development of failure and design criteria.

219. Graphite Development and Testing - DOE Contact J. E. Fox, (301) 353-3985; ORNL Contact W. P. Eatherly, (615) 574-5220

- o Selection, characterization, and qualification of graphite materials; evaluation of high temperature corrosion resistance and mechanical properties (tensile, creep, fatigue, fracture mechanics, etc.)
- o Fabrication, testing, and evaluation of irradiation experiments; development of high strength, oxidation resistant graphites with high resistance to irradiation damage.

220. Metals Technology Development - DOE Contact J. E. Fox, (301) 353-3985; GA Technologies Contact W. R. Johnson, (619) 455-2905

- o Characterize and qualify the metallic materials selected for application in the near-term steam cycle/cogeneration HTR system.
- o Develop base technology required for selection of alloys for advanced HTR systems.

221. Structural Materials Development - DOE Contact J. E. Fox, (301) 353-3985; ORNL Contact P. L. Rittenhouse, (615) 574-5103

- o Selection, characterization, and qualification of high temperature alloys; evaluation of effects of exposures in simulated environments on mechanical properties (creep, fatigue, fracture mechanics).
- o Development of the database and correlations required for qualification.

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 develop acceptable technologies for the treatment and immobilization of nuclear fuel cycle and special types of radioactive waste.

Materials Preparation, Synthesis, Deposition, Growth or Forming

222. Technical Support to West Valley Demonstration Project - DOE Contact E. Maestas, (716) 942-4314; PNL Contact R. A. Brouns, (509) 376-0731

   o Provide technical assistance in supernatant treatment and borosilicate glass formulation for West Valley Demonstration Project waste.

Materials Properties, Behavior, Characterization or Testing

223. Materials Characterization Center Testing of West Valley Formulation Glass - DOE Contact H. F. Walter, (301) 353-5510; PNL Contact M. Kreiter, (509) 375-2666

   o Evaluate, using various MCC test methods, samples of glass having the expected composition of West Valley borosilicate glass incorporating high-level waste.

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

   o Development of borosilicate glass waste form test methods.

   o Testing of nonradioactive reference West Valley Demonstration Project waste formulation glass.

225. Process and Product Quality Optimization for West Valley Waste Form - DOE Contact E. Maestas, (716) 942-4313; AU Contact L. D. Pye, (607) 871-2432

   o Attempt to maximize optimum conditions for producing acceptable quality borosilicate glass waste form product.

   o Development of methods for control of product quality during routine manufacture of the West Valley Demonstration Project waste form.

Device or Component Fabrication, Behavior or Testing

226. Special Waste Form Lysimeter for Arid Regions - DOE Contact M. W. Shupe, (208) 526-1288; EG&G Idaho Contact D. Halford, (208) 526-2163

- o Conduct waste form leaching tests in a field facility in order to determine typical source terms generated by commercial solidified low-level waste in an arid climate.

- o Identify the chemical and physical processes that control the concentrations of radionuclides in the surrounding soil.
- o Determine methods for representing the source term boundary conditions for transport models.

227. Special Waste Form Lysimeter for Humid Regions - DOE Contact M. W. Shupe, (208) 526-1288; EG&G Idaho Contact D. Halford, (208) 526-2163

- o Conduct waste form leaching tests in a field facility in order to determine typical source terms generated by commercial solidified low-level waste in a humid climate.

- o Identify the chemical and physical processes that control the concentration of radionuclides in the surrounding soil.

- o Compare radionuclide emigration from solidified commercial low-level waste in order to evaluate the benefits of solidification.

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 in an economical, reliable, safe, secure, and environmentally acceptable manner that will assure a reasonable return on 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 more than 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: to stabilize DOE's market share through the issuance of a new more flexible enrichment contract; to reduce prices to competitive levels; to enhance DOE customer services and marketing activities; and to 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 Office of the Deputy Assistant Secretary for Uranium Enrichment, reporting to the Assistant Secretary for Nuclear Energy, is responsible for the management of the uranium enrichment enterprise. This Secretariat is composed of four major 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 1987 were $1549 million.

Materials R&D activities within the Office of Uranium Enrichment are varied and, for the most part, classified Restricted Data. In FY 1987, approximately $8,785,000 million was used in these endeavors and $17,462,000 is planned for FY 1988. The Appendix summarizes these activities for the purpose of this report. The DOE contact is A. P. Litman, (301) 353-5777.

Device or Component Fabrication, Behavior or Testing

228. 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.

229. 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.

230. AVLIS: Separator Materials

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

231. AVLIS: Uranium Processing

- o Design, fabrication and operation of uranium electrolysis cells for AVLIS feed. Bath chemistry, solubility and construction materials studies.
- o 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

Division 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

232. 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.

233. Pyroprocess Development - DOE Contact David L. Hoff, (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.

234. 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.

235. 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.

236. 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-costing furnace, semi-automated pin processor and engineering-scale pyroprocessing equipment for the ultimate commercial fuel cycle facility design and costs.

237. Design Methodology Development and Applications - DOE Contact John Lewellen, (301) 353-3684, FTS 233-3684; ANL Contact D. C. Wade, (312) 972-4858, FTS 972-4858

- o Conduct and develop neutronics, thermal hydraulics, structural and seismic methods and computer codes for metal fuel liquid metal reactors. Evaluate reactor core design, safety analysis methods, and state-of-the-art computer codes.

238. Innovative Design Key Feature Test - DOE Contact C. Chester Bigelow, (301) 353-4299, FTS 233-4299; ANL Contact Dean R. Pedersen, (312) 972-3335, FTS 972-3335

- o The goal of the key features testing program are to validate the design features and analytic design tools, provide design data, verify performance predictions, aid in optimizing designs, and reduce conservatisms for advanced LMR concepts.

239. Reactor Systems Component Development - DOE Contact Eli I. Goodman, (301) 353-2966, FTS 233-2966; ANL Contact Richard W. Weeks, (312) 972-4931, FTS 972-4931

- o Conduct reactor systems component development, testing of high temperature insulation for EM pumps, and thermal hydraulic testing of advanced concepts.

Structural Materials and Design Methodology

Materials, Properties, Behavior, Characterization and Testing

240. 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

- o 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.

241. 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

- o 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.

242. 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

- o 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.

243. Nuclear Systems Materials Handbook - DOE Contact C. Chester Bigelow, (301) 353-4299, FTS 233-4200; ORNL Contact Martin F. Marchbanks, (615) 574-1091, FTS 624-1091

- o 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.

244. Materials Survey - DOE Contact David L. Hoof, (301) 353-2964, FTS 233-2964; ORNL Contact P. Rittenhouse, (615) 574-5103, FTS 233-5103

- o Conduct a broad review of materials with the potential of application to the design and use of out-of-core materials and problems of LMR systems.

245. Absorber and Reflector Procurement - DOE Contact Andrew Van Echo, (301) 353-3930, FTS 233-3930; WHC Contact Robert Leggett, (509) 376-2505, FTS 444-2505

- o Continue procurement of materials and alloys to fabricate FFTF reflector and control rod assemblies with improved reliability, safety, and longer life. Conduct PIE on in-reactor creep behavior and irradiation effects on mechanical properties of ferritic and dispersion-strengthened ferritic (DSF) alloy steels.

246. 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

- o Fabricate MOTA test train and vehicle to irradiate and test materials, HT-9, DSF and others, in a controlled environment in FFTF.

247. 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

- o Conduct, test, and evaluate irradiated absorber experiments to extent the FFTF absorber lifetimes, support Series III control and rod design and update design codes CONRD and CRPBOW.

248. FFTF Metal Core - DOE Contact Andrew Van Echo, (301) 353-3930, FTS 233-3930; WHC Contact Robert D. Leggett, (509) 376-2505, FTS 444-2505

- o 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.

249. 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

- o Continue CDE irradiation in FFTF to extend the fuel lifetime to 1,200 EFPD, conduct TREAT tests and PIE and TREAT tests and pins from ACO-1 and FO-2 lead tests.

250. FFTF Assembly Operations - DOE Contact Robert G. Lange, (301) 353-5338; WHC Contact LeRoi H. Rice, (509) 376-4080, FTS 444-4080

- o Fabricate metal fuel (U-Zr) and mixed oxide (U-Pu-O) fuel pins and fuel assemblies for FFTF and continue support of activities under DOE/PNC Fuels and Materials agreement.

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

251. Development of Improved Thermoelectric Materials for Space Nuclear Power Systems - DOE Contact W. Barnett, (301) 353-3097; General Electric Co., Space Systems Division Contact P. D. Gorsuch, (215) 354-5047

- o 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.

252. Development of an Improved Process for the Manufacture of DOP-26 Iridium Alloy Blank - DOE Contact W. J. Barnett, (301) 353-3097; ORNL Contact R. L. Heestand, (615) 574-4352

- o Development of a consumable arc melt/extrusion route process for the production of DOP-26 iridium alloy sheet and foil.

253. Carbon Bonded Carbon Fiber Insulation Manufacturing Process Development and Product Characterization - DOE Contact W. J. Barnett, (301) 353-3097; ORNL Contact W. P. Eatherly, (615) 574-5220

- o 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

254. Nondestructive Testing Methods Development and Application to Thermoelectric Materials and Devices - DOE Contact W. J. Barnett, (301) 353-3097

- o 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

255. Characterization of State-of-the-Art Thermoelectric Device/ Materials and Exploratory Studies of Rare Earth Sulfide Thermoelectric Materials - DOE Contact W. J. Barnett, (301) 353-3097; Iowa State University Contact B. Beaudry, (515) 294-1366

- o 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 $65 million in FY 1987 including approximately $35 million as the cost for irradiation testing in the Advanced Test Reactor. The Naval Reactors contact is Robert H. Steele, (703) 557-5565.

OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT

	FY 1987
Office of Civilian Radioactive Waste Management - Grand Total	$10,563,000
Office of Storage and Transportation Systems	$ 819,000
Development of Criteria for Nuclear Spent Fuel Storage in Air	733,000
Development of Zircaloy Deformation and Creep Rupture Models for Predicting Cladding Behavior During Interim Dry Storage	67,000
PWR and BWR Spent Fuel Assembly Crud Composition, Characterization, and Effects on Operations	19,000
Office of Civilian Radioactive Waste Management/Nevada Nuclear Waste Storage Investigations Project (OCRWM/NNWSI)	$ 9,419,000
Materials Properties, Behavior, Characterization or Testing	$ 7,999,000
Waste Package Environment	945,000
Waste Form Testing	2,745,000
Metal Barrier Testing	1,321,000
Other Engineered Barrier Waste Package Components	137,000
Integrated Testing	1,298,000
Waste Package - Performance Assessment	638,000
Research on Geochemical Modeling of Radionuclide Interaction with a Fractured Rock Matrix	915,000
Device or Component Fabrication, Behavior or Testing	$ 1,420,000
Waste Package - Design, Fabrication and Prototype Testing	1,168,000
Waste Package Environmental Field Tests	252,000
Sandia National Laboratories: Brittle Fracture Technology Program	$ 325,000
Materials Structure and Composition	$ 50,000
Microstructure Investigations of Nodular Cast Iron	25,000
Composition Investigation of Nodular Cast Iron	25,000

	Page
Sandia National Laboratories: Brittle Fracture Technology Program (continued)	
Materials Properties, Characterization, Behavior or Testing	$ 145,000
Generate Material Property Database for Nodular Cast Iron	140,000
Investigate the Feasibility of Using Depleted Uranium as a Structural Component in Cask Construction	5,000
Instrumentation and Facilities	$ 130,000
Evaluate Current NDE Methods for Applicability to Thick Section Nodular Cast Iron	130,000

OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT

Office of Storage and Transportation Systems

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

256. Development of Criteria for Nuclear Spent Fuel Storage in Air - DOE Contact D. E. Shelor, (202) 586-2836; PNL Contact E. R. Gilbert, (509) 375-2533

- o Testing spent fuel and unclad UO_2 in air to determine the temperature dependence and fuel type dependence of degradation by oxidation.
- o Develop methodology to derive storage criteria to prevent degradation of spent fuel in air by oxidation.

257. Development of Zircaloy Deformation and Creep Rupture Models for Predicting Cladding Behavior During Interim Dry Storage - DOE Contact D. E. Shelor, (202) 586-2836; PNL Contact E. R. Gilbert, (509) 375-2533

- o Analysis of existing data on deformation and creep rupture for nonirradiated Zircaloy.
- o Development of theoretical models for deformation and creep rupture for spent fuel under dry storage conditions.
- o Comparison of models with FRG deformation and creep rupture data on spent fuel and irradiated Zircaloy cladding.
- o Prediction of spent fuel cladding behavior under dry storage conditions.
- o Documentation of models and transfer to computer.

258. PWR and BWR Spent Fuel Assembly Crud Composition, Characterization, and Effects on Operations - DOE Contact D. E. Shelor, (202) 586-2836; 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/Nevada Nuclear Waste Storage Investigations Project (OCRWM/NNWSI)

The primary goal of the OCRWM/NNWSI 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. Many of the activities described in the FY 1986 Annual Report continued into FY 1987 but were terminated in mid-FY 1988.

Materials Properties, Characterization or Testing

259. Waste Package Environment - DOE Contact C. P. Gertz, (702) 295-8920; 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.

260. Waste Form Testing - DOE Contact D.L. Vieth, (702) 295-8920; LLNL Contact David Short, (415) 422-1287

- Perform the testing and evaluation necessasry 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.

261. Metal Barrier Testing - DOE Contact C. P. Gertz, (702) 295-8920; LLNL Contact David Short, (415) 422-1287

- o 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.

- o Six austenitic phase alloys and copper/copper based alloys are being evaluated as candidate materials.

262. Other Engineered Barrier Waste Package Components - DOE Contact C. P. Gertz, (702) 295-8920; LLNL Contact David Short, (415) 422-1287

- o Characterize the properties and behavior of other engineered barrier waste package components that may be present in a repository.

263. Integrated Testing - DOE Contact C. P. Gertz, (702) 295-8920; LLNL Contact David Short, (415) 422-1287

- o Characterize the integrated behavior of the waste form, barrier materials, and surrounding environment.

264. Waste Package - Performance Assessment - DOE Contact C. P. Gertz, (702) 295-8920; LLNL Contact David Short, (415) 422-1287

- o Provide a quantitative prediction of long-term waste package performance.

265. Research on Geochemical Modeling of Radionuclide Interaction with a Fractured Rock Matrix - DOE Contact C. P. Gertz, (702) 295-8920; LLNL Contact David Short, (415) 422-1287

- o 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.

266. Waste Package - Design, Fabrication and Prototype Testing - DOE Contact C. P. Gertz, (702) 295-8920; LLNL Contact David Short, (415) 422-1287

- o Develop, analyze, fabricate, and test waste package designs that incorporate qualified materials and that are fully compatible with the repository design.

- o 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.

267. Waste Package Environmental Field Tests - DOE Contact C. P. Gertz, (702) 295-8920; LLNL Contact David Short, (415) 422-1287

- o Develop and conduct field experiments designed to determine and evaluate the thermal, mechanical, thermomechanical, hydrothermal and chemical phenomena for welded tuff.
- o 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

268. Microstructure Investigations of Nodular Cast Iron - DOE Contact F. F a l c i , (301) 353-3595; SNL Contact K. B. Sorenson, (505) 844-5360

- o Investigation of the effect of microstructure on material properties.
- o Study of the effect of graphite nodule size and spacing on fracture toughness.

269. Composition Investigation of Nodular Cast Iron - DOE Contact F. Falci, (301) 353-3595; SNL Contact K. B. Sorenson, (505) 844-5360

- o Investigation of the effect of material composition on material properties.
- o Study of the effect of material composition on fracture toughness and tensile properties.

Materials Properties, Behavior, Characterization, or Testing

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

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

271. 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

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

Instrumentation and Facilities

272. 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

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

OFFICE OF DEFENSE PROGRAMS

	FY 1987
Office of Defense Programs - Grand Total	$48,806,500
Office of Waste Research and Development	$ 8,500
Materials Properties, Behavior, Characterization or Testing	$ 8,500
Waste Form Qualification	4,000
Immobilization/Volume Reduction/In-place Stabilization	4,500
Office of Weapons, Research, Development and Testing	$48,798,000
Inertial Fusion Division	$ 3,000,000
Fusion Research Branch	$ 3,000,000
Device or Component Fabrication, Behavior or Testing	$ 3,000,000
Target Fabrication	1,500,000
Laser Materials and Optical Components	1,500,000
Weapons Research Division	$45,798,000
Sandia National Laboratories - Albuquerque	$20,370,000
Solid State Sciences Directorate, 1100	$ 7,420,000
Ion Implantation and Radiation Physics Research Department, 1110	$ 1,920,000
Materials Properties, Behavior, Characterization or Testing	$ 1,920,000
Ion Implantation Studies for Friction and Wear	500,000
Silicon-Based Radiation Hardened Microelectronics	770,000
New Concepts in Microsensors	650,000
Laser and Chemical Physics Department, 1120	$ 750,000
Materials Properties, Behavior, Characterization or Testing	$ 750,000
Tungsten Deposition	350,000
Laser-Based Aluminum Etching	200,000
Gas Phase Studies	200,000

OFFICE OF DEFENSE PROGRAMS (Continued)

	FY 1987
Condensed Matter and Surface Science Department, 1130	$ 1,250,000
Materials Properties, Behavior, Characterization or Testing	$ 1,250,000
Shock Chemistry	500,000
Initiation of Granular Explosives	350,000
Surface Science	400,000
Compound Semiconductor and Device Research Department, 1140	$ 2,000,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 2,000,000
Materials Growth by Molecular Beam Epitaxy (MBE)	500,000
Materials Growth by MOCVD	400,000
Strained Layer Superlattices for IR Detectors	300,000
Novel Processing Technology for Semiconductor Technologies	500,000
Materials Processing for Sensors	300,000
Solid State Research Department, 1150	$ 1,500,000
Materials Properties, Behavior, Characterization or Testing	$ 1,500,000
Superconductivity	300,000
Semiconductors	300,000
Surface Science	450,000
Disordered Materials	450,000
Organic and Electronic Materials Department, 1810	$ 1,525,000
Chemistry of Organic Materials Division, 1811	$ 550,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 400,000
Dyed Antireflective Photoresist Material	150,000
Sulfonated Aromatic Polysulfones	100,000
Carbon Foams	150,000
Materials Properties, Behavior, Characterization or Testing	$ 150,000
Radiation Hardened Dielectrics	150,000

	FY 1987
Physical Chemistry and Mechanical Properties of Polymers Division, 1812	$ 585,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 305,000
Polysilane, Photoresists, Photoconductors, and Non-Charring Dielectrics	125,000
Mechanistic Studies of Polysilane Synthesis	70,000
Chemistry of Plasma Etching and Deposition Processes	110,000
Materials Structure and Composition	$ 280,000
Materials Structure, Dynamics, and Properties Studies by Multinuclear Pulsed NMR Spectroscopy	70,000
Studies of Adhesion at the Molecular Level by Surface Science Techniques	210,000
Physical Properties of Polymers Division, 1813	$ 390,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 300,000
Microporous Foam Development	150,000
Development of Removable Encapsulants	150,000
Materials Properties, Behavior, Characterization or Testing	$ 90,000
Mechanical Properties of Encapsulants	20,000
The Strength of Kevlar Narrow Fabrics	70,000
Electronic Property Materials Division, 1815	$ 300,000
Materials Properties, Behavior, Characterization or Testing	$ 300,000
High Electric Field Varistors	100,000
Hydrogen Effects in Silicon	100,000
Rapid Thermal Processing of Gate Oxides	100,000

OFFICE OF DEFENSE PROGRAMS (Continued)

	FY 1987
Materials Characterization Department, 1820	$ 1,140,000
Analytical Chemistry Division, 1821	$ 200,000
Instrumentation and Facilities	$ 200,000
Development of Automated Methods for Chemical Analysis	200,000
Electron Optics and X-Ray Analysis Division, 1822	$ 240,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 40,000
Thermomechanical Treatment of U Alloys	40,000
Instrumentation and Facilities	$ 200,000
Advanced Methods for Electron Optical X-Ray, and Image Analysis	200,000
Surface Chemistry and Analysis Division, 1823	$ 700,000
Instrumentation and Facilities	$ 700,000
Advanced Methods for Surface and Optical Analysis	700,000
Thermophysical Properties Division, 1824	$ 180,000
Instrumentation and Facilities	$ 180,000
Design and Fabrication of a Multi-Source X-Ray Gauge	80,000
Infrared Reflectometer Development	50,000
Flash Thermal Diffusivity Measurements on Multilayer Samples	50,000

	FY 1987
Metallurgy Department, 1830	$ 3,355,000
Coating Technology Division, 1831	$ 890,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 450,000
Plasma Deposition of Amorphous Metal Alloys	70,000
Electrophoretically-Deposited Coatings	150,000
Near-Net-Shape Processing of Nickel-Based Alloys	150,000
High Temperature Semiconductors	80,000
Materials Properties, Behavior, Characterization or Testing	$ 240,000
Optical Diagnostics for Materials Processing	240,000
Device or Component Fabrication, Behavior or Testing	$ 200,000
Development of Materials for Magnetic Fusion Reactors	200,000
Physical Metallurgy Division, 1832	$ 1,040,000
Materials Properties, Behavior, Characterization or Testing	$ 1,040,000
Toughness of Ductile Alloys	330,000
Properties of Ni-B Alloys	50,000
Analytical Electron Microscopy of Engineering Alloys	130,000
Friction and Wear of Modified Surfaces	230,000
Alloy Deformation Response and Constitutive Modeling	300,000
Process Metallurgy Division, 1833	$ 955,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 120,000
Vacuum Arc Remelting	60,000
Investment Costing	60,000

	FY 1987
Process Metallurgy Division, 1833 (continued)	
Device or Component Fabrication, Behavior or Testing	$ 835,000
Aluminum Laser Welding	40,000
Copper Brazing to Carbon	20,000
Dissimilar Metal Welds	200,000
Welding of Nickel-Based Alloys	225,000
Plasma Arc Welding	175,000
Laser Welding	175,000
Surface and Interface Technology Division, 1834	$ 470,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 80,000
Deposition of Amorphous Materials with a Dual-Beam Ion System	80,000
Materials Properties, Behavior, Characterization or Testing	$ 35,000
Modification of Mechanical Properties by Ion Implantation	35,000
Device or Component Fabrication, Behavior or Testing	$ 265,000
Development of Materials for Magnetic Fusion Reactors	200,000
Plasma Cleaning Studies	65,000
Instrumentation and Facilities	$ 90,000
Ion Beam Reactive Deposition System	50,000
In-Situ Friction, Wear, and Electrical Contact Resistance System	40,000
Chemistry and Ceramics Department, 1840	$ 6,930,000
Ceramics Development Division, 1845	$ 3,280,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 2,600,000
Ceramic Processing	2,600,000

OFFICE OF DEFENSE PROGRAMS (Continued)

	FY 1987
Chemistry and Ceramics Department, 1840 (continued)	
Ceramics Development Division, 1845 (continued)	
Materials Properties, Behavior, Characterization or Testing	$ 680,000
Fracture of Ceramics	680,000
Inorganic Materials Chemistry Division, 1846	$ 2,500,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 2,500,000
Glass and Glass-Ceramic Development	2,500,000
Corrosion Division, 1847	$ 1,150,000
Materials Properties, Behavior, Characterization or Testing	$ 1,150,000
Corrosion	1,150,000
Sandia National Laboratories - Livermore	$ 3,375,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 1,100,000
Powder Metallurgy	200,000
Advanced Electrodeposition Studies	100,000
Metal Forming	200,000
Advanced Organic Materials	200,000
Particulate Technology	50,000
Tritium Getter Technology	50,000
Molded Desiccant Foam	100,000
Plasma Processing	200,000
Materials Properties, Behavior, Characterization or Testing	$ 1,725,000
Helium-Induced 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	75,000
Tritium-Metal Interaction	350,000
Measurement of Multilayer Thin Film Structures	50,000

OFFICE OF DEFENSE PROGRAMS (Continued)

	FY 1987
Lawrence Livermore National Laboratory	$ 6,722,000
Instrumentation and Facilities	$ 550,000
New Spectroscopy	50,000
Tritium Facility Upgrade for Materials Characterization and Testing	500,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 1,777,000
Ion Beam Modification of Materials	230,000
Formation of Metastable Surface Alloys	180,000
Synthesis Project (Explosives)	120,000
Synthesis and Reactivity of Transition Metal Fluorocarbon Complexes	104,000
Advanced Ceramics Synthesis and Processing	157,000
Sputtering (Plutonium Alloys)	241,000
Kinetic Models (Hydrogen, Methane Oxidation)	15,000
Investigation of Multifilamentary NBN Superconductors	180,000
Grinding Glass in the Ductile Regime	140,000
Basic Study of the Single-Point Cutting Process	410,000
Materials Structure and Composition	$ 319,000
Theory of Polar Fluid Structure and Dynamics	49,000
Structures of Actinide-Hydrogen Compounds and Solutions at High Pressures	150,000
Actinide Thermochemistry	120,000
Materials Properties, Behavior, Characterization or Testing	$ 3,111,000
Influence of Cooling Rate on the Microstructure of Duplex Austenitic-Ferritic Stainless Steel	65,000
Role of Interfaces in Metallic-LayeredThin Films	70,000
Capillary Structures (in Foams)	190,000
Pre-transformation Behavior in Alloys	90,000
Polymer Modeling	100,000
Nuclear Spin Polarization	200,000
Plutonium Martensic Transformation Plasticity	100,000
Theory of Deflagration at High Pressures	140,000
High-Pressure High-Temperature Raman Spectroscopy of Energetic Materials	130,000
Hot Spot Microdynamics/High Explosives R&D	140,000

	FY 1987
Lawrence Livermore National Laboratory (continued)	
Roles of Post-Yield Properties and Physical Aging on the Fracture of Highly-Crosslinked Networks	90,000
Studies of Material Properties of HighTemperatures	72,000
Catalytic Properties of Actinide Compounds	174,000
Computer Molecular Dynamics	100,000
Dislocation Microstructure of Aluminum Deformed to Large Steady-State CreepStrains	140,000
In Situ Reversed Deformation Experiments	20,000
Hyperfine Studies and Radiation Effects	110,000
Actinide Phase Diagrams	30,000
Modeling and Experimental Measurement of Residual Stress	170,000
Numerical Modeling of Crack Growth and Plastic Deformation Material Model	192,000
Study of Residual Stress for Epoxy-Resin Composites	305,000
High Temperature Metal Alloy Radiant Property Measurements in Conjunction withAdvanced Surface Spectroscopy	80,000
Evaluation of Thermo-Plastic Material Model	126,000
Strength of Composite Materials	50,000
Integrated Engineering Applications Software (IDEAS) Project	100,000
High Strain Rate Tensile Testing	127,000
Instrumentation and Facilities	$ 1,515,000
Shockwave Fiber Optics Probe	150,000
Laser Induced Chemistry	238,000
Synchrotron Radiation Studies	345,000
Scanning Tunneling Microscope	150,000
Study of Solid Deformation Processes Using a Novel Calorimetric Technique	80,000
Scanning Tunneling Microscopy (STM) as a Detector	90,000
Research in Quantitative Ultrasonic Nondestructive Evaluation	247,000
Research in Computerized Tomographic Imaging	100,000
Contour Measurement with Capacitance Sensor	115,000
Tritium Facility Upgrade	(1,500,000)[1]
Dedication, Weapons Materials Research and Development Facility	(28,300,000)[1]

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

OFFICE OF DEFENSE PROGRAMS (Continued)

	FY 1987
Los Alamos National Laboratory	$15,331,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$ 8,561,000
Actinide Alloy Development	1,350,000
Plutonium Oxide Reduction	150,000
Plutonium Oxide Removal	150,000
Replacement Noble-Metal Alloys	150,000
Powder Preparation by Plasma Chemical Synthesis	270,000
Synthesis of SiC Whisker-$MoSi_2$ Composites for Elevated Temperature Applications	50,000
Whisker Reinforced Structural Ceramics	225,000
Low Density Metal "Smokes"	50,000
Ion-Beam Implantation	200,000
Electroplating Low-Atomic-Number Materials	120,000
Three New Conducting Polymers	50,000
New Highly Conductive Doped Polyacetylene	200,000
Liquid-Crystal Polymer Development	200,000
Surface-Property-Modified Plastic Components	130,000
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	866,000
Tritiated Materials	590,000
Salt Fabrication	395,000
Slip Casting of Ceramics	150,000
Whisker Growth Technology	120,000
New Hot Pressing Technology	300,000
Glass and Ceramic Coatings	10,000
Cold Pressing, Cold Isostatic Pressing, and Sintering	175,000
Plasma-Flame Spraying Technology	185,000
Rapid Solidification Technology	200,000
Superplastic Forming	150,000
Microwave Sintering/Processing	200,000
Materials Structure or Composition	$ 1,360,000
Actinide Surface Properties	700,000
Neutron Diffraction of Pu and Pu Alloys	160,000
Surface Studies	500,000

	FY 1987
Los Alamos National Laboratory (continued)	
Materials Properties, Behavior, Characterization or Testing	$ 2,770,000
Mechanical Properties of Uranium	60,000
High Strain Rate Testing	200,000
Mechanical Properties of Plutonium and Its Alloys	450,000
Phase Transformation in Pu and Pu Alloys	450,000
Isobaric Expansion of Actinides	300,000
Plutonium Shock Deformation	350,000
Dielectric Loss Measurements in Ceramics	200,000
Plutonium Doping for Self-Irradiation Damage in Ceramics	220,000
Nondestructive Evaluation	450,000
Powder Characterization	90,000
Device or Component Fabrication, Behavior or Testing	$ 2,640,000
Radiochemistry Detector Coatings	250,000
Target Fabrication	1,500,000
Filament Winder	150,000
Polymeric Laser Rods	100,000
High Energy Density Joining Process Development	410,000
Arc Welding Process Development	150,000
Ceramic Technology	60,000
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 wepons 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, while continuing progress toward development of final waste disposal strategies at Hanford and 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. Alternatives evaluated in the Hanford Defense Waste ES include: geological

disposal, in-place stabilization and disposal, continued storage, and a reference alternative which incorporates elements of the first two disposal alternatives.

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

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

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

274. Immobilization/Volume Reduction/In-place Stabilization - DOE Contact Ken Chacey, (301) 353-4970 and Marv Furman, (509) 376-7062; Westinghouse Hanford Company Contact Dave Turner, (509) 376-8365

   o Process flowsheets for treatment of HLW streams at Richland and Idaho.

Office of Weapons Research, Development and Testing

Inertial Fusion Division

Fusion Research Branch

Device or Component Fabrication, Bahavior or Testing

275. Target Fabrication - DOE Contact Carl B. Hilland, (301) 353-3687; LANL Contact Dave Duchane, (505) 667-9893; KMS Fusion, Inc. Contact Timothy Henderson, (313) 769-8500, ext. 302; LLNL Contact W. Hatcher, (415) 422-1100

   o Targets filled with dueterim-tritium gas are irradiated with a laser or particle beam to produce a fusion burn.

276. Laser Materials and Optical Components - DOE Contact Carl B. Hilland, (301) 353-3687; LLNL Contact E. Storm, (415) 422-0400; KMS Fusion, Inc. Contact Jon Larsen, (313) 769-8500; University of Rochester Contact R. McCrory, (716) 275-5286

   o Development of Nd:glass amplifier discs and optical components for kilojoule-class laser systems.

Division of Weapons Research

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 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, 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

277. Ion Implantation Studies for Friction and Wear - DOE Contact A. E. Evans, (301) 353-3098; SNL Contacts D. M. Follstaedt, (505) 844-2102; S. M. Myers, (505) 844-6076; 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.

278. 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; 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.

279. 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

- o New concepts in microsensors are being developed for a variety of stimuli, including radiation, magnetic fields, chemical species and viscosity, using principles of semiconductor device operation and fabrication, surface acoustic wave propagation, and optical properties of solids.

Laser and Chemical Physics 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

280. Tungsten Deposition - DOE Contact A. E. Evans, (301) 353-3098, FTS 233-3098; SNL Contact Ken Greenberg, (505) 844-1243

- o Deposition of tungsten on a variety of materials using an abnormal glow discharge. Deposited thin films adhere well to all materials studied and have IC-device-quality conductivity.

281. Laser-Based Aluminum Etching - DOE Contact A. E. Evans, (301) 353-3098, FTS 233-3098; SNL Contact Wayne Johnson, (505) 844-8782

- o Developed a laser-based system to etch aluminum interconnects on high-density ICs without damaging nearby circuit elements and to deposit new networks of polysilicon and/or tungsten interconnects on ICs. System is useful for IC design error corrections and customization.

282. Gas Phase Studies - DOE Contact A. E. Evans, (301) 353-3098, FTS 233-3098; SNL Contact Ken Greenberg, (505) 844-1243

- o Gas phase studies of species densities in plasma etch reactors for the purpose of model validation.

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; and (2) 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, modification and control of surface properties, the early stages of oxidation and corrosion, adhesion of

metals to polymers, and the mechanism of operation of metal-insulator-semiconductor (MIS) electronic gas sensors.

Materials Properties, Behavior, Characterization, or Testing

283. Shock 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.

- Studies of the mechanisms and materials parameters which determine the electrical output of shock-activated thermal batteries are being carried out.

- A revolutionary time-resolved dynamic stress gauge using the piezoelectric polymer PVF_2 is being developed for laboratory, field testing and component diagnostics application. The mechanism for the operation of the gauge is being investigated.

284. Initiation of Granular Explosives - DOE Contact A. E. Evans, (301) 353-3098; Sandia Contact R. E. Setchell, (505) 844-5459

- Experimental and theoretical efforts are being directed at developing a fundamental understanding of the mechanisms involved in the shock wave initiation and growth to detonation of heterogeneous granular explosives.

- Materials of current interest include hexanitrostilbene and PBX 9404.

285. Surface Science - DOE Contact A. E. Evans, (301) 353-3098; SNLA Contact D. W. Goodman, (505) 844-5435

- 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, 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.

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, semiconductor physics (theory and experiment) and materials science in a coordinated effort. 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 switching.

Materials Preparation, Synthesis, Deposition, Growth or Forming

286. Materials Growth by Molecular Beam Epitaxy (MBE) - DOE Contact A. E. Evans, (301) 353-3098, FTS 233-3098; Sandia Contact L. R. Dawson, (505) 846-3451

- o Growth of AlGaAs/GaAs, InAsSb/InAs and InGaAs/GaAs strained layer superlattice (SLS) and strained quantum well (SQW) structures for electronic and optoelectronic applications.

287. Materials Growth by MOCVD - DOE Contact A. E. Evans, (301) 353-3098, FTS 233-3098; Sandia Contact R. M. Biefield, (505) 844-1556

- o 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 8-12um wavelength region.

288. Strained Layer Superlattices for IR Detectors - DOE Contact A. E. Evans, (301) 353-3098, FTS 233-3098; Sandia Contact P. S. Peercy, (505) 844-4309

- o 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 um range. These IR materials are being grown by both MBE and MOCVD techniques.

289. 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.

- o This program involves studies of new technologies for formation of diffusion barriers for improved epitaxial growth, novel metallurgies for Shottky barrier and Ohmic contact formation, and development of new metallurgical techniques for deposition of reactive alloys.

290. Materials Processing for Sensors - DOE Contact A. E. Evans, (301) 353-3098, FTS 233-3098; Sandia Contacts D. S. Ginley, (505) 844-8863 and R. J. Baughman, (505) 844-6337

- o Growth of high quality semimagnetic semiconductors for magnetic field sensors, development of processing technologies for fabricating fiber-optic based strain and chemical sensors, and thin dielectric and organic films for chemical sensors.

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.

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

- o Transport measurements to access the fundamental factors which limit the performance of ceramic superconductors.
- o Heat capacity studies to elucidate the mechanism of superconductivity.
- o Development of theoretical models of high temperature superconductivity.
- o Development of new processing technologies for ceramic superconductors.

292. 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

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

293. Surface Science - DOE Contact A. E. Evans, (301) 353-3098, FTS 233-3098; Sandia Contact D. R. Jennison, (505) 844-5909

- o Detection and analysis of neutral atoms and molecules desorbed from surfaces.
- o Theory of electronically stimulated desorption.
- o Theory of surface electronic structure.
- o Hydrogen in metals.

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

- o Application of polymeric synthesis routes to ceramic materials.

- o Gas phase materials processing.
- o Gelation in foam precursors and sol-gel glasses.
- o 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

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

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

296. 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

   - o Sulfonated aromatic polysulfones have been developed as stable ionic battery membranes and are now in testing in prototype batteries.

297. Carbon Foams - DOE Contact A. E. Evans, (301) 353-3098, FTS 233-3098; Sandia Contract Roger Clough, (505) 844-3492

- o Development of a new type of microporous carbon foam.
- o High-temperature carbonization of polymer foams.
- o Application as target pellets for fusion experiments.

Materials Properties, Behavior, Characterization or Testing

298. Radiation Hardened Dielectrics - DOE Contact A. E. Evans, (301) 353-3098; Sandia Contacts R. L. Clough, (505) 844-3492, S. R. Kurtz, (505) 844-5436 and C. Arnold, (505) 844-8728

- o Polymer dielectrics have been developed that display a minimum radiation-induced conductivity (RIC).
- o 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.

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 Properties, Behavior, Characterization or Testing

299. Polysilane Photoresists, Photoconductors, and Non-Charring Dielectrics - DOE Contact A. E. Evans, (301) 353-3098; Sandia Contact J. M. Zeigler, (505) 844-0324

- o Alkyl-substituted polysilanes and related materials are currently being developed as improved self-developing photoresists for use in microelectronic circuit manufacture.
- o Different polysilane structures are under investigation as high temperature, non-charring dielectrics.

Materials Preparation, Synthesis, Deposition, Growth or Forming

300. 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) 844-8547, R. G. Kepler, (505) 844-7520, K. Schweizer, (505) 846-7536

- o Synthesis of improved polysilane self-developing photoresists.
- o For use in simplified microelectronic circuit on PC board manufacture.
- o Emphasis on understanding fundamental photochemistry and photophysics.

301. 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

- o Study of chemistry of glow discharge plasmas using molecular beam and laser techniques.
- o Application to selectivity in etching for microelectronic fabrication.
- o Also applied to production of solar cell materials and their carbon/hydrogen films.

Materials Structure and Composition

302. Materials Structure, Dynamics, and Property Studies by Multinuclear Pulsed NMR Spectroscopy - DOE Contact A. E. Evans, (301) 353-3098; FTS 233-3098; SNLA Contacts J. M. Zeigler, (505) 844-0324, and R. H. Assink, (505) 844-6372

- o Use of ^{13}C and ^{1}H spectroscopy of precursor liquids for encapsulants and foams.
- o Analysis of chemical structures of new explosives.
- o Study of degradation pathways and products in organic materials.
- o Imaging techniques for liquid and solid foams.

303. Studies of Adhesion at the Molecular Level by Surface Science Techniques DOE Contact A. E. Evans, (301) 353-3098; FTS 233-3098; SNLA Contacts J. M. Zeigler, (505) 844-0324 and J. A. Kelber, (505) 844-5436

- o Study of mechanism of polymer-polymer and polymer-metal adhesion using ESD, PSD, XPS, and Auger spectroscopies.
- o Relevant to problem of delamination of printed circuit boards.

- 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

304. Microporous Foam Development - DOE Contact A. E. Evans, (301) 353-3098; Sandia Contacts J. H. Aubert, (505) 844-5604 or P. B. Rand, (505) 844-7953

- We have discovered a new way to produce carbon foams of low density and small cell size. The process involves the production of polyacrylonitrile (PAM) by a solution-gelation technique followed by CO_2 solvent extraction. The resulting PAN foam is then carbonized by exposure to elevated temperatures. These foams are of potential use in several weapons applications.

305. Development of Removable Encapsulants - DOE Contact A. E. Evans, (301) 353-3098; FTS 233-3098; SNLA 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

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

- The bulk modulus of polymeric encapsulants is essential for predicting internal stresses from thermal cycling. Up to now, only estimated values of the bulk modulus have been used since it is a difficult quantity to evaluate. Recently, we have demonstrated that the bulk modulus can be obtained by using the tri-axial testing facility. Preliminary measurements indicate significant departures from previous estimates of the bulk modulus for polymeric encapsulants.

307. The Strength of Kevlar Narrow Fabrics - DOE Contact A. E. Evans, (301) 353-3098; Sandia Contact R. H. Ericksen, (505) 844-8333

- The influence of variables important for parachute applications of Kevlar was studied and tests to determine the fabric deformation mechanisms are underway.

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

308. High Electric Field Varistors - DOE Contact A. E. Evans, (301) 353-3098; SNL Contacts R. G. Kepler, (505) 844-7520 and G. E. Pike, (505) 844-7562

- ZnO varistors are being prepared from fine powders precipitated from chemical solutions, yielding switching electric fields from 30 to 100 kV/cm.

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

- Measurements mode 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.

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

- Characterization of 20 nm layers of SiO_2.
- Capacitance-voltage techniques to study X-ray radiation defects.
- Fowler-Nordheim current measurements for dielectric breakdown measurements.

Materials Characterization Department, 1820

Department 1820 performs chemical, physical, and thermophysical analyses of materials in support of weapons and energy programs throughout the Laboratories. The department also has the responsibility for the development of advanced analytical techniques to meet existing or anticipated needs. Consulting and process reviews are other important functions of the department.

Analytical Chemistry Division, 1821

The Analytical Chemistry Division, 1821, is responsible for performing chemical analyses in support of weapon and energy programs at Sandia. The division is equipped to analyze a variety of samples such as gases, polymers, liquids, solutions, solids, organics, inorganics, glasses, alloys, ceramics, and geological materials. Analyses are performed by a variety of techniques using absorption and emission spectroscopy, gas chromatography, gas chromatography/mass spectrometry, ion chromatography, neutron activation analysis, electrochemistry, combustion, and classical methods of chemical analysis.

Instrumentation and Facilities

311. Development of Automated Methods for Chemical Analysis - DOE Contact A. E. Evans, (301) 353-3912; Sandia Contact S. H. Weissman, (505) 846-0820

   - New, highly automated methods and software for artificial intelligence for search/match routines are being developed for the identification and quantitative analysis of a broad range of materials.

Electron Optics and X-Ray Analysis Division, 1822

Materials Preparation, Synthesis, Deposition, Growth or Forming

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

   - Thermomechanical treatments of uranium alloys as a means of improving properties and ease of processing. Methods have been found for significantly reducing the quench severity required in U-Ti alloys, and for simultaneously increasing yield strength and ductility in U-0.75%Ti.

Instrumentation and Facilities

313. 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 to improve resolution, accuracy, and efficiency. Improvements in in situ electronic

diffraction analysis are a recent accomplishment. A new system in advanced centralized image analysis interfaces with several optical and electron optical instruments.

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

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

- Recent accomplishments include improvements in the multivariate least squares software package for quantitative Fourier transform infrared spectroscopy and improved software for automated data acquisition and reduction for the laser Raman microprobe system. Also, a combined gas chromatography/Fourier transform infrared spectrometer has been constructed for use in reaction studies on organic materials.

Thermophysical Properties Division, 1824

The mission of Division 1824 is the measurement and analysis of thermal and optical properties of engineering materials in support of Sandia's weapons and energy programs. Capabilities include thermal conductivity and diffusivity measurements, calorimetry, densitometry, dilatometry, optical reflectance, optical emittance, and ellipsometry.

Instrumentation and Facilities

315. Design and Fabrication of a Multi-Source X-Ray Gauge - DOE Contact A. E. Evans, (301) 353-3098; Sandia Contact W. D. Drotning, (505) 844-7934

- A new system is being constructed based on attenuation of monochromatic gamma rays from a radioactive isotopic source to analyze special materials for a strategic defense initiative program. This is a nondestructive method that yields quantitative elemental analysis. More complex systems using multi-isotopic sources are being constructed and tested for complex materials.

316. Infrared Reflectometer Development - DOE Contact A. E. Evans, (301) 353-3098; Sandia Contact H. L. Tardy, (505) 846-6548

- o A new infrared reflectometer has been designed and construction is almost completed. This system will be used in support of a strategic defense initiative program and for reentry systems.

317. Flash Thermal Diffusivity Measurements of Multilayer Samples - DOE Contact A. E. Evans, (301) 353-3098; FTS 233-3098; SNLA Contact W. F. Chambers, (505) 844-6163

- o Development of advanced methods of automated electron and X-ray instrumental analysis to improve resolution, accuracy, and efficiency.
- o Construction of a microstructural image analysis system.
- o Use of automated analytical electron microscope.

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.

Coating Technology Division, 1831

The Coating Technology Division conducts basic and applied research in two areas: (1) coatings and (2) optical diagnostics for processes. Coating research is currently being conducted in the areas of plasma deposition, chemical vapor deposition, electrophoretic deposition, and sputtering. In addition, this division provides support for design engineers in the specification of processes and transfer of technology involving coatings.

Materials Preparation, Synthesis, Deposition, Growth or Forming

318. Plasma Deposition of Amorphous Metal Alloys - DOE Contact A. E. Evans, (301) 353-3098; Sandia Contact A. K. Hays, (505) 844-9996

- o Amorphous metal alloys composed of Ni, P and C have been produced by decomposing $Ni(CO)_4$ and PH_3. The time-temperature transformation and electron transport properties of these materials have been studied. The diffusion of H_2 through these films is under investigation.

319. Electrophoretically-Deposited Coatings - DOE Contact A. E. Evans, (301) 353-3099; Sandia Contact D. J. Sharp, (505) 844-8604

- Electrophoretic deposition technology is being developed for three applications: (1) to apply electrically insulating coatings on large, irregularly shaped objects; (2) to apply IEMP hardeners on electronic component packages; and (3) to apply nuclear fuel (UO_2) to metal substrates to produce unique energy sources.

320. Near-Net-Shape Processing of Nickel-Based Alloys - DOE Contact A. E. Evans, (301) 353-3098; Sandia Contact A. W. Mullendore, (505) 844-6833

- High hardness Ni-B alloys have been produced from the chemical vapor deposition of $Ni(CO)_4$ and B_2H_6. Injection moldings for fiber optic connectors have been produced to near-net-shape.

321. High Temperature Semiconductors - DOE Contact A. E. Evans, (301) 353-3098; Sandia Contact A. W. Mullendore, (505) 844-6833

- Single crystals of boron carbide grown using a chemical vapor deposition process. These specimens have been studied (i.e., electron transport properties have been measured) to determine the applicability of boron-based compounds for use as high temperature semiconductors.

Materials Properties, Behavior, Characterization or Testing

322. Optical Diagnostics for Materials Processing - DOE Contact A. E. Evans, (301) 353-3098; Sandia Contact H. C. Peebles, (505) 846-3454

- Emission spectroscopy has been used to investigate laser light absorption during plume formation that occurs during a laser welding process. Similar techniques are being developed to obtain species concentration and temperature profiles in a vacuum arc remelter.

Device or Component Fabrication, Behavior or Testing

323. 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 developed to deposit ceramic/metal coatings. The coatings are being considered for first wall surfaces or for graded thermal expansion layers.

Physical Metallurgy Division, 1832

The mission of the Physical Metallurgy Division 1832 is to provide the characterization and understanding of the 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 capabilities are part of this division, and extensive use is made of the analytical capabilities at Sandia.

Materials Properties, Behavior, Characterization or Testing

324. 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

   o Elastic-plastic fracture toughness (J_{Ic}) is being studied to determine if it can be used as the basis for structural design. This includes a study of both the experimental techniques used to measure toughness at high loading rates and the application of the parameter in computer code calculations. The correlation between microstructure and toughness is also examined. Current emphasis is on the study of ductile cast iron for nuclear material shipping casks.

325. Properties of Ni-B Alloys - DOE Contact A. E. Evans, (301) 353-3098; Sandia Contact A. N. Campbell, (505) 844-7452

   o The mechanical response of a Ni-B alloys produced by chemical vapor deposition is being characterized. Microstructural examination is being performed to explain and model the deformation processes for this material.

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

   o 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.

327. 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

   o 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.

328. 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

- o 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.

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

329. Vacuum Arc Remelting - DOE Contact A. E. Evans, (301) 353-3098; Sandia Contact F. J. Zanner, (505) 844-7073

- o 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

330. Aluminum Laser Welding - DOE Contact A. E. Evans, (301) 353-3098; Sandia Contact M. J. Cieslak, (505) 846-7500

- o 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.

331. Copper Brazing to Carbon - DOE Contact A. E. Evans, (301) 353-3098; Sandia Contact F. M. Hosking, (505) 844-8401

- o Solid state welding and solid-liquid interdiffusion techniques have been evaluated for joining copper flex circuits in the 373-450°K range. High quality welds were produced with the use of indium and indium-silver alloy interlayers.

332. Dissimilar Metal Welds - DOE Contact A. E. Evans, (301) 353-3098; Sandia Contacts M. J. Cieslak, (505) 846-7500 and G. A. Knorovsky, (505) 844-1109

- o Fusion welding procedures for dissimilar-metal welds are being developed with emphasis on avoidance of hot-cracking. A Nb(C,N) phase was found to form in the weld metal of 15-5 PH/HP 9-4-20 welds during the terminal transient stage of solidification and is the cause of hot-cracking.

333. 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

- o 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.

334. 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

- o 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.

335. Laser Welding - DOE Contact A. E. Evans, (301) 353-3098; Sandia Contact J . L. Jellison, (505) 844-6397

- o Both pulsed and CW laser welding is being developed for application to component closures. Mechanisms of beam-plume interactions are being evaluated for various material-process combinations. These results, along with a new understanding of the roles of reflectivity and convention, are being incorporated into models of the processes. Thermal blooming of the beam as it passes through the plume and weld pool convection are under study.

Surface and Interface Technology Division, 1834

The Surface Metallurgy Division 1834 is concerned with the influence of surface and near-surface regions to 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

336. Deposition of Amorphous Materials with a Dual Beam Ion System - DOE Contact A. E. Evans, (301) 353-3098; Sandia Contact J. K. G. Panitz, (505) 844-8604

- o A dual beam ion system has been developed to sputter- deposit films onto selected substrates. Concurrent ion bombardment with inert and reactive gas ions increases the adhesive strength of the deposited film.

Materials Properties, Behavior, Characterization or Testing

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

- o 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

338. Development of Materials for Magnetic Fusion Reactors - DOE Contact A. E. Evans, (301) 353-3098; SNL Contact M. F. Smith, (505) 846-4270

- o Tests are continuing to evaluate materials used in magnetically confined fusion energy devices. The two materials developed for these applications are a beryllium limiter assembly and a low-pressure chamber plasma spray process.

339. Plasma Cleaning Studies - DOE Contact A. E. Evans, (301) 353-3098; Sandia Contact R. R. Sowell, (505) 844-1038

- o Fluorocarbon plasmas have been used to remove metal oxide films from the surface of Inconel 718 that are formed during an S-glass-to-Inconel metal sealing process.

Instrumentation and Facilities

340. Ion Beam Reactive Deposition System - DOE Contact A. E. Evans, (301) 353-3098; Sandia Contact D. E. Peebles, (505) 844-1647

- o A system has been constructed for reactive ion beam deposition of compound films. The mechanism of compound film formation will be characterized for TiN and then complex film deposition of compounds not readily obtained by current methods will be studied.

341. 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

- o An in situ friction, wear, and electrical contact resistance device has been assembled 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. The department also supports the Laboratories through the study of metallurgical corrosion and oxidation. Electrochemistry constitutes a major element of these studies. Initiative is taken to stimulate advanced weapons and energy related concepts by providing new materials and developing 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

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

- o High purity homogeneous PZT powders have been prepared by sol-gel chemistry techniques. The total mixture has been co-precipitated to insure

homogeneity. The most important element is considered to be the ZrO_2 and most of the efforts have focused on this component.

- o ZnO varistor material has been prepared by sol-gel chemistry techniques. High purity material and doped materials have been prepared and are being evaluated.

Materials Properties, Behavior, Characterization or Testing

343. Fracture of Ceramics - DOE Contact A. E. Evans, (301) 353-3098; Sandia Contact F. P. Gerstle, Jr., (505) 844-4304

- o Basic research to better understand fracture processes and to develop tougher ceramics based on this understanding.

Inorganic Materials Chemistry Division, 1846

Division 1846 has responsibility for relating the chemical properties of inorganic materials to their application in a variety of Sandia weapons, energy, and reactor safety programs. The division has programs in the chemical preparation of glasses and ceramics including sol-gel chemistry of glasses for coatings and monolithic structure and electroactive ceramic powders, precipitation of ion exchangeable transition metal oxides for catalysts, thin-film capacitors, and solution stabilization to yield homogeneous, monodispersed structural and electronic ceramics. The division also has programs to study the properties and survivability of inorganic materials in reactive environments, e.g., solvent (aqueous, acidic and basic, corrosive) dissolution of inorganic glasses, ionic conductivity of high temperature electrolytes, and the physical and chemical properties, especially thermal stability, of inorganic materials at high temperature.

Materials Preparation, Synthesis, Deposition, Growth or Forming

344. Glass and Glass-Ceramic Development - DOE Contact A. E. Evans, (301) 353-3098, FTS 233-3098; Sandia Contact D. H. Doughty, 505-844-1933

- o A glass has been developed for use in Li/SO_2 batteries. This glass was developed to resist the environment of Li batteries for five years. A model of Li under potential deposition was proposed and used to define a glass chemistry resistant to attack.

Corrosion Division, 1847

Division 1847 personnel perform research to understand and control the corrosion and oxidation of metals, and they also characterize gas-metal reactions involving species such as hydrogen and ammonia. Corrosion research is directed toward: (a) developing new and improved materials; (b) defining boundaries for applying existing materials; and (c) performing failure analyses. Emphasis is on understanding the mechanistic nature of corrosion processes. The division maintains expertise in the areas of corrosion by

aqueous and non-aqueous electrolytes; corrosion by gases; stress corrosion cracking; gas-metal interactions including scattering, adsorption, and desorption; and electrodeposition.

Materials Properties, Behavior, Characterization or Testing

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

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

Sandia National Laboratories - Livermore

Materials Preparation, Synthesis, Deposition, Growth or Forming

346. 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

   o 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.

347. 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

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

348. Metal Forming - DOE Contact A. E. Evans, (301) 353-3098; Sandia Contacts J. Lipkin, (415) 422-2417 and T. C. Lowe, 415-422-3187, and D. A. Hughes, (415) 294-2686

   o Nonelastic deformation is being examined through crystal plasticity modeling and experimentation. Results are used to guide design of phenomenological models for use in finite element simulations of forming and of failure of anisotropic materials.

349. 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

- o An understanding of methods for producing microstructural modifications in organic foams has enabled the production of polymeric foams with unique physical properties.

350. 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

- o We have developed methods to produce extremely fine actinide oxide particles of controlled morphology: spheres, plates and needles.

351. Tritium Getter Technology - DOE Contact A. E. Evans, (301) 353-3098; FTS 233-3098; Sandia Contacts D. L. Lindner, (415) 294-3306 and D. A. Nissen, (415) 294-2767

- o We have demonstrated that certain solid organic alkenes can be used to getter tritium. These materials have been shown to form stable, solid species that do not release the bound tritium or degrade into low molecular weight species.

352. 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

- o 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.

353. Plasma Processing - DOE Contact A. E. Evans, (301) 353-3098; FTS 233-3098; Sandia Contacts W. L. Hsu, (415) 294-2379

- o The synthesis of diamond and amorphous carbon by plasma processing is being studied.

Materials Properties, Behavior, Characterization or Testing

354. Helium-Induced 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; J. E. Costa, 415-422-2352

- o The effect of helium on the low temperature mechanical properties of fcc metals is being investigated theoreticalloy and experimentally. Tritium decay is used to introduce helium into metals without inducing radiation damage.

355. 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.

356. 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. Spingarn, (415) 294-2719

- The stability, compatibility, and joining of polymer matrix composite materials are under investigation. Focus is upon graphite fiber reinforced materials. Identification of moisture adsorption sites in thermosetting resins is underway. Coatings to increase stability for special designs are being studied. Joining studies include adhesives, mechanical fasteners and the welding of thermoplastics.

357. Compatibility, Corrosion, and Cleaning of Materials - DOE Contact, A. E. Evans, (301) 353-3098; Sandia Contacts H. R. Johnson, (415) 422-2822 and D. K. Ottesen, (415) 294-2787

- Sophisticated electroanalytical and spectroscopic techniques are being used to examine surfaces to assess compatibility, corrosion, and cleanliness.

358. 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.

359. 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.

Instrumentation and Facilities

360. 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

- o 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.

361. 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

- o New laboratory capabilities within the Tritium Research Laboratory include the development of equipment for quantitative helium analysis and a high pressure, high temperature apparatus for T_2 exposure of test specimens.

Lawrence Livermore National Laboratory

Materials Preparation, Synthesis, Deposition, Growth or Forming

362. Ion Beam Modification of Materials - DOE Contact A. E. Evans, (301) 353-3098; FTS 233-3098; LLNL Contact R. G. Musket, (415) 422-0483

- o 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.

363. Formation of Metastable Surface Alloys - DOE Contact A. E. Evans, (301) 353-3098; FTS 233-3098; LLNL Contact E. N. Kaufman, (415) 422-2640

- o This program uses directed-energy electron and laser beams to form surface alloys for potential programmatic applications and to study the microscopic mechanisms of their formations.

364. Synthesis Project (Explosives) - DOE Contact A. E. Evans, (301) 353-3098; FTS 233-3098; LLNL Contact C. L. Coon, (415) 422-6311

- o The primary objectives of this research are (1) to synthesize new, energetic materials which have the potential of surpassing HMX in terms of performance and safety, and (2) developing new synthetic approaches to the synthesis of nitro and nitramino compounds.

365. Synthesis and Reactivity of Transition Metal Fluorocarbon Complexes - DOE Contact A. E. Evans, (301) 353-3098; FTS 233-3098; LLNL Contact R. D. Sanner, (415) 423-3875

- The objectives are to synthesize new transition metal fluorocarbon complexes and to investigate the reactivity of the compounds.

366. Advanced Ceramics Synthesis and Processing - DOE Contact A. E. Evans, (301) 353-3098; FTS 233-3098; LLNL Contact J. B. Holt, (415) 422-8003

- Study specific solid combustion reactions in order to develop a process to synthesize ultra-fine grained (0.1-0.5u) B_4C powders. Powders of this size range should be sinterable without the use of additives.

367. Sputtering (Plutonium Alloys) - DOE Contact A. E. Evans, (301) 353-3098; FTS 233-3098; LLNL Contact H F. Rizzo, (415) 422-6369

- Determine how triode sputtering parameters can be controlled to synthesize amorphous and metastable Pu alloys; study how changes in Pu/solute atomic size mismatch and Pu electronic (5-f electrons) effects influence the compositional ranges for formation of amorphous and metastable Pu alloys; and model the substrate physics to understand the formation of observed amorphous- and metastable-sputtered deposits.

368. Kinetic Models (Hydrogen, Methane Oxidation) - DOE Contact A. E. Evans, (301) 353-3098; FTS 233-3098; LLNL Contact J. R. Creighton, (415) 423-7949

- To produce simplified models of hydrogen and methane oxidation and compare the models with experimental data.

369. An Investigation of Multifilamentary NbN Superconductors - DOE Contact A. E. Evans, (301) 353-3098; FTS 233-3098; LLNL Contact L. Summers, (415) 423-6574

- We have developed methods of fabricating brittle superconductors in a stabilized multifilamentary geometry. These techniques can be continuously applied for producing the long lengths of conductor needed to fabricate magnets.

370. Grinding Glass in the Ductile Regime - DOE Contact A. E. Evans, (301) 353-3098; FTS 233-3098; LLNL Contact K. L. Blaedel, (415) 422-0290

- We are developing techniques for grinding glass in a ductile fashion. Ductile grinding causes less surface damage than brittle grinding, thus minimizing the subsequent polishing required to finish the optic.

371. A Basic Study of the Single-Point Cutting Process - DOE Contact A. E. Evans, (301) 353-3098; FTS 233-3098; LLNL Contact R. Donaldson, (415) 422-1916

- We are making significant progress toward developing a fundamental understanding of how various materials are cut by sharp diamond edges. This understanding will lead to improvements in the design of precision machine tools and may determine their ultimate cutting accuracy.

Materials Structure and Composition

372. Theory of Polar Fluid Structure and Dynamics - DOE Contact A. E. Evans, (301) 353-3098; FTS 233-3098; LLNL Contact D. Calef, (415) 422-7797

- Develop theoretical models for the structure and dynamics of polar fluids and processes involving charge motion in those fluids, especially at higher densities.

373. Structures of Actinide-Hydrogen Compounds and Solutions at High Pressures - DOE Contact A. E. Evans, (301) 353-3098; FTS 233-3098; LLNL Contact R. H. Condit, (415) 422-8729

- This is a search for (1) new and interesting crystal phases in actinide hydrides (uranium, neptunium, plutonium) and (2) the effect of hydrogen on the phases produced in actinide metals under high pressure and over a range of temperatures.

374. Actinide Thermochemistry - DOE Contact A. E. Evans, (301) 353-3098; FTS 233-3098; LLNL Contact M. G. Adamson, (415) 523-2024

- To develop a general capability to predict equilibrium compositions and thermodynamic activities in complex multiphase mixtures containing actinides and to assemble an evaluated set of actinide (Pu) alloy and actinide compound thermochemical data for use in the selected thermochemical modeling code(s).

Materials Properties, Behavior, Characterization or Testing

375. The Influence of Cooling Rate on the Microstructure of Duplex Austenitic-Ferritic Stainless Steel - DOE Contact A. E. Evans, (301) 353-3098; FTS 233-3098; LLNL Contact J. W. Elmer, (415) 423-8235

- Investigations of high energy density welds and rapidly solidified melts have shown large differences between the microstructures which develop at high cooling rates and those which develop at low cooling rates. This investigation studies the microstructure of stainless steel alloys which have been solidified at low, intermediate and high cooling rates.

376. The Role of Interfaces in Metallic-Layered Thin Films - DOE Contact A. E. Evans, (301) 353-3098; FTS 233-3098; LLNL Contact A. F. Jankowski, (415) 423-519

- This study examines the role of interfaces in the physical properties of multilayered thin films. This information provides the basis for understanding the stress state effects on interfacial solid-state bonding.

377. 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.

378. 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.

379. Polymer Modeling - DOE Contact A. E. Evans, (301) 353-3098; FTS 233-3098; LLNL Contact R. Cook, (415) 422-6993

- This program is aimed at improving our understanding of polymeric materials through theoretical and computer simulation studies of polymer chain dynamics under a variety of conditions.

380. 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.

381. Plutonium Martensitic Transformation Plasticity - DOE Contact A. E. Evans, (301) 353-3098; FTS 233-3098; LLNL Contact P. H. Adler, (415) 423-4417

- This project is directed toward the development of a tough, ductile and highly dense form of Pu. This work involves examination of the crystallography, thermodynamics, and kinetics of the $\delta \leftrightarrow \alpha$ transformation. This would lead to development of the constitutive relations governing this mechanically-induced phase transformation and allow design of an α-alloy of the correct metastability

382. Theory of Deflagration at High Pressures - DOE Contact A. E. Evans, (301) 353-098; FTS 233-3098; LLNL Contact D. Calef, (415) 422-7797

- Develop theoretical models to understand the deflagration (or burning) of solid materials at very high pressures. Find meaningful functional forms for these processes that can then be used in macroscopic modelling.

383. High-Pressure High-Temperature Raman Spectroscopy of Energetic Materials - DOE Contact A. E. Evans, (301) 353-3098; FTS 233-3098; LLNL Contact M. S. Costantino, (415) 422-6923

- The objectives of this research are (1) establish a diamond anvil cell/Raman spectroscopy facility, (2) explore the equilibrium chemistry of decomposition reactions of various energetic materials and (3) obtain these same spectra as a function of time to obtain information on decomposition kinetics.

384. Hot Spot Microdynamics/High Explosives R&D - DOE Contact A. E. Evans, (301) 353-3098; FTS 233-3098; LLNL Contact R. Simpson, (415) 423-0379

- The motivation behind this research has been to establish the diagnostic capability of precisely synchronizing radiometric measurements on high explosives with known hydrodynamic states during initiation and detonation. This technology enables determination of detonation temperatures which can be used as an evaluation of equations of state (EOS).

385. Roles of Post-Yield Properties and Physical Aging the Fracture of Highly-Crosslinked Networks - DOE Contact A. E. Evans, (301) 353-3098; FTS 233-3098; LLNL Contact J. D. LeMay, (415) 423-3599

- The primary objectives of this work were: (1) develop test methods for attaining the post-yield condition and high strains in highly-crosslinked epoxy polymers; (2) to study the properties of bulk polymers thus deformed, and (3) to determine the compatibility of these properties with molecular fracture models.

386. Studies of Material Properties at High Temperatures - DOE Contact A. E. Evans, (301) 353-3098; FTS 233-3098; LLNL Contact O. H. Krikorian, (415) 422-8076

- This work combines correlation methods with theory to predict material behavior and properties for high temperature materials for which such data do not exist.

387. 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 play in the reactivity of solid actinide compounds with gases and vapors.

388. Computer Molecular Dynamics - DOE Contact A. E. Evans, (301) 353-3098; FTS 233-3098; LLNL Contact A. M. Karo, (415) 422-7800

- A primary objective of our current research is to understand the plasma-wall interaction zone of fusion plasmas in enough detail so that results from the calculations can be used to interpret contemporary ion-source operation, thereby providing a basis for extrapolation to high-power systems.

389. Dislocation Microstructure of Aluminum Deformed to Large Steady-State Creep Strains - DOE Contact A. E. Evans, (301) 353-3098; FTS 233-3098; LLNL Contact M. E. Kassner, (415) 423-2329

- This research was directed towards experimentally identifying (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.

390. In Situ Reversed Deformation Experiments - DOE Contact A. E. Evans, (301) 353-3098; FTS 233-3098; LLNL Contact M. E. Kassner, (415) 523-2329

- Continue the world's first in situ cyclic or reversed plastic deformation tests in the high-voltage transmission electron microscope (HVEM).

391. Hyperfine Studies and Radiation Effects - DOE Contact A. E. Evans, (301) 353-3098; FTS 233-3098; LLNL Contact C. E. Violet, (415) 422-7728

- Measure the melting curve of Pu-Ga-Fe alloys. Measure 14 MeV neutron damage to $Nd_2Fe_{14}B$.

392. Actinide Phase Diagrams - DOE Contact A. E. Evans, (301) 353-3098; FTS 233-3098; LLNL Contact M. E. Kassner, (415) 423-2329

- The systems to be evaluated include, Pu-Ga, Pu-Al, Th-Al, Np-Al, Am-Al and U-Al.

393. 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

- We have made progress in modeling and experimentally measuring deformation-induced residual stress. We find that bulk measurement of residual stress by diffraction is most reliable and that finite-element analyses produce valid results for isotropic materials.

394. Numerical Modeling of Crack Growth and Plastic Deformation Material Model - DOE Contact A. E. Evans, (301) 353-3098; FTS 233-3098; LLNL Contact R.A. Riddle, (415) 423-7541

- We are developing new analytical tools to predict the effect of cracks and other defects on the strength of structural components. We are updating a J Integral post-processor for the finite-element code NIKE2D to include the effects of thermal stresses and strains, residual stresses, and body forces.

395. A Study of Residual Stress for Epoxy-Resin Composites - DOE Contact A. E. Evans, (301) 353-3098; FTS 233-3098; LLNL Contact W. Feng, (415) 422-8701

- 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 will be used to minimize residual stress and, hence, improve the integrity of composite structures.

396. 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

- A knowledge of the optical radiative properties of the surfaces of high purity metals at temperatures up to and above the melting point is of considerable technical importance for a number of applications. These include welding by TIG, E-beam and laser methods; smelting and casting; developing thermal and E-beam evaporative sources for thin film and composite deposition; and Laser Isotope Separation (LIS).

397. Evaluation of a Thermo-Plastic Material Model - DOE Contact A. E. Evans, (301) 353-3098; FTS 233-3098; LLNL Contact D. R. Lesuer, (415) 422-9633

- We are progressing toward an understanding of the suitability and limitations of the isotropic, rate-independent, thermoplastic material models typically

used in LLNL NIKE computer codes. These unproven material models have been widely used in a number of problems involving thermoplastic behavior, including thermal mismatch, solid-state bonding and weld shrinkage.

398. Strength of Composite Materials - DOE Contact A. E. Evans, (301) 353-3098; FTS 233-3098; LLNL Contact S. E. Groves, (415) 422-1331

- o Th objective of this development project was to significantly improve our ability to accurately predict the strength of composite materials, both experimentally and theoretically.

399. Integrated Engineering Applications Software (IDEAS) Project - DOE Contact A. E. Evans, (301) 353-3098; FTS 233-3098; LLNL Contact N. Nguyen, (415) 422-7458

- o 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.

400. High Strain Rate Tensile Testing - DOE Contact A. E. Evans, (301) 353-3098; FTS 233-3098; LLNL Contact D. H. Lassila, (415) 423-9537

- o New analysis techniques have been developed for the tensile Hopkinson bar test to determine stress-strain behavior of materials at high strain rates.

Instrumentation and Facilities

401. Shockwave Fiber Optics Probe - DOE Contact A. E. Evans, (301) 353-3098; FTS 233-3098; LLNL Contact G. Haugen, (415) 422-7779

- o To develop an ultrafast pressure sensor to measure the profile of shockwaves.

402. Laser Induced Chemistry - DOE Contact A. E. Evans, (301) 353-3098; FTS 233-3098; LLNL Contact C. Stevens, (415) 422-6208

- o To establish a research facility using lasers to both stimulate and probe gas-phase chemical reactions.

- o To understand the spectroscopy and dynamics of laser-excited vibrational overtones of polyatomic molecules and influence the subsequent outcome of chemical reactions.

403. Synchrotron Radiation Studies - DOE Contact A. E. Evans, (301) 353-3098; FTS 233-3098; LLNL Contact J. Kinney, (415) 423-1126

- To explore high-resolution, chemically-specific tomograph which may ultimately have applications in support of the advanced materials characterization needs.

- To develop advanced digital image processing capabilities.

404. Scanning Tunneling Microscope - DOE Contact A. E. Evans, (301) 353-3098; FTS 233-3098; LLNL Contact W. Siekhaus, (415) 422-6884

- The scanning tunneling microscope (STM) is a new device which can analyze the physical and the electronic structure of surfaces of conducting materials with a resolution below 1 Å. The technical objectives of this program are to develop STMs capable of operating in fluids (air, water, oil) and in ultra-high vacuum (UHV).

405. Study of Solid Deformation Processes Using a Novel Calorimetric Technique - DOE Contact A. E. Evans, (301) 353-3098; FTS 233-3098; LLNL Contact R. E. Lyon, (415) 423-8323

- Design and construct a high sensitivity deformation calorimeter.

- Utilize the deformation calorimeter to study the thermodynamics of reversible and irreversible deformation of solids.

- Develop a theory of large reversible deformation, including compressibility, to correlate experimental results on elastomers.

406. Scanning Tunneling Microscopy (STM) as a Detector - DOE Contact A. E. Evans, (301) 353-3098; FTS 233-3098; LLNL Contact W. Siekhaus, (415) 422-6884

- Scanning tunneling microscopy (STM), in conjunction with the atomic force microscope (AFM), can now be used to detect and characterize submicron-size defects on optical components. Such measurements are applicable to single-point diamond tools whose sharp radii of curvature now approach tens of Angstroms.

407. Research in Quantitative Ultrasonic Nondestructive Evaluation - DOE Contact A. E. Evans, (301) 353-3098; FTS 233-3098; LLNL Contact G. A. Clark, (415) 423-9759

- We have developed methods of removing distortion from ultrasonic measurement signals and have used them to process signals from controlled laboratory experiments and several actual programmatic applications.

408. Research in Computerized Tomographic Imaging - DOE Contact A. E. Evans, (301) 353-3098; FTS 233-3098; LLNL Contact J. Brase, (415) 422-6992

- o Computed Tomography (CT) has demonstrated the ability to produce accurate three-dimensional images of the human body. We have made significant progress in developing quantitative CT techniques for producing high-resolution images of materials in interest to LLNL researchers.

409. Contour Measurement with Capacitance Sensor - DOE Contact A. E. Evans, (301) 353-3098; FTS 233-3098; LLNL Contact S. Patterson, (415) 422-6133

- o The contour of a curved, conducting workplace can be determined with nanometer accuracy by measuring the capacitance between the surface and a movable, noncontacting probe. Accuracy of computer models is currently limited by the precision of the available finite-element code.

410. Tritium Facility Upgrade - DOE Contact A. E. Evans, (301) 353-3098; FTS 233-3098; LLNL Contact G. M. Morris, (415) 423-1770

- o Upgrade of the Tritium Facility to include a cleanup system and an office/mechanical technician shop addition.

411. Dedication of the Weapons Materials Research and Development Facility - DOE Contact A. E. Evans, (301) 353-3098; FTS 233-3098; LLNL Contact M. G. Adamson, (415) 423-2024

- o Groundbreaking ceremonies for the $28.3M Weapons Materials Research and Development Facility were held in 1983; construction was completed in August 1986; the building was dedicated August 21, 1987.

Los Alamos National Laboratory

Materials Preparation, Synthesis, Deposition, Growth or Forming

412. 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

- o Development of new alloys of plutonium, including casting, thermo-mechanical working, sputtering, and stability studies.

- o Measurements of resistivity, thermal expansion and bend ductility to evaluate fabrication processes and alloy stability.

413. Plutonium Oxide Reduction - DOE Contact G. Bennett (301) 353-3197, FTS 233-3197; LANL Contact D. Peterson, (505) 667-5181, FTS 843-5181

- o Determination of thermodynamics of interactions used in direct-oxide reduction of plutonium.

414. Plutonium Oxide Removal - DOE Contact G. Bennett, (301) 353-3197, FTS 233-3197; LANL Contact P. Kleinschmidt, (505) 667-6945, FTS 843-6945

- o Identification of ways to remove residual plutonium contamination from iridium.

415. Replacement Noble-Metal Alloys - DOE Contact G. Bennett, (301) 353-3197, FTS 233-3197; LANL Contact T. George, (505) 667-4931, FTS 843-4931

- o Development of new noble-metal-based alloys to provide improved containment for plutonium oxide in space power systems.

416. Powder Preparation by Plasma Chemical Synthesis - DOE Contact A. E. Evans, (301) 353-3098, FTS 233-3098; LANL Contact G. J. Vogt, (505) 667-5813, FTS 843-5813

- o Development of plasma-assisted chemical vapor deposition for the production of ultrafine, ultrapure ceramic powders.

417. Synthesis of SiC Whisker-MoS_2 Matrix Composites for Elevated Temperature Applications - DOE Contact J. Eberhardt, (202) 586-5377; LANL Contact F. Gac, (505) 667-5126, FTS 843-5127

- o Incorporation of SiC whiskers in $MoSi_2$ for reinforcement.
- o Toughens material or lower temperatures.
- o Strengthens material or higher temperature.

418. 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

- o Producing reinforcing materials for structural ceramics such as SiC and Si_3N24.
- o Use technology developed at Los Alamos to grow long VLS SiC whiskers and use them in the development of staple yarns and subsequent woven cloth configurations.

419. Low Density Metal "Smokes" - DOE Contact A. E. Evans, (301) 53-3098, FTS 233-3098; LANL Contact D. V. Duchane, (505) 667-6887, FTS 843-6887

- o Production of low-density metal "smoke" by vacuum deposition.
- o Gold "smoke" density as low as 1 percent of full density.

420. 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

- o Exploration of ion implantation for surface modification.
- o Goals of improved surface hardness and corrosion resistance.

421. 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

- o Investigation of electroplating low atomic number metals (aluminum and beryllium) by using non-aqueous plating baths.

422. 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

- o Synthesis of one polyphenylguinoxaline and two polypyrrones showing unique electrically conductive properties when treated with appropriate doping agents.

423. 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

- o Use of new cesium electride to induce a high level of electrical conductivity and to improve the stability in polyacetylene films.

424. 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

- o Synthesis of a liquid crystal polymer with strength in three dimensions.

425. 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

- o Modification of surface properties of plastic components by a solvent infusion process.

- o Use of process to improve the biocompatibility properties of such plastics as acrylics and silicones.

426. 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

- o Manufacture of microstructural polyolefin foams with densities between 0.01 g/cc and 0.2 g/cc by a nonconventional foaming process.

427. Target Coatings - DOE Contact A. E. Evans, (301) 353-3098, FTS 233-3912; LANL Contact D. V. Duchane, (505) 667-3238, FTS 843-3238

- o Development of single and multilayer metallic and nonmetallic thin film coatings, smooth and uniform in thickness.

428. 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

- o Physical vapor deposition and sputtering to produce materials for structural applications, corrosion resistance, optical properties, and thin film transducers.

429. 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

- o Development of techniques for low temperature deposition of tungsten, molybdenum, rhenium, and nickel on hollow substrates of spherical and cylindrical shapes.

- o Fabrication of ultra-thin, free-standing shapes.

430. 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

- o Investigation of feasibility of synthesis of a broad range of metallic glasses by electrodeposition.

- o Applications: hard coatings, corrosion-resistant coatings, weapons physics, inertial confinement fusion.

431. 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

- o Development of fabrication processes, and evaluation and testing of commercial plastic materials for weapons programs.

- o Development of highly filled polymers, reinforced composites, cushioning materials, and high-explosives compatible adhesives.

- o 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.

432. 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

- o Advanced R&D on low-Z, tritiated materials with the emphasis on Li(D,T) (salt) and other metal tritides.

- o Studies of new methods for preparing, fabricating, and containing such compounds, and for measurement of properties.

433. 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

- o Development and evaluation of fabrication processes for lithium tritide deuteride.

- o Use of hot pressing and hot isostatic pressing to near net shape to improve part shape versatility, density, and surface quality.

- o Conduct of component integrity studies involving radiation induced growth and outgassing.

434. 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

- o Slip casting of many ceramics including alumina, magnesia, and thoria.

- o Use of colloidal chemistry and powder characterization theory along with materials engineering.

435. Whisker Growth Technology - DOE Contact A. E. Evans, (301) 353-3098, FTS 233-3098; LANL Contact H. Casey, (505) 667-4365, FTS 843-4365

- o Growth of silicon carbide whiskers by a vapor-liquid-solid process which produces very long fibers.

- o Improving control over the process itself to obtain mono-sized whiskers of regular morphology; processing whiskers to remove detritus and impurities; characterizing the whiskers and relating their properties to structural features; and growth of Si_3N_4 whiskers by same process.

436. 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

- o 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.

437. Glass and Ceramic Coatings - DOE Contact A. E. Evans, (301) 353-3098, FTS 233-3098; LANL Contact H. Casey, (505) 667-4365, FTS 843-4365

- o Develop vitreous enamels and general ceramic coatings to provide radiation-hardened, electrical-insulating components for accelerator technology.

438. 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

- o Use of cold pressing and cold isostatic pressing to consolidate ceramic and metal powders in support of laboratory programs.

439. 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

- o Fabrication of free-standing shapes, and metallic and ceramic coatings by plasma spraying.

440. Rapid Solidification Technology - - DOE Contact A. E. Evans, (301) 353-3098, FTS 233-3098; LANL Contact H. Casey, (505) 667-4365, FTS 843-4365

- o Development of RSR technologies such as melt spinning, splat cooling, and rapid solidification plasma spraying.
- o Alloy development, microstructural analysis, properties testing, process development, modeling.

441. Superplastic Forming - DOE Contact A. E. Evans, (301) 353-3098, FTS 233-3098; LANL Contact H. Casey, (505) 667-4365, FTS 843-4365

- o Investigation of superplastic forming of titanium and uranium alloys.
- o Evaluation of fine grained U-6 wt% Nb (2m grain size) in biaxial forming.

442. Microwave Sintering/Processing - DOE Contact A. E. Evans, (301) 353-3098, FTS 233-3098; LANL Contact J. Katz, (505) 667-1424, FTS 843-1424

- o Investigating techniques of bonding and sintering ceramics such as $A1_2 0_3$ and glass.
- o Use of very high frequency microwaves which suscept directly to the area in which the heat is needed.
- o Investigation of the control of the heating and its effect on microstructure.

Materials Structure or Composition

443. 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

- o Characterization of actinide metal, alloy and compound surfaces using the techniques of x-ray photoelectron spectroscopy, Auger analysis, ellipsometry and Fourier-transform infrared spectroscopy.
- o Studies of surface reactions, chemisorption, attack by hydrogen, nature of associated catalytic processes.

444. 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

- o Neutron diffraction studies of plutonium and its alloys conducted at the Los Alamos WNR pulsed neutron source.
- o Time-of-flight technique used to measure diffraction at elevated temperatures and pressures.

445. Surface Studies - DOE Contact A. E. Evans, (301) 353-3098, FTS 233-3912; LANL Contact H. K. McDowell, (505) 667-4686, FTS 843-4686

- o Studies of surface structures and atomic and electronic properties of uranium alloys and intermetallics, UO_2 and ThO_2 single crystals, heavy fermion systems, and palladium/hydrogen systems.
- o Develop essential atomic-level understanding of surface properties of materials and physical and chemical processes.
- o Study of surface modification, synchrotron radiation of uranium, UPt_3 surface properties, valence bands of UO_2, residues on electropolished/oxidized uranium, and use of MeV ion beams to probe surface structure.

- o Use of techniques such as Low Energy Electron Diffraction (LEED), Auger and Loss Spectroscopies, Ion-Scattering Spectroscopy (ISS), Ultraviolet Photoelectron Spectroscopy (UPS), Synchrotron Radiation, and MeV-ion-beam scattering.

Materials Properties, Behavior, Characterization or Testing

446. Mechanical Properties of Uranium - DOE Contact A. E. Evans, (301) 353-3098, FTS 233-3098; LANL Contact P. Armstrong, (505) 667-4889, FTS 843-4889

- o Investigation of mechanical properties of U-6 wt% Nb and pure U at high strain rates.
- o Study of the effects of crystallographic texture on high rate (shock regime) uranium deformation.

447. High Strain Rate Testing - DOE Contact A. E. Evans, (301) 353-3098, FTS 233-3098; LANL Contact P. S. Follansbee, (505) 667-8021, FTS 843-8021

- o Testing of metals at rates up to, but not including the shock-wave regime to elicit fundamental understanding of changes in mechanism as a function of deformation rate.

448. 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

- o Study relationship of mechanical properties of Pu and Pu alloys to their microstructures.
- o Use of optical and electron microscopy, X-ray, electron, and neutron diffraction.

449. 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

- o Investigation of mechanisms, crystallography, and kinetics of transformations in plutonium and alloys using pressure and temperature dilatometry, optical metallography, and X-ray diffraction.

450. 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

- o Study of P-V relationships in liquid actinide elements by isobaric expansion.

451. Plutonium Shock Deformation - DOE Contact A. E. Evans, (301) 353-3098, FTS 233-3098; LANL Contact R. Gray, (505) 667-5452, FTS 843-5452

- o Plutonium alloys subjected to shock deformation, recovered and examined to determine effects of shock on microstructures and mechanical properties.

452. Dielectric Loss Measurement in Ceramics - DOE Contact Marvin Cohen, 301-353-4253; LANL Contact H. M. Frost, (505) 667-1290, FTS 843-1290

- o Loss tangent measurements in ceramics at very high frequencies to evaluate effects of neutron damage for magnetic fusion energy applications.
- o Evaluation of microwave sintering properties of ceramics for fabrication purposes.

453. Plutonium Doping for Self-Irradiation Damage in Ceramics - DOE Contact A. E. Evans, (301) 353-3098, FTS 233-3098; LANL Contact F. W. Clinard, Jr., (505) 667-5102, FTS 843-5102

- o Use of short-lived Pu isotope to study self-irradiation damage in titanate and silicate ceramics.
- o Material converts from crystalline to amorphous state.

454. Nondestructive Evaluation - DOE Contact A. E. Evans, (301) 353-3098, FTS 233-3098; LANL Contact A. Wilson, (505) 667-6404, FTS 843-6404

- o Development of nondestructive evaluation techniques that produce quantitative estimates of material properties.
- o Application of multivariate analysis to welding processes. Use of tomographic techniques to extend radiographic inspections.

455. Powder Characterization - DOE Contact A. E. Evans, (301) 353-3098, FTS 233-3098; LANL Contact H. Casey, (505) 667-4365, FTS 843-4365

- o Characterization of starting powders (RF plasma SiC, commercial powders of ThO_2, tungsten, copper, Si_3N_4, MgO and Al_2O_3).
- o Determination of particle size and distribution, morphology, state of agglomeration, zeta potential, and surface area.

Device or Component Fabrication or Testing

456. 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

- o Physical vapor deposition of coatings for radiochemical detectors.

457. 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

- o Hydrocarbon polymer applied by plasma polymerization to glass microspheres.
- o Micromachining, plasma etching, plasma polymerization.
- o Targets filled with deuterium tritium gas.

458. Filament Winder - - DOE Contact A. E. Evans, (301) 353-3098, FTS 233-3098; LANL Contact E. Eaton, (505) 667-5261, FTS 843-5261

- o Four-axis computer-programmed winding machine.
- o Winding envelopes to 4 ft. diameter, 10 ft. long.
- o Winds helixes, cones, spheres, closed-end vessels of glass, kevlar, carbon, tungsten, and alumina fibers.

459. 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

- o Development of polymeric-host dye-laser rods.
- o In situ polymerization of dye/monomer mixture.
- o Inexpensive "disposal" laser rods.

460. 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

- o Development of microcomputer technology and signal analysis for process control and multiaxis, programmable component manipulation for high-voltage electron beam welding.
- o Operation of a high-voltage electron beam welder for fabrication of products in the fissile material area.

- o Investigation of real-time diagnostics of laser welding efficiency.
- o Study of plasma effects on laser welding efficiency.
- o Correlation of photodiode, acoustic, light-spectral and electron current measurements with high speed cinematography and resultant weld geometry.

461. 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

- o Video monitoring and Varistraint testing established as techniques to investigate crack susceptibility of gas-tungsten-arc welds.

462. Ceramic Technology - DOE Contact A. E. Evans, (301) 353-3098, FTS 233-3098; LANL Contact H. Casey, (505) 667-4365, FTS 843-4365

- o Fabrication of castable ceramics for energy technologies.

463. Solid State Bonding - DOE Contact A. E. Evans, (301) 353-3098, FTS233-3098; LANL Contact H. Casey, (505) 667-4365, FTS 843-4365

- o Evaluating aluminum solid-state bonding for seamless ICF targets.
- o Evaluation of bond load modulation and ion bombardment cleaning.
- o Investigation of bonding technique optimization.

OFFICE OF FOSSIL ENERGY

	FY 1987
Office of Fossil Energy - Grand Total	$6,850,000
Office of Technical Coordination	$6,165,000
Advanced Research and Technology Development Program	$6,165,000
Materials Preparation, Synthesis, Deposition, Growth or Forming	$1,045,000
Consolidation of Rapidly Solidified Aluminide Metal Powders	75,000
Investigation of Electrospark Deposited Coatings for Protection of Materials in Advanced Steam Cycle Superheater Applications	50,000
Short Fiber Reinforced Structural Ceramics	225,000
Fabrication of Fiber-Reinforced Composites by CVD Infiltration	187,000
Characterization of Fiber-CVD Matrix Interfacial Bonds	125,000
Microwave Sintering of Sol-Gel Derived Ceramic Superconductors	73,000
Transfer of CVD Infiltration Technology to Industry	50,000
Development of Advanced Fiber Reinforced Ceramics	160,000
Development and Microstructural Evaluation of Austenitic Alloys	100,000
Materials Properties, Behavior, Characterization or Testing	$3,325,000
Mechanical Properties and Microstructural Stability of Advanced Steam Cycle Materials	140,000
Transformation, Metallurgical Response and Behavior of the Weld Fusion and Heat Affected Zone in Cr-Mo Steels for Fossil Energy Applications	0[1]
Analysis of Hydrogen Attack on Pressure Vessel Steels	0[1]
Investigation of the Weldability of Ductile Alumindes	50,000
Development of Iron and Nickel Aluminides	160,000
Joining of Advanced Aluminides	75,000
Corrosion and Mechanical Properties of Alloys in FBC and Mixed-Gas Environments	320,000
Investigation of Corrosion Mechanisms of Coal Combustion Products on Alloys and Coatings	80,000
Investigation of the Effects of Microalloy Constituents, Surface Treatment, and Oxidation Conditions on Development and Breakdown of Protective Oxide Scales	215,000
Investigation of the Effects of Microalloy Constituents, Surface Treatment, and Oxidation Conditions on Development and Breakdown of Protective Oxide Scales	215,000

[1]Prefunded in FY 1986.

	FY 1987
Office of Technical Coordination (Continued)	
Advanced Research and Technology Development Program (Continued)	
Materials Properties, Behavior, Characterization, or Testing (Continued)	
Investigation of the Effects of Microalloy Constituents, Surface Treatment, and Oxidation Conditions on Development and Breakdown of Protective Oxide Scales	215,000
Mechanical Properties of Oxide Films and Correlation with Metal/Oxide Interface	50,000
A Study of Erosive Particle Rebound Parameters	80,000
In situ Scanning Electronic Microscopy Studies of Erosion-Corrosion	200,000
Study of Particle Rebound Characteristics and Material Erosion at High Temperature	0[2]
Development of Nondestructive Evaluation Techniques for Structural Ceramics	190,000
Effect of Flaws on the Fracture Behavior of Structural Ceramics	125,000
Joining of Silicon Carbide Reinforced Ceramics	75,000
Nondestructive Evaluation of Advanced Ceramic Composite Materials	75,000
Investigation of the Mechanisms of Failure of Ceramic Materials for Hot Gas Filtration	0[3]
High-Temperature Creep Behavior of Refractory Bricks	0[3]
Weldability Studies of Advanced Austenitic Alloys	100,000
Investigation of Corrosion-Resistant Oxide Sales on Iron-Based Alloys in Mixed Gas Environments	225,000
Solid Particle Erosion in Turbulent Flows Past Tube Banks	60,000
Modeling of Fibrous Preforms for CVD Infiltration	45,000
Structural Reliability and Damage Tolerance of Ceramic Composites	200,000
Improved Ceramic Composites Through Controlled Fiber-Matrix Interaction	150,000
Ceramic Catalyst Materials	150,000
Evaluation of Mechanical Properties of Advanced Austenitic Alloys	130,000

[2]Prefunded in FY 1986.

[3]Prefunded in FY 1985.

OFFICE OF FOSSIL ENERGY (Continued)

	FY 1987
Office of Technical Coordination (Continued)	
Advanced Research and Technology Development Program (Continued)	
Device or Component Fabrication, Behavior or Testing	$ 740,000
"Materials and Components in Fossil Energy Applications" Newsletter	100,000
Studies of Materials Erosion in Coal Conversion and Utilization Systems	250,000
Mechanisms of Galling and Abrasive Wear	75,000
Thermomechanical Modeling of Refractory Brick Linings for Slagging Gasifiers	65,000
Alkalai Attack of Coal Gasifier Refractory Linings	0[4]
Thermodynamic Properties and Phase Relations for Refractory-Slag Reactions in Slagging Coal Gasifiers	0[4]
Evaluation of Candidate Materials for Solid Oxide Fuel Cells	150,000
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[4]
Development of a Design Methodology for High-Temperature Cyclic Application of Materials Which Experience Cyclic Softening	100,000
Instrumentation and Facilities	$ 370,000
Management of the AR&TD Fossil Energy Materials Program	350,000
Coal Conversion and Utilization Plant Support Services	20,000
Office of Surface Coal Gasification	$ 685,000
Surface Gasification Materials Program	$ 685,000
Materials Preparation, Synthesis, Deposition Growth or Forming	$ 685,000
Development of Iron Aluminides for Coal Gasification Systems	215,000
Ceramic Fiber-Ceramic Matrix Hot-Gas Filters	90,000
Protective Coatings and Claddings: Application/Evaluation	230,000
Materials Development for Solid Oxide Oxygen Production Unit	150,000

[4]Prefunded in FY 1986.

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

Advanced Research and Technology Development 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 resesarch; 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 programs supports workshops to identify research needs in all fossil energy technologies and manages selected training programs for faculty and students at Energy Technology Centers.

Materials Preparation, Synthesis, Deposition, Growth or Forming

464. Consolidation of Rapidly Solidified Aluminide Metal Powders - DOE Contact E. E. Hoffman, (615) 576-0735; Idaho National Engineering Laboratory Contacts J. E. Flinn and R. N. Wright, FTS 583-8127

   o Determination of the most effective means of, and associated parameters for, consolidating rapidly solidified nickel-iron aluminide powders.

465. Investigation of Electrospark Deposited Coatings for Protection of Materials in Advanced Steam Cycle Superheater Applications - DOE Contact E. E. Hoffman, (615) 576-0735; Hanford Engineering Development Laboratory Contact R. N. Johnson, (509) 376-0715

   o Examination of the use of the electrospark deposition coating process for the application of corrosion-, erosion-, and wear-resistant coatings to candidate superheater alloys.

466. Short Fiber Reinforced Structural Ceramics - DOE Contact E. E. Hoffman, (615) 576-0735; LANL Contacts P. D. Shalek, (505) 667-6863

   o Investigate the utility of whisker reinforcement technology for producing structural ceramic composites of improved strength and fracture toughness.

467. Fabrication of Fiber-Reinforced Composites by CVD Infiltration - DOE Contact E. E. Hoffman, (615) 576-0735; ORNL Contacts R. A. Lowden and D. P. Stinton, (615) 574-4559

   o Develop a ceramic composite having higher than normal toughness and strength yet retaining the typical ceramic attributes of refractories and high resistance to abrasion and corrosion.

468. Characterization of Fiber-CVD Matrix Interfacial Bonds - DOE Contact E. E. Hoffman, (615) 576-0735; ORNL Contacts R. A. Lowden and D. P. Stinton, (615) 574-4559

   o Optimize the strength and toughness of fiber-reinforced ceramic composites by tailoring the strength of the bonds between the fiber and the matrix

469. Microwave Sintering of Sol-Gel Derived Ceramic Superconductors - DOE Contact E. E. Hoffman, 615-576-0735; ORNL Contacts M. A. Janney and H. D. Kimrey, (615) 574-4281

- o Conduct coordinated research and development on ceramic superconducting materials with major emphasis on the sol-gel synthesis and processing of these materials at INEL and microwave processing of these new ceramics at ORNL.

470. Transfer of CVD Infiltration Technology to Industry - DOE Contact E. E. Hoffman, (615) 576-0735; ORNL Contact T. M. Besmann, (615) 574-4551

- o Transfer AR&TD-developed CVD infiltration technology to Babcock and Wilcox as part of a joint R&D program with Babcock and Wilcox Research Laboratories.

471. Development of Advanced Fiber Reinforced Ceramics - DOE Contact E. E. Hoffman, (615) 576-0735; Georgia Institute of Technology, Georgia Tech Research Institute Contact T. L. Starr, (404) 894-3678

- o 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.

472. Development and Microstructural Evaluation of Austenitic Alloys - DOE Contact E. E. Hoffman, (615) 576-0735; ORNL Contact R. W. Swindeman, (615) 574-5108

- o Alloys based on modifications to four groups of alloys will be developed on the basis of attributes required for advanced steam cycle superheater service.

Materials Properties, Behavior, Characterization or Testing

473. Mechanical Properties and Microstructural Stability of Advanced Steam Cycle Materials - DOE Contact E. E. Hoffman, (615) 576-0735; Cornell University Contact Che-Yu Li, (607) 256-4349

- o Mechanical testing and ranking of the strengths and metallurgical stabilities of advanced steam cycle superheater alloys at temperatures ranging from 650-760°C.

474. Transformation, Metallurgical Response and Behavior of the Weld Fusion and Heat Affected Zone in Cr-Mo Steels for Fossil Energy Applications - DOE Contact E. E. Hoffman, (615) 576-0735, FTS 626-0735; University of Tennessee Contact C. D. Lundin, (615) 974-5310

- o Develop fundamental information on the metallurgical behavior of the heat affected zone of welds in chromium-molybdenum alloys.

475. Analysis of Hydrogen Attack on Pressure Vessel Steels - DOE Contact E. E. Hoffman, (615) 576-0735; University of California at Santa Barbara Contact G. R. Odette, (805) 961-3525

- o Refine previous analyses and confirm the adequacy of the basic thermodynamic information available in the literature.
- o Describe the initiation and development of methane damage in carbon steel, C-Mn-Si steels, 2 1/4 Cr-1 Mo steel, and weldments.

476. Investigation of the Weldability of Ductile Aluminides - DOE Contact E. E. Hoffman, (615) 576-0735; Colorado School of Mines Contact G. R. Edwards, (303) 273-3773

- o Determine the role of microstructure in the intergranular cracking of nickel-iron alumindes, with special emphasis on weld cracking susceptibility.

477. Development of Iron and Nickel Aluminides - DOE Contact E. E. Hoffman, (615) 576-0735; ORNL Contact C. T. Liu, (615) 574-4459

- o Design and test materials that will use Al_2O_3 as the main protective layer to prevent sulfidation attack and that will possess good mechanical properties at high temperatures.

478. Joining of Advanced Aluminides - DOE Contact E. E. Hoffman, (615) 576-0735; Idaho National Engineering Laboratory Contact D. E. Clark, FTS 583-0746

- o Investigate weldability problems limiting the use of aluminides in welded structures.

479. Corrosion and Mechanical Properties of Alloys in FBC and Mixed-Gas Environments - DOE Contact E. E. Hoffman, (615) 576-0735; Argonne National Laboratory Contact K. Natesan, (312) 972-5103

- o Provide a basic understanding of the corrosion behavior of commercial and model alloys after exposure to multi-component gas mixtures.
- o Evaluate mechanisms of the formation and breakaway behavior of protective scales on base metals and weldments exposed to atmospheres containing O, S, and Cl.

480. Investigation of Corrosion Mechanisms of Coal Combustion Products on Alloys and Coatings - DOE Contact E. E. Hoffman, (615) 576-0735; University of Pittsburgh Contact G. H. Meier, (412) 624-5316

- o Investigate the formation and breakdown of protective oxide scales in mixed oxidant gases.

481. Investigation of the Effects of Microalloy Constituents, Surface Treatment, and Oxidation Conditions on Development and Breakdown of Protective Oxide Scales - DOE Contact E. E. Hoffman, (615) 576-0735, FTS 626-0735; Battelle Columbus Laboratories Contact I. G. Wright, (614) 424-4377

- o 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

482. Investigation of the Effects of Microalloy Constituents, Surface Treatment, and Oxidation Conditions on Development and Breakdown of Protective Oxide Scales - DOE Contact E. E. Hoffman, (615) 576-0735, FTS 626-0735; Case Western Reserve University Contact K. M. Vedula, (216) 368-4211

- o Effects of reactive element additions on the protectiveness of oxide scales formed in sulfidizing/oxidizing atmospheres

483. Investigation of the Effects of Microalloy Constituents, Surface Treatment, and Oxidation Conditions on Development and Breakdown of Protective Oxide Scales - DOE Contact E. E. Hoffman, (615) 576-0735, FTS 626-0735; Universal Energy Systems, Inc., Contact V. Srinivasan, (513) 426-6900

- o 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

484. Mechanical Properties of Oxide Films and Correlation with Metal/Oxide Interrace -DOE Contact E. E. Hoffman, (615) 576-0735; Oak Ridge National Laboratory Contact J. H. DeVan, (615) 574-4451

- o Conduct joint high temperature gas-metal reaction studies with researchers in Harwell's Materials Development and Metallurgy and Materials Physics Division.

485. A Study of Erosive Particle Rebound Parameters - DOE Contact E. E. Hoffman, (615) 576-0735; University of Notre Dame Contact T. H. Kosel, (219) 239-5642

- o Systematic investigation of the effects of materials properties and experimental variables on the rebound directions and velocities of erodent particles.

486. In Situ Scanning Electron Microscopy Studies of Erosion-Corrosion - DOE Contact E. E. Hoffman, (615) 576-0735; ORNL Contact J. R. Keiser, (615) 574-4453

- o Microscopically evaluate erosion-corrosion of alloys before and after being subjected to a flowing gas stream of erodent particles.

487. Study of Particle Rebound Characteristics and Material Erosion at High Temperature - DOE Contact E. E. Hoffman, (615) 576-0735; University of Cincinnati Contact W. Tabakoff, (513) 475-2849

- o 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.

488. Development of Nondestructive Evaluation Techniques for Structural Ceramics - DOE Contact E. E. Hoffman, (615) 576-0735; ANL Contact W. A. Ellingson, (312) 972-5068

- o Study and develop acoustic and radiographic techniques as well as possible novel techniques to characterize structural ceramics with regard to various properties and flaws.

489. Effect of Flaws on the Fracture Behavior of Structural Ceramics - DOE Contact E. E. Hoffman, (615) 576-0735; ANL Contact J. P. Singh, (312) 972-5123

- o Establish correlations between the composition, microstructure, and mechanical properties of structural ceramics with well-defined flaws.
- o Provide information to relate mechanical properties to nondestructive evaluation results.

490. Joining of Silicon Carbide Reinforced Ceramics - DOE Contact E. E. Hoffman, (615) 576-0735; Idaho National Engineering Laboratory Contact D. N. Coon, FTS 583-9738

- o Identify and develop techniques for joining silicon carbide fiber-reinforced composite materials.

491. Nondestructive Evaluation of Advanced Ceramic Composite Materials - DOE Contact E. E. Hoffman, (615) 576-0735; Idaho National Engineering Laboratory Contact J. B. Walter, FTS 583-0033

- o Develop an effective capability for nondestructive evaluation of ceramic fiber reinforced ceramic composites focusing on ultrasonic and radiographic techniques.

492. Investigation of the Mechanisms of Failure of Ceramic Materials for Hot Gas Filtration - DOE Contact E. E. Hoffman, (615) 576-0735; United Kingdom Coal Research Establishment/Oak Ridge National Laboratory Contact R. R. Judkins, (615) 574-4572

- o Investigate the mechanisms of failure of high temperature ceramic filters used for removing particulates from gas streams and apply the results to similar rigid ceramic filters.

493. High-Temperature Creep Behavior of Refractory Bricks - DOE Contact E. E. Hoffman, (615) 576-0735; Iowa State University Contact T. D. McGee, (515) 294-9619

- o Study of the creep behavior of high-chromia refractories suitable for lining the hot section of slagging gasifiers.

494. Weldability Studies of Advanced Austenitic Alloys - DOE Contact E. E. Hoffman, (615) 576-0735; ORNL Contact R. W. Swindeman, (615) 574-5108

- o 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.
- o Development of a suitable filler metal.

495. Investigation of Corrosion-Resistant Oxide Scales on Iron-Based Alloys in Mixed Gas Environments - DOE Contact E. E. Hoffman, (615) 576-0735; ORNL Contact J. H. DeVan, (615) 574-4451

- o 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 600-800°C.

496. Solid Particle Erosion in Turbulent Flows Past Tube Banks -DOE Contact E. E. Hoffman, (615) 576-0735; University of California, Berkeley, Contact R. Greif, (415) 642-6462

- o Investigation to improve the understanding of erosion processes in gas streams.

497. Modeling of Fibrous Preforms for CVD Infiltration - Doe Contact E. E. Hoffman, (615) 576-0735; Georgia Institute of Technology Contact T. L. Starr, (404) 894-3678

- o Development of an analytical model for the fabrication and infiltration of fibrous preforms.

- o 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.

498. Structural Reliability and Damage Tolerance of Ceramic Composites - DOE Contact E. E. Hoffman, (615) 576-0735; NBS Contacts E. R. Fuller and S. J. Schneider, (301) 921-2901

- o Characterization of the high temperature failure mechanisms of structural ceramics, especially silicon carbide and silicon nitride based materials, for use in coal conversion applications.

499. Improved Ceramic Composites Through Controlled Fiber-Matrix Interaction - DOE Contact E. E. Hoffman, (615) 576-0735; Pacific Northwest Laboratory Contact J. L. Bates, (509) 375-2579

- o Understand and control the fiber-matrix interface to improve the performance of ceramic matrix composites in fossil energy systems

500. Ceramic Catalyst Materials - DOE Contact E. E. Hoffman, (615) 576-0735; Sandia National Laboratory Contact B. Granoff, FTS 844-8145

- o Investigation of the role of ceramic materials properties in the activity and selectivity of novel catalytic materials.

501. Evaluation of Mechanical Properties of Advanced Austenitic Alloys - DOE Contact E. E. Hoffman, (615) 576-0735; ORNL Contact R. W. Swindeman, (615) 576-5108

- o Creep-rupture data on alloys developed in an earlier task will be gathered in the temperature range 600-760°C for times from 10 to 10,000 h.

Device or Component Fabrication, Behavior or Testing

502. "Materials and Components in Fossil Energy Applications" Newsletter - DOE Contact E. E. Hoffman, (615) 576-0735; Battelle-Columbus Laboratories Contact I. G. Wright, (614) 424-4377

- o Publish a periodic newsletter to address current developments in materials and components in fossil energy applications.

503. Studies of Materials Erosion in Coal Conversion and Utilization Systems - DOE Contact E. E. Hoffman, (615) 576-0735; LBL Contact A. V. Levy, (415) 486-5822

- o Determine the erosion-corrosion behavior of materials used in the flow passages of liquid slurries under conditions representative of those in coal liquefaction systems.

504. Mechanisms of Galling and Abrasive Wear - DOE Contact E. E. Hoffman, (615) 576-0735; National Bureau of Standards Contact L. K. Ives, (301) 921-2943

- o Study of the wear mechanisms of materials associated with valves in coal conversion systems.

505. Thermomechanical Modeling of Refractory Brick Linings for Slagging Gasifiers - DOE Contact E. E. Hoffman, (615) 576-0735; Massachusetts Institute of Technology Contact Oral Breyukozturk, (617) 253-7186

- o Study of the failure mechanisms of refractory-brick-lined coal gasification vessels under transient temperature loadings.

506. Alkali Attack of Coal Gasifier Refractory Linings - DOE Contact E. E. Hoffman, (615) 576-0735; Virginia Polytechnic Institute and State University Contact J. J. Brown, Jr., (703) 961-6777

- o Investigate the physical and chemical characteristics of alkali attack of coal gasifier linings under nonslagging conditions.

507. Thermodynamic Properties and Phase Relations for Refractory-Slag Reactions in Slagging Coal Gasifiers - DOE Contact E. E. Hoffman, (615) 576-0735; Pennsylvania State University Contact Arnulf Muan, (814) 865-7659

- o Determine the chemical constraints affecting the performance of refractory material under experimental conditions corresponding to those prevailing in slagging gasifiers.

508. Evaluation of Candidate Materials for Solid Oxide Fuel Cells - DOE Contact E. E. Hoffman, (615) 576-0735; Pacific Northwest Laboratory Contact J. L. Bates, (509) 375-2579

- o Develop highly electronically conducting oxides for use as cathodes in SOFCs

509. 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 Contact E. E. Hoffman, (615) 576-0735; Acurex Corporation Contact J. W. Sawyer, (415) 961-5700

- o Determination of the principal causes of failure of ceramic filters used for removal of fine particulates from high-temperature, high-ressure gas streams in coal conversion and utilization systems.

510. Development of a Design Methodology for High-Temperature Cyclic Application of Materials Which Experience Cyclic Softening - DOE Contact E. E. Hoffman, (615) 576-0735; University of Illinois Contact D. L. Marriott, (217) 333-7237

- o Develop a design methodology for high-temperature cyclic conditions, taking into account the effects of strain softening.

Instrumentation and Facilities

511. Management of the AR&TD Fossil Energy Materials Program - DOE Contact E. E. Hoffman, (615) 576-0735; ORNL Contacts R. R. Judkins, P. T. Carlson, (615) 574-4572

- o Management of the AR&TD Fossil Energy Materials Program under DOE approved guidelines.

512. Coal Conversion and Utilization Plant Support Services - DOE Contact E. E. Hoffman, (615) 576-0735; ORNL Contact J. R. Keiser, (615) 574-4453

- o Provide screening data on the susceptibility to corrosion and stress-corrosion cracking of potential materials of construction for coal conversion and utilization plants.

- o Provide failure analyses and on-site examination for the Wilsonville, Alabama, Advanced Coal Liquefaction Research and Development Facility and other coal conversion plants as needed.

Office of Surface Coal Gasification

Surface Gasification Materials Program

Materials Preparation, Synthesis, Deposition, Growth or Forming

513. Development of Iron Aluminides for Coal Gasification Systems - DOE Contacts G. F. Wheeler, (301) 353-3511, FTS 233-3511, and D. Dubis (METC), (304) 291-4399, FTS 923-4399; ORNL Contact C. T. Liu, (615) 574-5120

   o Development of low cost, low density intermetallic alloys for use as components in advanced fossil energy conversion and utilization systems.

514. Ceramic Fiber-Ceramic Matrix Hot-Gas Filters - DOE Contacts G. F. Wheeler, (301) 353-3511, FTS 233-3511, and D. Dubis (METC), (304) 291-4399, FTS 923-4399; ORNL Contact D. P. Stinton, 615-574-4556

   o Development of a ceramic fiber-ceramic matrix composite that will be suitable as a high-temperature particulate filter for use in hot-gas cleanup systems.

515. Protective Coatings and Cladding: Application/Evaluation - DOE Contacts G. F. Wheeler, (301) 353-3511, FTS 233-3511, and D. Dubis (METC), (304) 291-4399, FTS 923-4399; ANL Contact D. J. Baxter, (312) 972-5117

   o Experimental evaluation and thermodynamic analysis of metallic protective coatings for coal gasifier waste heat steam generators and superheaters.

   o Development of coating inspection methods.

516. Materials Development for Solid Oxide Oxygen Production Unit - DOE Contacts G. F. Wheeler, (301) 353-3511, FTS 233-3511, and D. Dubis (METC), (304) 291-4399, FTS 923-4399; Argonne National Laboratory Contacts E. E. Hoffman, (615) 576-0735 and R. B. Poeppel, (312) 972-5118

   o Development and implementation of solid oxide ceramic oxygen-generating devices in coal gasification systems.

PARAGRAPH DESCRIPTIONS

OFFICE OF ENERGY UTILIZATION RESEARCH

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

Energy Conversion and Utilization Technologies Division

The mission of 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) 586-5377; FTS 896-5377) 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 Tom Kollie ((615) 574-4571; FTS 624-4571). 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 1987 $50,000

DOE Contact: D. Mello, (202) 586-9345
The Pennsylvania State University (IAA No. DE-AI02-830R21350) 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. 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.

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

2. Tribological Surface Modifications and Coatings — FY 1987 $635,000

DOE Contact: D. Mello, (202) 586-9345
ANL (Contract No. W-31-109-ENG-38) Contact: Fred Nichols, (312) 972-8292

This program will provide quantitative experimental and theoretical information on improving tribological properties of solid materials for use under extreme conditions. Program emphasis will be on developing wear resistant and low friction surfaces for tribological systems operating under extreme conditions, such as high temperature (>600°C), high speed, high stress, and high chemical activity. This project commenced with two tasks: (1) the development of hard coatings for high speed steel cutting tools to improve tool life and performance; and (2) the development of novel coatings and surfaces for tribological systems operating under extreme environments. The initial process to be explored in the latter task is ion implantation and ion-beam-enhanced deposition. This will also include a modeling effort.

Keywords: Surface Modification, Coatings, Tribology, Friction, Wear, Ion Implantation

3. Modeling of Hard Coatings for Tribological Systems Operating Under Extreme Conditions — FY 1987 $ 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 has been written 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, 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 1987.

Keywords: Coatings, Friction, Wear, Metals, Machining

4. Tribological Studies on Coated High Speed Steel Cutting Tools — FY 1987 $ 0

DOE Contact: D. Mello, (202) 586-9345
University of California in Los Angeles (Contract No. DE-A102-84CE90227) Contact: Rointan Bunshah, (213) 825-2210

Hard coatings on T-15 tool steels were prepared by a patented Actuated Reactive Evaporation Process as part of the program on hard coatings being conducted at ANL, GWU and Borg-Warner. This project was concluded in FY 1987.

Keywords: Coatings, Friction, Wear, Metals, Machining

5. Abrasion and Impact Resistant Coatings — FY 1987 $125,000

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.

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

6. Mechanical Interactions of Rough Surfaces — FY 1987 $ 0

DOE Contact: D. Mello, (202) 586-9345
SKF Industries, Inc. (Contract No. DE-AC02-84ER13163) Contact: John McCool, (215) 265-1900, Ext. 267

This project is a joint effort with the Office of Basic Energy Sciences. The project is exploring the behavior of lubricated, concentrated contacts involving microscopically rough surfaces under conditions of combined rolling, sliding and spinning, with and without the presence of contaminating particles. It also is developing processing principles and techniques for the analysis of digitized rough surface profiles to yield surface descriptors that are predictive of functional performance and which have acceptable systematic and random error. It consists of both experimental and analytical work. This project is concluding in FY 1987.

7. Coordination of ECUT Plastics Recycling and Reuse Efforts

FY 1987
$35,000

DOE Contact: Stanley M. Wolf, (202) 586-5377
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. Currently, work, to be solicited by an open competition in FY 1988, is being planned 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

8. Ceramic Wear Microcontact Modeling

FY 1987
$100,000

DOE Contact: D. Mello, (202) 586-9345
SKF Industries, Inc. (Contract No. DE-AC02-87CE90001) Contact: John McCool, (215) 265-1900, ext. 267

This project is investigating the comparative tribological performance of ceramics and surface modified materials based on microgeometrical effects, and utilizing a microcontact model.

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

9. Assessment of the Economic Potential of Plastics Reuse

FY 1987
$10,000

DOE Contact: Stanley M. Wolf, (202) 586-5377
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, Economics

10. Laser Surface Modifications of Ceramics — FY 1987 $75,000

DOE Contact: Stanley M. Wolf, (202) 586-5377
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, Si_3N_4, or Al_2O_3 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.

Keywords: Structural Ceramics, Coatings and Films, Laser Annealing

11. Plasma-Assisted Sintering of Ceramics — FY 1987 $110,000

DOE Contact: Stanley M. Wolf, (202) 586-5377
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

12. Ion Implantation of Ceramics — FY 1987 $345,000

DOE Contact: Stanley M. Wolf, (202) 586-5377
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

13. Compositionally Modified Ceramics — FY 1987 $225,000

DOE Contact: Stanley M. Wolf, (202) 586-5377
ORNL (Contract DE-AC05-84OR21400) Contact: Rodney McKee, (615) 574-5144

This research task contains three elements: (1) materials synthesis and characterization, (2) mechanics and mechanical behavior studies, and (3) electrical and optical properties measurements. The ceramic system under initial investigation is layered structures of aluminum oxide and titanium oxides. The mechanical property characterization techniques used include: (1) dynamic resonance for studying the elastic-inelastic behavior, (2) ultra-low load microindentation for quantitative measurements of plastic deformation, and (3) conventional materials testing for strength and ductility studies.

Keywords: Structural Ceramics, Molecular Beam Epitaxy, Layers

14. Injection Molding of Electrosterically-Stabilized Oxide Suspensions in an Aqueous Medium — FY 1987 $65,000

DOE Contact: Stanley M. Wolf, (202) 586-5377
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 Molding, Polymers

15. Assessment of the State of the Art in Machining and Surface Preparation of Ceramics — FY 1987 $20,000

DOE Contact: Stanley M. Wolf, (202) 586-5377
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.

Keywords: Structural Ceramics, Machining, Surface Preparation

16. Microporous Ceramics — FY 1987 $160,000

DOE Contact: Stanley M. Wolf, (202) 586-5377
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

17. Chemical Vapor Deposition of Ceramic Composites — FY 1987 $160,000

DOE Contact: Stanley M. Wolf, (202) 586-5377
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

18. Thin-Wall Hollow Ceramic Spheres from Slurries — FY 1987 $240,000

DOE Contact: Stanley M. Wolf, (202) 586-5377
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 Al_2O_3-Cr_2O_3 was followed by experimental assessment of the structural and thermal insulation potential for these unique low density materials using both simulated models

and experimental measurements. 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

19. Strain Tolerant Ceramic Fibers from Liquid Crystal Polymer Precursors — FY 1987 $50,000

DOE Contact: Stanley M. Wolf, (202) 586-5377
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

20. Synthesis of SiC Whisker - $MoSi_2$ Matrix Composites for Elevated Temperature Applications — FY 1987 $50,000

DOE Contact: Stanley M. Wolf, (202) 586-5377
LANL (Contract W-7405-Eng-36) Contact: Frank Gac, (505) 667-5452

SiC whisker-$MoSi_2$ 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 $MoSi_2$. Initial room temperature mechanical property measurements indicate a composite strength nearly twice that of the pure $MoSi_2$, and a composite fracture toughness 30% higher than that of the pure $MoSi_2$.

Keywords: Metals, Alloys, Ceramics, Composites, Whiskers

21. Ordered Metallic Alloys for Lightweight Applications

FY 1987
$200,000

DOE Contact: Stanley M. Wolf, (202) 586-5377
ORNL (Contract No. DE-AC05-84OR21400) Contact: Wally Porter, (615) 574-5143
Dartmouth (ORNL Subcontract 19X-55918C) Contact: Erland Schulson, (603) 646-2888

The objective of this effort is to explore the potential of ordered intermetallic alloys for possible use as lightweight structural materials. Initial efforts are concentrating on magnesium-based alloys. Alloys based on Mg-Si, Mg-Si-Li, and Mg-Al were identified as candidates for initial development and have been under study.

Keywords: Non-ferrous Metals, Intermetallics, Magnesium

22. Assessment of Curing and Joining of Polymers

FY 1987
$10,000

DOE Contact: Stanley M. Wolf, (202) 586-5377
ORNL (Contract No. DE-AC05-84OR21400) Contact: Thomas Kollie, (615) 574-4571 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.

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

23. Separation of Impurities from Molten Metals Using MHD Forces

FY 1987
$135,000

DOE Contact: Stanley M. Wolf, (202) 586-5377
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

Materials Structures and Composition

24. Mechanisms of Adherence at Ceramic Joints — FY 1987 $160,000

DOE Contact: Stanley M. Wolf, (202) 586-5377
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/Welding, Adherence

25. Modeling of Boron-Effect in Ni_3Al — FY 1987 $860,000

DOE Contact: Stanley M. Wolf, (202) 586-5377
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 Ni_3Al 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-Ni_3Al.

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

26. Predictions of Ordered Intermetallics — FY 1987 $175,000

DOE Contact: Stanley M. Wolf, (202) 586-5377
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

27. Predictions of Super-Strong Liquid Crystal Polymers

FY 1987
$100,000

DOE Contact: Stanley M. Wolf, (202) 586-5377
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

28. Predictions of Polymer Decompositions

FY 1987
$140,000

DOE Contact: Stanley M. Wolf, (202) 586-5377
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

29. Influence of Electronic Structure on Ordered Intermetallics

FY 1987
$20,000

DOE Contact: Stanley M. Wolf, (202) 586-5377
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.

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

30. Reactive Polymer Processing Assessment — FY 1987 $ 0 ($15,000 in FY 1986)

DOE Contact: Stanley M. Wolf, (202) 586-5377
ORNL (Contract No. DE-AC05-84OR21400) Contact: Thomas Kollie, (615) 574-4571
University of Pittsburgh (ORNL Subcontract 32X-SA254V) Contact: Tom Lindt, (412) 624-5308

In order for polymeric materials to be used cost effectively to a greater extent in structural components of ground transportation vehicles, it is necessary that the speed of processing be increased. The purpose of this assessment is to determine technology research and development needs in reactive processing of polymers that could eventually facilitate the greater use of lightweight polymer-based structural components in energy-conserving applications in ground transportation vehicles.

Keywords: Polymers, Reactive Processing, Lightweight Materials

31. Liquid Crystalline Polymers Assessment — FY 1987 $ 0 ($25,000 in FY 85)

DOE Contact: Stanley M. Wolf, (202) 586-5377
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.

Keywords: Polymers, Liquid Crystals

32. Inorganic Polymers Assessment — FY 1987 $ 0 ($60,000 from FY 1985 and FY 1986)

DOE Contact: Stanley M. Wolf, (202) 586-5377
Pennsylvania State University (ORNL Consultant Subcontract) Contact: Harry Allcock, (814) 865-3527
ORNL (Contract No. DE-AC05-84OR21400) Contact: Randall Curlee, (615) 576-4864

The objective of this effort is to determine if there is a potential role for ECUT in supporting long-term, high-risk, base technology research and development that could result in the greater use of inorganic polymers. These materials are attractive for energy

conservation as they do not require a petroleum-based feedstock and they may have properties superior to the usual carbon-based polymers.

Keywords: Polymers, Inorganic, Lightweight Materials

33. Thermosetting Resins with Reversible Crosslinks — FY 1987 $75,000

DOE Contact: Stanley M. Wolf, (202) 586-5377
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

34. Biobased Polymers — FY 1987 $150,000

DOE Contact: Stanley M. Wolf, (202) 586-5377
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

35. Assessment of DoD/NASA Thermal Insulation Technology — FY 1987 $20,000

DOE Contact: Stanley M. Wolf, (202) 586-5377
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.

Keywords: Thermal Insulations, Aerospace

36. The Role of Inert Gas Entrapped in Rapidly Solidified Materials — FY 1987 $400,000

DOE Contact: Stanley M. Wolf, (202) 586-5377
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, Solidification-Rapid, Powder Synthesis

37. Novel Technique for Particulate Removal from Molten Metals — FY 1987 $100,000

DOE Contact: Stanley M. Wolf, (202) 586-5377
ORNL (Contract No. DE-AC05-84OR21400) Contact: D. O. Hobson, (615) 574-5109

This research is directed toward development of a device to remove particulates from a flowing molten metal stream just before it solidifies. Such removal is very important because of the recent trend toward near-net-shape castings. The device is electromagnetic and creates differential forces in the particles, causing them to migrate through the liquid stream.

Keywords: Removal, Particulates, Molten Metal

Materials Properties, Characterization, Behavior, or Testing

38. Ordered Metallic Alloys for High Temperature Applications — FY 1987 $690,000

DOE Contact: Stanley M. Wolf, (202) 586-5377
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: Non-ferrous Metals, High Temperature Service, Alloys, Ordered Intermetallics

39. Measurements of Grain Boundary and Surface Energies of Metals and Ceramics — FY 1987 $50,000

DOE Contact: Stanley M. Wolf, (202) 586-5377
ORNL (Contract DE-AC05-84OR21400) Contact: Thomas Kollie, (615) 574-4571

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

40. Effects of Laser Machining of Silicon Nitride — FY 1987 $50,000

DOE Contact: Stanley M. Wolf, (202) 586-5377
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

41. Assessment of Energy Conservation Implications of Corrosion — FY 1987 $15,000

DOE Contact: Stanley M. Wolf, (202) 586-5377
ORNL (Contract DE-AC05-84OR21400) Contact: Randy Curlee, (615) 576-4864
Battelle Columbus Laboratories (ORNL Subcontract 11X-78994V) Contact: W. Halder Fisher, (614) 424-6424

The objective of this study was to reexamine the database developed by BCD as part of a previous NBS study on the cost of metallic corrosion in the United States from the viewpoint of energy costs with energy conservation potential of solutions to corrosion problems being identified. Overall, the energy costs were estimated to be about 7 quads/year with about 2 quads/year as the estimate for potential energy savings with full application of current technologies.

Keywords: Corrosion, Energy Conservation

Device or Component Fabrication, Behavior, or Testing

42. Friction and Wear Research and Development — FY 1987 $350,000

DOE Contact: D. Mello, (202) 586-9345
ORNL (Contract No. DE-AC05-840R21400) Contact: Peter Blau, (615) 574-5377

Tribological experiments are run on high technology ceramics of current interest to determine apparent friction coefficients and wear rates and the ceramics are analyzed to elucidate the active wear mechanisms. A 5 X 5 matrix experiment was run in which pins of five types of ceramics were run against disks of themselves and the other four ceramic types. Ceramics studied included a Si_3N_4, a SiC, a toughened Al_2O_3, an

untoughened Al_2O_3, and a partially stabilized ZrO_2. Tests were conducted in air and dry nitrogen at room temperature, 400°, and 800°F, at speeds of 1 foot per second and nominal loads of 40 pounds per square inch (2 lb. normal load on 1/4-inch diameter pin). Further work is concentrating on defining the limits of the "no-" or "low-wear" region for these and other ceramics. A high temperature tribometer was constructed. Wear properties of ion-implanted titanium diboride are being investigated.

Keywords: Ceramics, Friction, Wear

43. Development of a Wear Theory of Ceramics — FY 1987 $100,000

DOE Contact: D. Mello, (202) 586-9345
Georgia Institute of Technology (ORNL Subcontract 780219X-15) Contact: Ward Winer, (404) 894-3270

The objectives of this effort are: (1) to observe and measure the temperature of "hot spots" during pin-on-disk tests of ceramics and (2) to develop a theory for the severe wear of ceramics based on plastic flow or melting of the hot spots. Pins of partially stabilized zirconia or silicon nitride are tested against sapphire (Al_2O_3) disks. The wear on the ends of the pins is observed optically through the transparent disk. The output expected from this work is a better understanding of the mechanisms of wear of ceramics, ultimately leading to improvements in the wear resistances of ceramics.

Keywords: Ceramics, Erosion and Wear

44. Lubricant Research and Development — FY 1987 $650,000

DOE Contact: D. Mello, (202) 586-9345
National Bureau of Standards: Gaithersburg (Interagency Agreement OR-21350) Contact: Stephen Hsu, (301) 921-2113

One objective of this effort is to improve the understanding of the influences of lubricant molecular structure on the lubricant qualities. Three commercial base stock (without additives) oils, commonly used in formulating engine oils, were separated into various molecular fractions and each fraction tested for friction and wear in a specially devised four-ball test and for oxidation stability in a unique micro-oxidation test. Chemical species produced during both tests are identified. The mechanisms for additive effectiveness are also investigated. New analytical and mechanical tests are developed. Measurements indicated there were significant differences in the lubricant qualities of the various molecular constituents of base stock oils. The most lubricous molecular constituent has been identified and its structure is being investigated. An in-situ micro-Raman spectroscope has been developed and is being utilized for lubricant film tribochemical analysis.

Keywords: Metals, Oils, Friction, Wear, Engines

45. Energy Efficient Gears — FY 1987 $50,000

DOE Contact: D. Mello, (202) 586-9345
Northwestern University (NBS Subcontract No. 60NANBD0547) Contact: Herbert Cheng, (312) 491-7062

This project has developed a friction model in partial-elastohydrodynamic and boundary lubrication for prediction of power loss in spur gears due to rolling and sliding. A new two-disk friction testing machine has been designed and constructed and experiments have been conducted which validate the model. A dynamic time dependent wear model for partial-elastohydrodynamic contact is under development.

Keywords: Gears, Oils, Frictions, Wear, Engines

46. Modeling of Solid Ceramic Joints — FY 1987 $ 0 ($175,000 in FY 1986)

DOE Contact: Stanley M. Wolf, (202) 586-5377
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.

Keywords: Ceramics, Metals, Joining, Models

47. Electromagnetic Joining of Ceramics - Laboratory Proof of Concept — FY 1987 $100,000

DOE Contact: Stanley M. Wolf, (202) 586-5377
Quest Research Corporation (formerly DHR, Incorporated) (ORNL Subcontract 86X-00217C) Contact: Richard Silberglitt, (703) 893-6401
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

48. Development of Tests for Ceramic-Ceramic and Ceramic-Metal Joints FY 1987 $120,000

DOE Contact: Stanley M. Wolf, (202) 586-5377
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/Welding, Tests

49. Nondestructive Evaluation (NDE) of Ceramic Joints FY 1987 $120,000

DOE Contact: Stanley M. Wolf, (202) 586-5377
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.

Keywords: Structural Ceramics, Joining/Welding, NDE

50. NMR of Green State Ceramics FY 1987 $ 0 ($ 75,000 in FY 1986)

DOE Contact: Stanley M. Wolf, (202) 586-5377
ANL (Contract W-31-109-Eng-30) Contact: Bill Ellingson, (312) 972-5068

This work explores the use of advanced nuclear magnetic resonance (NMR) imaging methods to characterize green-state ceramic materials, particularly the detection and mapping of binder/plasticizer distribution and porosity. An existing NMR imaging system has been highly modified and a set of well-defined ceramic test specimens is used to determine the sensitivities of NMR to gross inhomogeneities in the green-state.

Keywords: Structural Ceramics, NDE, Green State

51. Assessment of Energy Conservation Implications of High Temperature Superconductors FY 1987 $20,000

DOE Contact: Stanley M. Wolf, (202) 586-5377
ORNL (Contract No. DE-AC05-84OR21400) Contact: Thomas Kollie, (615) 574-4571

The objective of this effort was to determine if there is enough energy conservation potential in possible future applications of the recently discovered high temperature (transition temperatures on the order of 100°K) superconductors to warrant more detailed assessments. These would help ECUT to establish a proper role in the future support of research and development aimed at eventual applications of such materials in energy conserving systems. Completed in May 1987 by ORNL staff members, the assessment concluded that the theoretical (upper bound) energy conservation potential is enormous but it also warned that so little is known at present about the materials or even the possible applications that it was impossible to state how much of that upper bound, theoretical potential could reasonably be expected to ever be realized even in the long term. A larger, more in-depth assessment effort, to be jointly funded by DOE ECUT and Fossil Energy and the Electric Power Research Institute (EPRI), was being organized for early FY 1988.

Keywords: Superconductors, Ceramics, Assessment

Instrumentation and Facilities

52. Assessment of X-ray Methods for Investigations of Ceramic Wear Surfaces FY 1987 $37,500

DOE Contact: Stanley M. Wolf, (202) 586-5377
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.

Keywords: Ceramics

53. Thin Film Thermocouples for Heat Engines — FY 1987 $100,000

DOE Contact: Stanley M. Wolf, (202) 586-5377
National Bureau of Standards: 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 (nisil-nicrosil); and platinum- platinum 6% 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.

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 Sam Tagore, (202) 586-9210.

Materials Properties, Behavior, Characterization or Testing

54. Unguarded Thin Heater Tester

FY 1987
$100,000

DOE Contact: Sam Tagore, (202) 586-9210
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

55. Studies of Loose-Fill Insulation

FY 1987
$90,000

DOE Contact: Sam Tagore, (202) 586-9210
ORNL Contact: David McElroy, (615) 574-5976

Loose-fill cellulosic and mineral fiber insulating materials are being subjected to both laboratory and field studies to determine the effects of settling on density and R-value. These materials are typically sold on the basis of the R-value as-installed. R-value is a function of insulation thickness and density, and pronounced settling results in a lower than anticipated insulating capacity for a given quantity of material. Laboratory testing involves vibration of these materials in a simulated wall cavity. The in situ studies consist of repeated visits to sites in several parts of the country, over as long as two years, to record measurements of insulation depth and density in residential attics. A series of reports and technical presentations will result from this effort.

Keywords: Building Insulation, Settled Density, Nondestructive Evaluation

56. Heat Flow Modeling

FY 1987
$50,000

DOE Contact: Sam Tagore, (202) 586-9210
ORNL Contact: David McElroy, (615) 574-5976

There are two aspects in this effort. The first is the mathematical modeling of heat transfer along longitudinal and radial coordinates. One dimensional heat flow studies in various materials are being undertaken and calculation of errors associated with edge heat loss effects are also considered.

The second component involves the physical description of heat transfers in a material with respect to "apparent" thermal conductivity. The factors that contribute to heat transfer phenomena are being studied in detail.

Keywords: Building Insulation, Heat Transfer, Mathematical Modeling

57. Heat Flux Transducer Calibration Design — FY 1987 $30,000

DOE Contact: Sam Tagore, (202) 586-9210
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 was initiated 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. The task will be completed in FY 1989.

Keywords: Calibration, Heat Flux Transducers, Roof Tester Panels

58. Variable R/Switchable Surface Analysis — FY 1987 $40,000

DOE Contact: Sam Tagore, (202) 586-9210
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

59. Building Materials Research Plan and Moisture Studies — FY 1987 $140,000

DOE Contact: Sam Tagore, (202) 586-9210
NJIT Contact: Erv Bales, (201) 596-3010

There are two aspects in this effort. The first is a chapter presenting the national need for research on building materials by the Building Thermal Envelope Coordinating Committee. This resulted in a Research Agenda with 81 project description. The second aspect is a study of moisture interactions with buildings materials to establish threshold

conditions for temperature and humidity for mildew initiation and propagation. Models for mildew growth will be developed from experimental parameters.

Keywords: National Needs for Research, Research Agenda, Mildew, Moisture

60. Analysis of Metal Building Behavior — FY 1987 $70,000

DOE Contact: Sam Tagore, (202) 586-9210
BNL Contact: W. Loss, (516) 666-2052

This project includes testing and analysis of heat transfer associated with a metal building at Brookhaven. The building was instrumented to guide an ASHRAE type analysis of U-values and infiltration rates. The overall U-value was 12 Btu/ft^2-F-day despite large fastener losses. Suggestions are provided for reducing heat losses by 30 percent.

Keywords: Metal Building, Fasteners, Infiltration, U-Values

61. Assessment of Properties of Wood — FY 1987 $20,000

DOE Contact: Sam Tagore, (202) 586-9210
Forest Products Laboratory Contact: A. Ten Wolde, (608) 264-5629

This assessment is to determine the variability and significance of thermal properties of wood products as a function of moisture content and species. The voids in the data base will be identified.

Keywords: Wood, Wood Products, Thermal Conductivity, Specific Heat, Moisture Content

62. Recommended R-Levels - ZIP Program — FY 1987 $45,000

DOE Contact: Sam Tagore, (202) 586-9210
NBS Contact: Steve Petersen, (301) 975-6136

This effort has two thrusts. 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 thrust is to document the computer program ZIP used to provide the recommendations. This documentation and the ZIP program will be available in FY 1988 for use by the energy conservation community.

Keywords: Recommended R-Values, Computer Program, Cost-Effective Analysis

63. Impact of CFC Restrictions — FY 1987 $40,000

DOE Contact: Sam Tagore, (202) 586-9210
NBS Contact: H. Fanney, (301) 975-5864

Restrictions on CFC gas availability may remove thermally efficient insulations from use. This study evaluates the thermal performance and economics of alternative insulations that contain smaller or zero levels of CFC on wall and roof applications.

Keywords: Insulation Sheathing, Walls, Roofs, Economic Analysis

64. Gas Diffusion and Effective Conductivity of Foam Insulation Versus Age — FY 1987 $95,000

DOE Contact: Sam Tagore, (202) 586-9210
MIT Contact: Leon Glicksman, (617) 253-2233

Freon-blown rigid urethane foam insulation is being investigated under this task, to quantify the degree to which the effective thermal conductivity of insulation foamed with low thermal conductivity refrigerants changes due to diffusional effects as the insulation ages. A quasi-one dimensional model with upper and lower limits is used to examine heat conduction through the solid and gas in the foam insulation, and to study the effect of cell-wall geometry and cell arrangement on the thermal resistance, as well as the effect of the thermal conductivity of the solid and the amount of solid in the corners of the nodules. 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

65. Improved Standard Reference Materials — FY 1987 $50,000

DOE Contact: Sam Tagore, (202) 586-9210
NBS Contact: Hunter Fanney, (301) 975-5864

Candidates for improved standard reference materials are being investigated under this task, using a one meter diameter line-heat-source guarded hot plate. At present, only two materials are available from NBS for calibrating guarded hot plates and heat flow meters. A need exists to supply the measurement community with calibration samples whose apparent thermal conductivity and thermal resistance is both higher and lower than those now available, either using materials that more nearly resemble those that will be measured in current production or using an entirely new calibration material approach.

The results of this effort will be, first, an assessment of candidate materials and, later, an improved standard reference material.

Keywords: Building Insulation, Heat Transfer, Nondestructive Evaluation

66. High Temperature Insulation Standard Reference Materials

FY 1987
$75,000

DOE Contact: Sam Tagore, (202) 586-9210
NBS Contact: D. R. Smith, (303) 497-3733

Ceraboard and a high temperature loose-fill insulation are candidates to be investigated for use as new Standard Reference Materials (SRM), using a new 800°K guarded hot plate being completed as part of this effort. High temperature SRMs are needed in the industrial insulation field, and it is expected that this effort will complete certification testing of one such material during FY 1987.

Keywords: Industrial Insulation, Heat Transfer, Nondestructive Evaluation

67. Assessment of Low Density Concretes and Cement Insulation

FY 1987
$30,000

DOE Contact: Sam Tagore, (202) 586-9210
NBS Contact: Walter Rossiter, (301) 975-6719

A study is being conducted to review existing information and building practices concerning the use of lightweight concrete in construction and foamed cement insulation in wall cavities. The review focuses on the properties and composition of the materials, test methods used for evaluating the materials, the effect of the materials on other building components, types of applications and constructions for which they are used, and installation techniques. Gaps in technical knowledge regarding the use and characterization of these materials will be identified and used to define subsequent research in this area.

Keywords: Building Insulation, Cements and Concrete, Foam Generation, Autoclaving, Conventional Solidification

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

68. Composite Cathode Material Development — FY 1987 $150,000

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

TiB_2-Graphite samples will be tested in commercial cells to determine optimum composition and factors that affect long term life. Configuration and voltage reduction tests will be performed in a 6000 ampere test cell. This project will be completed in FY 1989.

Keywords: Composites, Cathode

69. Cerox Inert Anode Material — FY 1987 $150,000

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

The addition of CeO_2 to molten cryolite produces a coating on oxygen evolving electrodes. The factors controlling the in situ formation of the coating, the coating characteristics, and the coating stability have been evaluated. Additionial studies are planned for FY 1988. Metal purity and voltage drops will be determined for commercial aluminum reduction cell operating conditions.

Keywords: Coatings, Anode, Ceramics

70. Corrosion Resistant Amorphous Metallic Films — FY 1987 $246,000

DOE Contact: William Sonnett, (202) 586-2389
JPL Contact: Edward Cuddihy, (818) 354-3188

A technology is being developed for depositing amorphous metallic films having high corrosion resistance on carbon steel shapes of industrial interest. Magnetron sputtering is being used to deposit mixtures of MoCrB and TiCrPC. The objective is to provide a construction material that will reduce the impact of corrosion on heat transfer, equipment maintenance and capital cost. The project will end in FY 1988.

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

71. Investigation of Material for Inert Electrodes in Aluminum Electrodeposition Cells — FY 1987 $ 0

DOE Contact: M. J. McMonigle, (202) 586-2082
MIT Contact: J. S. Haggarty, (617) 253-3300

Materials prepared and tested are variations of $NiO\text{-}NiFe_2O_4$ for inert anodes and TiB_2 for stable cathodes. Laser units were used to generate ultra pure powders and single crystals of candidates. Electrical conductivity and rate of solution tests in cryolite melts will be run. Test results have lead to the development of a selection criteria for stable electrode materials. This project was completed in FY 1987.

Keywords: Ceramics, Material Science, Aluminum, Cryolite

Materials Properties, Behavior, Characterization or Testing

72. Diagnostic Sources of Current Inefficiency in Industrial Molten Salt Electrolytic Cells by Raman Spectroscopy — FY 1987 $ 0

DOE Contact: M. J. McMonigle, (202) 586-2082
MIT Contact: D. R. Sadoway, (617) 253-3300

Aluminum chloride and magnesium chloride melts have been analyzed with Raman spectroscopy to determine bath chemistry during electrolysis. Reports will be published early FY 1988. Identification of molten species in cryolite melts will lead to the identification of process chemical steps and possible sources of current efficiency losses. This project will be completed the second quarter of FY 1988.

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

73. Expand and Control Inert Electrode Cell Operating Conditions — FY 1987 $800,000

DOE Contact: M. J. McMonigle, (202) 586-2082
PNL Contact: Pat Hart, (509) 375-2906
MIT Contact: John Haggarty, (617) 253-3487

Cermets of Ni-Fe spinels with copper additions have been tested. Operating conditions have been identified that provide 99.8 aluminum and low anode wear rates. Confirmation tests and boundary conditions for operations will be determined in FY 1988. Failure mechanisms for TiB_2 based materials have been investigated. TiB_2 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 Properties, Behavior, Characterization or Testing

74. Advanced Heat Exchanger Material Technology Development — FY 1987 $800,000

DOE Contact: S. Richlen, (202) 586-2078
ORNL Contact: E. Long, (615) 574-5172

This project conducts research to develop improved materials and fabrication processes and to expand the materials data base for advanced ceramic heat exchangers. Currently the project is studying the effects of corrosive waste stream constituents on candidate ceramic 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

75. Assessment of Strength Limiting Flaws in Ceramic Heat Exchanger Components — FY 1987 $344,000

DOE Contact: S. Richlen, (202) 586-2078
Babcock & Wilcox Contact: T. Powers, (804) 522-5038

This project studies the flaw populations and the effect of operating environments on flaw populations of ceramic heat exchanger components. Currently the project is

studying flaw populations and population changes under exposure to thermal environments by using various advanced non-destructive evaluation techniques. 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

76. National Laboratory Support to Assessment of Strength Limiting Flaws in Ceramic Heat Exchanger Components — FY 1987 $168,000

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.

Keywords: Structural Ceramics, NDE, Structure

Device or Component Fabrication, Behavior or Testing

77. HiPHES System Design Studies — FY 1987 $400,000

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

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

Keywords: Composite Ceramics, Heat Exchangers

78. Fiber Architecture Design Studies — FY 1987 $200,000

DOE Contact: S. Richlen, (202) 586-2078
ORNL Contact: J. Blass, (615) 574-0721

This project will develop design methods for ceramic composites to support design of HiPHES components.

Keywords: Composite Ceramics, Fiber Architecture

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

79. Silicon Carbide Powder Synthesis — FY 1987 $ 0

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. Ray Johnson, (615) 576-6832
Standard Oil Engineered Materials 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, which has been completed, 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 is nearing completion, incorporates the following elements:

- Scale-up of the process 5-10X over the laboratory scale process has been achieved.
- As soon as the system is successfully brought on-line, confirmatory experiments and 3-5 experimental runs to confirm laboratory scale results and to fine-tune operating conditions will be performed.
- Process flowsheets will then be developed and economic analyses performed to identify capital and operating costs for the commercial production of gas phase SiC in conjunction with the process development program.

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

80. Turbomilling of SiC — FY 1987 $124,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: T. N. Tiegs, (615) 574-5173
Southern Illinois University Contact: Dale E. Whittmer, (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 has been expanded to 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

81. Sintered Silicon Nitride — FY 1987 $200,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. Ray Johnson, (615) 576-6832
Army Materials Technology Lab Contact: G. E. Gazza, (617) 923-5408

The program is concentrating on sintering compositions in the Si_3N_4-Y_2O_3-SiO_2 system using a two-step sintering method where the N_2 gas pressure is raised to 7-8 MPa during the second step of the process. During the sintering, dissociation reactions are suppressed by the use of high nitrogen pressure and cover powder of suitable composition over the specimen. Variables to be studied include sintering process parameters, source of starting powders, milling media and time, and specimen composition. Room temperature modulus of rupture, high temperature stress rupture, oxidation resistance, and fracture toughness will be determined.

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

82. Si_3N_4 Powder Synthesis — FY 1987 $478,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. Ray Johnson (615) 576-6832
Ford Contact: G. M. Crosbie, (313) 574-1208

The goal is to achieve major improvements in the quantitative understanding of how to produce sinterable Si_3N_4 powders having highly controlled particle size, shape, surface area, impurity content, and phase content. Of interest to the present powder needs is a silicon nitride powder of high cation and anion purity without carbon residue. The process study has been directed towards a modification of the low temperature reaction of $SiCl_4$ vapor with liquid NH_3.

A pilot plant design for the "vapor-chloride - liquid ammonia" direct reaction 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.

During the next phase of the project, the goal will be to test for unique properties of the ceramics sintered from low carbon powders, before committing to a pilot plant of the scale designed.

Keywords: Silicon Nitride, Powder Synthesis, Structural Ceramics

83. Processing Of Monolithics — FY 1987 $1,000,000

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 develop 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, resulting in a high-temperature ceramic with the strength and toughness required of an AGT rotor, and with a Weibull modulus of approximately 20.

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

84. Dispersion Toughened Si_3N_4 — FY 1987 $ 0

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: T. N. Tiegs, (615) 574-5173
Garrett Processing Company: 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.

A follow-on program has been planned to identify the key processing parameters for densified composite microstructure/ properties with improved strength and toughness from room temperatures for net-shape fabrication of high temperature composite components.

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

85. Dispersion Toughened Si_3N_4 FY 1987 $ 0

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: T. N. Tiegs, (615) 574-5173
Rockwell International Corp./Rocketdyne Div. Contact: G. D. Schnittgrund, (818) 710-5972

This work sought to develop high toughness, high strength refractory ceramic matrix composites that could be made at low cost and to near-net-shape for heat engine applications. The composite system selected for development was based on a silicon nitride matrix toughened by dispersions of ZrO_2, HfO_2, or $(Hf,Zr)O_2$ modified with suitable additions of other refractory ceramics to control the physical behavior. The desired microstructure and optimum mechanical properties were developed by expeditious laboratory process methods including colloidal suspension, press forming, sintering, and hot pressing.

Two composite systems composed of Si_3N_4 plus a dispersion of ZrO_2 particles were shown to exhibit improved properties over that of a Si_3N_4 matrix. HfO_2 (Y_2O_3) was successfully substituted for ZrO_2 (Y_2O_3) with an associated gain in strength. Colloidal processing produced composites with excellent dispersion and homogeneity.

Keywords: Silicon Nitride, Composites, Transformation, Sintering, Hot Pressing

86. Dispersion Toughened Si_3N_4 FY 1987 $200,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: M. A. Janney, (615) 574-4281
GTE Labs Contact: S. T. Buljan, (617) 890-8460

This task has three primary objectives: (1) to develop 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.

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

87. Composite Development — FY 1987 $560,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. Ray Johnson, (615) 576-6832
Norton Company Contact: C. A. Ebel, (617) 393-5950

The objective of this task is 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 is 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% SiC whiskers have been applied. Whiskers from domestic and foreign suppliers have been 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.

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

88. Advanced Composites — FY 1987 $168,000

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 work is to optimize the sintering procedure to densify silicon nitride-silicon carbide composites. Three matrix systems were chosen for the study: (1) Si_3N_4-Al_2O_3-AlN, (2) Si_3N_4-Al_2O_3-AlN-Y_2O_3, and (3) Si_3N_4-Al_2O_3-AlN-MgO.

Composites containing 20 percent whiskers in the system containing Y_2O_3 have been 90 percent densified, while samples with a density of over 80 percent have been obtained in the SiAlON system.

Keywords: Composites, Silicon Nitride, Whiskers, Silicon Carbide, Sintering, SiAlON

89. Dispersion Toughened Oxide Composites — FY 1987 $322,000

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.

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

90. Transformation Toughened Ceramics Processing — FY 1987 $362,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: P. F. Becher, (615) 574-5157
Norton Company Contact: Giulio A. Rossi, (617) 393-6600

The objective of this work is the production of improved zirconia toughened ceramics (ZTC) for advanced engine applications. The scope includes the powder synthesis and characterization of the sintered ceramics. Materials made from three powder sources have been evaluated: a rapid solidification from-the-melt powder, and two chemically derived powders.

Rapidly solidified powders showed better performance than chemically derived ones.

Keywords: Composites, tt-ZrO_2, Powder, Sintering, Alumina

91. Development of Toughened Ceramics — FY 1986 $107,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. Ray Johnson, (615) 576-6832
Ceramatec Contact: R. A. Cutler, (801) 486-5071

This project is working on 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 addresses processing methods for fabricating these layered composites via sintering.

These studies 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. Demonstration of the retention of residual stresses with temperature is a primary purpose of this project.

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

92. Sol-Gel Oxide Powder — FY 1987 $100,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. Ray Johnson, (615) 576-6832
ORNL Contact: W. D. Bond, (615) 574-7071

This project involved determination of the feasibility of sol-gel processes for (1) synthesizing powders of phase-stabilized zirconia and alumina and (2) for mullite preparation by reaction-sintering of Al_2O_3-SiO_2 gel powders.

Keywords: Powder Synthesis, Sintering, Sol Gel, Oxide Powder, Alumina, Zirconia, Yttria, Hafnia, Silicon Carbide, Whiskers

93. Advanced Transformation Toughened Oxides — FY 1987 $ 0

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

The objective was to develop a thermal insulating material which has sufficient strength and toughness for heat engine applications. The approach was to explore the composite materials in the system Al_2O_3:Cr_2O_3/ZrO_2:HfO_2. The ultimate goal of this research was to optimize toughness and strength of the composite material by controlling the microstructure using processing methods.

Specimens with a fracture strength of 900 MPa and a toughness of 11 $MN(m)^{1/2}$ were prepared in the laboratory.

Keywords: Composites, Transformation Toughened, Alumina, Mullite, Chromia

94. Injection Molded Composites — FY 1987 $186,000

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

95. Low Expansion Ceramics — FY 1987 $150,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. Ray Johnson, (615) 576-6832
Virginia Polytechnic Institute and State University Contact: J. J. Brown, Jr. (703) 961-6777

Research is being conducted to develop an isotropic, ultra-low 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.

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

96. Active Metal Brazing PSZ-Iron — FY 1987 $200,000

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. This work is focused on the joining of partially stabilized zirconia to nodular cast iron by brazing. The emphasis for this work for FY 1987 was to investigate: (1) the effect of thermal aging and testing temperature on the strength of joints between zirconia and cast iron, (2) the possibilities for using alternate ceramic and metallic materials in brazed components, and (3) residual stress patterns in ceramic-to-metal braze joints using indentation techniques.

A novel method for brazing zirconia to cast iron has been established.

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

Materials Properties, Behavior, Characterization or Testing

97. Ceramic Component Design Technology — FY 1987 $100,000

DOE Contact: Saunders B. Kramer, (202) 586-8012
NASA Contact: John Gyekenyesi, (216) 433-3210

The advanced finite element and probability codes required to design, analyze and optimize ceramic components are being developed. Enhancement of the SCARE code with new subroutines continues.

Keywords: Design Methodology, Engines

98. Microstructural Modeling of Cracks — FY 1987 $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. Because of this roughness, crack face interaction influences fracture initiation. Thus, the goal of this study is to investigate this effect under arbitrary stress states.

Keywords: Predictive Behavior Modeling, Structural Ceramics

99. Adherence of Coatings — FY 1987 $18,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: C. J. McHargue, (615) 574-4344
University of Tennessee Contact: J. E. Stoneking, (615) 974-2171

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

100. Dynamic Interfaces — FY 1987 $175,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: E. L. Long, Jr., (615) 574-5172
Battelle Columbus Labs 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 to be 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 to be carefully characterized before and after testing to provide detailed input into the model.

The need for lubrication at the ring/cylinder interface was 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.

Efforts for a second phase will address 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

101. Advanced Statistical Calculations — FY 1987 $60,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. Ray Johnson, (615) 576-6832
ORNL Contact: W. P. Eatherly, (615) 574-5220

The goal of this task was to design advanced statistical tools for characterizing the strength of structural ceramics in a meaningful and realistic way for use in design codes.

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

102. Advanced Statistics Calculations — FY 1987 $ 0

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: W. P. Eatherly, (615) 574-5220
GE Research Lab 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 or Technique Development

103. Physical Properties — FY 1987 $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 conductivities of toughened structural ceramics at high temperatures. The role of photon transport at high temperatures and the influence of second phase additions is 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

104. Translucence Effects — FY 1987 $3,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. L. McElroy, (615) 574-5976
Integral Technologies Inc. (ITI) Contact Thomas Morel, (312) 789-0003

The purpose of this task is 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 has been 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

105. Project Data Base — FY 1987 $103,000

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

106. Characterization of Transformation-Toughened Ceramics

FY 1987
$100,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. Ray Johnson, (615) 576-6832
U.S. Army Materials Technology Lab. (AMTL) Contact: Jeffrey J. Swab, (617) 923-5410

The task has several objectives. The main objective is to determine the effect of time-at-temperature on transformation toughened zirconias, especially tetragonal zirconia polycrystals (TZP) at engine operating temperatures (1000-1200°C). A preliminary study of the degradation of mechanical properties at low temperatures (200-400°C) in yttria-doped zirconias has also been initiated.

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 indicate that within the 200-400°C temperature range, the TZP material becomes "destabilized," resulting in a large loss of mechanical properties and even catastrophic failure of the test sample.

Keywords: Alumina, Transformation Toughened Zirconia Oxide, High Temperature Service, Engines, Fracture

107. Fracture Behavior of Toughened Ceramics

FY 1987
$207,000

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 is 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 were 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

108. Cyclic Fatigue of Toughened Ceramics — FY 1987 $215,000

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

109. Rotor Materials Data Base — FY 1987 $250,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. Ray Johnson, (615) 576-6832
ORNL Contacts: K. C. Liu, (615) 574-5116; M. K. Ferber, (615) 576-0818

The purpose of this activity is to generate high temperature mechanical properties data for candidate ceramic rotor materials.

Keywords: Creep, Engines, High Temperature Service, Structural Ceramics

110. Static Behavior of Toughened Ceramics — FY 1987 $15,000

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

The fatigue behavior of several commercially-available MgO partially stabilized zirconias (Mg-PSZ) was studied by measuring the strength (S_f) as a function of time, temperature, and applied stress level. The strength was determined using an interrupted fatigue (I.F.) test in which flexure samples were exposed at temperatures between 500 and 1000°C for times up to 1000 hours. The applied stress was maintained at a percentage of the short-term S_f value measured at the same temperature. SEM, TEM, optical microscopy, X-ray diffraction, micro-Raman spectroscopy, and dilatometry were used to characterize both the as-received and tested I.F. specimens.

Results indicated that the application of the Mg-PSZ ceramics as high temperature components would be limited to temperatures of 800°C and below, particularly when substantial mechanical stresses are involved.

Keywords: Fatigue, Fracture Strength, Toughened Ceramics, Structure, Static Behavior

111. Ceramic Durability Evaluation AGT — FY 1987 $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 35,000 hours will be evaluated.

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

112. Ceramic Corrosion Evaluation AGT — FY 1987 $100,000

DOE Contact: Saunders B. Kramer, (202) 586-8012
NASA Contact: Carl A. Stearns, (216) 433-5504

Ceramic material specimens, including silicon carbide, silicon nitride, and glass ceramic materials will be evaluated in a combustion rig simulating turbine engine conditions. After exposure to combustion products seeded with various impurities corrosion effects and strength will be determined.

Keywords: Structural Ceramics, Glass Ceramics, Corrosion

113. Corrosion/Erosion Effects — FY 1987 $50,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. Ray Johnson, (615) 576-6832
National Bureau of Standards (NBS) Contact: S. M. Wiederhorn, (301) 975-2000

The objective of this work is to identify the mechanisms of failure in structural ceramics subjected to mechanical loads in various test temperatures and environments. Of particular interest is the damage that accumulates in structural ceramics as a consequence of high temperature exposure to environments and stresses normally present in heat engines.

Early in the study, the corrosion reactions of molten sodium carbonate were studied using analytical scanning transmission electron microscopy. Thin films were used to identify interfacial reactions and compositions of corrosion scales on the surface of alpha-silicon carbide as a consequence of the reaction. Recently, reaction bonded silicon

carbide samples that had been subjected to deformation in bending and tension were studied extensively to determine the source of failure in these materials at elevated temperatures.

Keywords: Corrosion, Engines, Erosion, Structural Ceramics, Silicon Carbide, Surface, AGT, Combustion

114. Environmental Effects In Toughened Ceramics — FY 1987 $500,000

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 eight PSZ- and DTA-toughened ceramics using primarily the dynamic fatigue measurement. Flexure 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

115. High Temperature Fracture Toughness Measurement — FY 1987 $ 0

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: Victor J. Tennery, (615) 574-5123
University of Washington Contact: R. C. Bradt, (206) 543-2600

Improved fracture toughness test(s) are being developed and will be demonstrated for both monolithic and composite structural ceramics over the broad temperature range from 20°C to 1400°C. The objective is to develop simple and inexpensive methods to be considered as standard for measuring fracture resistance.

Keywords: Composites, Structural Ceramics, Fracture, High Temperature

116. High Temperature Tensile Testing — FY 1987 $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 Si_3N_4 tensile samples have been tested using the new ORNL self-aligning grip system at three stressing rates.

Fractography indicated that fracture was transgranular at room temperature and the fracture origins were normally porosities and occasionally inclusions.

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

117. Standard Tensile Test Development — FY 1987 $120,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. Ray Johnson, (615) 576-6832
National Bureau of Standards (NBS) Contact: S. M. Wiederhorn, (301) 975-2000

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

Keywords: Creep, Structural Ceramics, Tensile Testing

118. Fracture Toughness Determination of Thin Coatings — FY 1987 $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 indention experiments using the mechanical properties microprobe.

Keywords: Fracture, Structural Ceramics

119. Non-Destructive Evaluation — FY 1987 $141,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. Ray Johnson, (615) 576-6832
ORNL Contact: R. W. McClung, (615) 574-4466

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

120. Ceramic Component NDE Technology — FY 1987 $90,000

DOE Contact: Saunders B. Kramer, (202) 586-8012
NASA LeRC Contact: Alex Vary, (216) 433-6019

Advanced NDE techniques for screening and evaluating ceramic materials and components are being identified and developed.

Keywords: Ceramics, NDE

121. Computed X-Ray Tomography — FY 1987 $120,000

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 aim of this effort is to develop X-ray beam hardening corrections for polychromatic X-ray sources when used with computed tomography machines to inspect structural ceramics and to develop appropriate test phantoms for calibration of these scanners.

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

Technology Transfer and Management Coordination

122. Standard Reference Materials — FY 1987 $270,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. Ray Johnson, (615) 576-6832
NBS Contact: A. L. Dragoo, (301) 975-5785

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, NBS, Reference Material, Powder Characterization, Structural Ceramics

123. Technology Transfer Assessment, Support Contracts, IEA

FY 1987
$255,000

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 or Technique Development, Technology Transfer, Assessment, Research, Subcontractors, Exhibits, Meetings

124. Management And Coordination

FY 1987
$752,000

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

125. Metal-Ceramic Joints

FY 1987
$499,000

DOE Program 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/Welding, Metals, Structural Ceramics, AGT, Metal-Ceramic

126. Metal-Oxide Ceramic Joints — FY 1987 $625,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. Ray Johnson, (615) 576-6832
Battelle Columbus Laboratories Contact: R. A. Schmidt, (614) 424-4396

The objective of this project is to develop the analytical tools necessary to design reliable high strength ceramic oxide-to-ceramic oxide and ceramic oxide-to-metal joints. The technical work involves both analytical and experimental tasks. The goal of the analytical work is a predictive model that can be used in engineering design of ceramic joints. The experimental work will involve the fabrication and testing of first small scale and later scale-up sized joints.

Keywords: Engines, Joining/Welding, Metals, Structural Ceramics

127. Ceramic-Ceramic Joints — FY 1987 $639,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. Ray Johnson, (615) 576-6832
Norton Company Contact: Donald O. Patten, Jr., (617) 393-5963

The objective of this project is to develop the analytical tools for use in designing ceramic joints as a function of the mechanical and physical properties of the ceramics, the materials used in producing the joint, the geometry of the joint, externally imposed stresses both of a mechanical and thermal nature, temperature, and the effects of joints exposed for long times at high temperature in an oxidizing (heat engine) atmosphere. The maximum temperature of interest for application of silicon carbide and silicon nitride containing joints is 1530°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/Welding, Metals, Structural Ceramics

128. Advanced Coating Technology AGT — FY 1987 $351,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. Ray Johnson, (615) 576-6832
GTE Labs Contact: V. K. Sarin, (617) 890-8460

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 sintered Si_3N_4 for use in an advanced gas turbine engine. Chemical

vapor deposition (CVD) will be used to develop appropriate coating configurations to accommodate as many of the mechanical, thermal, and chemical requirements demanded of the application as possible.

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

129. Advanced Coating Technology — FY 1987 $75,000

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 reduce or eliminate the contact stress damage at ceramic-ceramic interfaces in gas turbine engines by chemically vapor depositing a coating that consists of Al_2O_3 and a solid lubricant to minimize the coefficient of sliding friction. Following satisfactory production of these coatings, tribological testing will be used to identify the optimum composition and concentration of lubricant to minimize the coefficient of friction.

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

130. Wear Resistant Coatings — FY 1987 $248,000

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

131. Wear Resistant Coatings — FY 1987 $244,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. P. Stinton, (615) 574-4556
Cummins Contact: Malcolm Naylor, (812) 377-5000

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. The coatings studied in this project will be deposited by several suppliers onto nickel-based alloy substrates. 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 shall be selected for further evaluation.

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

132. Sliding Seal Materials for Diesel Engines — FY 1987 $75,000

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

Friction and wear testing of metal and ceramic coated metal components are being conducted in a piston ring bench test rig to develop improved sliding seal materials for low heat rejection diesel engines.

Keywords: Erosion/Wear, Coatings, Diesel Engines, Tribology

133. High Temperature Solid Lubricant Coatings — FY 1987 $50,000

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

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

134. Thick Thermal Barrier Coatings — FY 1987 $200,000

DOE Contact: John Fairbanks, (202) 586-8066
NASA LeRC 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

135. Thick Thermal Barrier Coatings FY 1987 $200,000

DOE Contact: John Fairbanks, (202) 586-8066
NASA LeRC 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

136. Advanced Turbine Technology Applications Project (ATTAP, AGT-100) FY 1987 $4,500,000

DOE Contact: Saunders B. Kramer, (202) 586-8012
NASA LeRC Contact: Paul Kerwin, (216) 433-3409
General Motors, Allison Gas Turbine Division Contact: Phil Haley, (317) 230-2272

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

137. Advanced Turbine Technology Applications Project (ATTAP, AGT-101) FY 1987 $4,500,000

DOE Contact: Saunders B. Kramer, (202) 586-8012
NASA LeRC Contact: Thomas Strom, (216) 433-3408
Garrett Turbine Engine Co. Contact: Dan Kreiner, (602) 220-3465

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 (OESD)

The mission of the Office of Energy Storage and Distribution is to provide overall direction, interpret policy objectives and establish management procedures for a balanced program of technology planning, research and development, and test and evaluation, which will foster the establishment of a reasonable cross section of Electric Energy Distribution and Energy Storage Systems technology options.

The Office manages the electric energy distribution and storage systems groups of technologies in the formulation, and execution of appropriate national energy policies and programs and the verification of program balance and priorities among the technologies. 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.

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. Described below are the materials R&D efforts of the three subprograms: Electrochemical Energy Storage, Thermal Energy Storage and Chemical/Hydrogen Energy Storage.

Materials Preparation, Synthesis, Deposition, Growth or Forming

138. Medium Temperature Solid Electrolytes: Proton Conductors — FY 1987 $125,000

DOE Contact: M. Gurevich, (202) 586-1495
BNL Contact: C. Linkous, (516) 282-7949
Stanford Contact: R. Huggins, (415) 723-4110

Fundamental investigations are being pursued: the synthesis and characterization of modified high temperature polymers that may serve as proton conductors and, into a non-aqueous, molten salt hydride-ion conducting electrolyte. This work is ongoing at BNL and Stanford University. BNL aims at the introduction of ionomeric substituents in various polymers found to be stable in a steam environment. Efforts at Stanford University focus on the characterization of the novel electrolyte's conductivity and stability and the identification of H_2-permeable electrodes which can serve as electrodes for "sandwich" electrochemical structures which can be used in steam electrolysis.

Keywords: Polymers, Electrolytes

139. Hydrogen Production with Photoactive Semiconductor Catalysts — FY 1987 $125,000

DOE Contact: M. Gurevich, (202) 586-1495
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. Future efforts will focus on process reproducibility and more intensive analytical efforts to physically characterize the coatings. This will be followed by applying the coatings on semiconductor powders to be used in photochemical H_2 production experiments.

Keywords: Semiconductors, Plasma Polymerization, Coatings

140. Ceramics Research — FY 1987 $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 Methods, Fast Ion Conductors and Solid Electrolytes, Batteries

141. Metals and Alloys — FY 1987 $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 Compounds — FY 1987 $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 Cells, Batteries

143. Polymers — FY 1987 $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 1987 $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 1987 $ 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. High Temperature Steam Electrolysis — FY 1987 $50,000

DOE Contact:M. Gurevich, (202) 586-1495
Westinghouse R&D Center Contact: W. Feduska, (412) 256-1951

Subsequent to solid oxide electrolyte cell life testing, efforts have addressed the causes and remedies of cell performance degradation with time. Post-mortem analyses of test cell specimens have identified: electrolyte detachment or cracking; layer structure formation in the electrolyte; cathode sintering and loss of active surface area; electrolyte instability in the cathode structure. Westinghouse recommends improvement of cell fabrication, particularly in the electrochemical vapor deposition attachment of the nickel structure of the cathode to the electrolyte layer. Cathode doping improvements are recommended as well.

Keywords: Solid Oxide Electrolytes

147. Cold Storage of Hydrogen on Activated Carbon — FY 1987 $100,000

DOE Contact:M. Gurevich, (202) 586-1495
Syracuse University: J. Schwartz, (315) 423-2807

H_2 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. Future efforts will focus on characterization of storage capacity and kinetics as

a function of activated carbon compression, impurities, recycling. These data will be used to establish system design/performance specifications and requirements for H_2 storage system prototype fabrication.

Keywords: Hydrogen Storage, Catalysts

148. Use of Micro Particles as Heat Exchangers and Catalysts — FY 1987 $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

149. Evaluation of Heats of Mixing Systems for Thermal Energy Storage — FY 1987 $41,000

DOE Contact Eberhart Reimers: (202) 586-4563
ORNL Contact: John Tomlinson, (615) 574-0768
NY 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 Behavioral, Modelling

150. Development of Solid/Vapor Ammoniated Complexes as Thermal Energy Storage Materials — FY 1987 $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

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 Solar Buildings Technology Program focuses on solar energy products and designs that are economically competitive and can contribute significantly to building energy supplies. The objectives of the program are to: (1) develop solar energy technologies that can be practically used to supply 70-80 percent of building space heating, hot water, cooling, and lighting requirements at costs competitive with conventional technologies; and (2) provide industry with the information and techniques required to improve component and system reliability and durability to achieve acceptable system performance and equipment service life. 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

151. Thermochromic Materials Research for Optical Switching Films — FY 1987 $125,000

DOE Contact: M. M. Jenior, (202) 586-2998
Honeywell Contact: G. V. Jorgensen, (612) 378-4655

This research 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 (VO_2) 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 ultimate output of this research will be the development of undoped crystalline VO_2 pigments that switch and doped pigments produced by mixing VO_2 pigments with tungsten or tungsten oxide.

Keywords: Coatings and Films, Metallic Glasses, Photothermal, Low Temperature Service

152. Electrochromic Coatings R&D — FY 1987 $175,000

DOE Contact: M. M. Jenior, (202) 586-2998
SERI Contact: D. Benson, (303) 231-1162

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 energy efficiency of solar buildings. In FY 1987, SERI researched deposition of a range of amorphous metal oxide films, the most promising being molybdenum oxide. Optimum deposition parameters must be experimentally determined and basic mechanisms studies must be done to improve the understanding of electrochromic response in this material. SERI hopes to develop a potential laboratory-scale PE-CVD process for fabricating all of the layers required for a solid-state electrochromic coating. Patent rights for the process will be sold or licensed to a private manufacturer for commercial development.

Keywords: Coatings and Films, Transformation, Chemical Vapor Deposition, Low Temperature Service

153. Optical Switching Materials — FY 1987 $150,000

DOE Contact: M. M. Jenior, (202) 586-2998
LBL Contact: Steven Selkowitz, (415) 486-5064

The objectives of this activity are to identify, synthesize and characterize optical switching technologies that offer performance characteristics that meet the needs of apertures in different building applications in different climates. Dynamic control of aperture transmittance should make it possible to greatly reduce net heating, lighting, and cooling loads attributable to fenestration. There are three objectives: (1) research and synthesize new electrochromic materials that have a broadband or selective optical response different than that of existing materials using low-cost deposition techniques; (2) develop device designs based on (1); and (3) provide scientific evaluations for all DOE contractor research in the area of switching devices. In FY 1987, basic manganese oxide material studies were conducted and the performance of switching devices based on nickel

oxide/manganese oxide made by non-vacuum techniques, including switchable non-conducting media, were evaluated.

Keywords: Coatings and Films, Low Temperature Service

154. Solid State Electrochromic "Smart" Windows — FY 1987 $127,000

DOE Contact: M. M. Jenior, (202) 586-2998
EIC Contact: R. D. Rauch, (617) 769-9450

The purpose of this research 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 solar input to and radiation heat loss from building interiors to improve energy efficiency. Quantitative demonstration of the intrinsic electrochemical reversibility of lithium insertion/extraction has been achieved, thus establishing the framework for fabrication of an all-solid-state structure without cycle limitations. The expected output is an all-solid-state thin film electrochromic coating with a >50 percent to <10 percent transmittance range and a switching speed of <100 seconds.

Keywords: Coatings and Films, Low Temperature Service

155. Optics and Materials for Controlled Radiant Energy in Buildings — FY 1987 $187,000

DOE Contact: M. M. Jenior, (202) 586-2998
Tufts University Contact: R. B. Goldner, (617) 628-5000

The objective is development and modeling of all-solid optical switching devices based on films of electrochromic 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 research approach is four-fold: to demonstrate feasibility and identify candidate materials (Phase I completed); to improve and model each of the window layers and build prototypes (Phase II in progress); to use these prototypes to help solve the problems associated with large area electrochromic (ec) windows development (Phase III); and to transfer the technology (Phase IV). Electrically switchable glazings can control the radiant energy transfer in buildings and other enclosed spaces (e.g., vehicles) economically and automatically, thereby significantly improving their energy efficiency. The feasibility of variable reflectivity in (poly-) crystalline films of tungsten oxide (c-WO_3) and of solid state structures operable largely in the variable reflectivity mode have also been demonstrated.

Also, candidate materials for each window layer have been identified and their performance limits have been established. The expected outputs are highly practical CE, IC, and EC layers and laboratory-scale integrated structures that can be reproducibly fabricated.

Keywords: Coatings and Films, Transformation, Low Temperature Service

156. Holographic Diffractive Structures for Enhanced Daylighting — FY 1987 $46,000

DOE Contact: M. M. Jenior, (202) 586-2998
Advanced Environmental Research Group Contact: R. Ian-Frese, (617) 864-4982

This project involves the development of a low-cost holographic diffractive structure (HDS) system that maximizes the utilization of sunlight for daylighting. HDSs 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.

Keywords: Coatings and Films, Low Temperature Service

Materials Properties, Behavior, Characterization, or Testing

157. Generic Aperture Materials — FY 1987 $150,000

DOE Contact: M. M. Jenior, (202) 586-2998
LBL Contact: Steven Selkowitz, (415) 486-5064

The goal of this activity is to perform the research and development that is necessary to overcome present obstacles to commercial development of transparent silica aerogel insulating glazings. This involves basic and applied research to investigate and improve the properties of aerogels, investigations of better production methods, and the development of methods to protect them from the environment. Highly insulating windows can provide good thermal performance along with good daylighting alternatives in new and existing buildings. In FY 1987 this activity included research to develop preparation and sealing techniques to reduce the remaining light scattering from aerogels and studies to determine the effects of aerogel density on performance. In addition, a model to evaluate the energy performance of windows in response to spectrally selective

coatings to help determine the relative effectiveness of the various optical switching approaches was developed.

Keywords: Coatings and Films, Low Temperature Service

158. Exposure Testing — FY 1987 $30,000

DOE Contact: R. Hassett, (202) 586-8163
LANL Contact: S. Moore, (505) 667-2228

The objective of this project is to conduct exposure testing of collector and passive system materials and develop a data base for existing commercial materials and new state-of-the-art materials. Solar energy technologies are intimately dependent on the specialized materials they contain. The long-term success of the technologies depends on the long-term durability of the materials. This research activity maintains the currency of data on durability. Five- to eight-year real time exposure data is required to verify accelerated exposure test procedures. Solar radiation, elevated temperatures, and moisture exposure testing is being conducted at the high altitude exposure test facility. Information on insolation, temperature, humidity, and ultraviolet radiation is being collected and analyzed. The results will be used to aid in correlating short-term and accelerated tests and in developing degradation prediction models.

Keywords: Coatings and Films, Polymers, Photothermal

159. Thermal Energy Storage Materials R&D — FY 1987 $175,000[1]

DOE Contact: R. Hassett, (202) 586-8163
SERI Contact: D. Benson, (303) 231-1162

This project is designed to conceive, develop, and evaluate thermal energy storage (TES) materials options for possible use in solar heated or energy conserving buildings. The objective is to complete analyses and laboratory-scale research and testing on each new TES materials concept in order to prove its practical potential well enough for private industry to adopt the concept and develop products based upon it. Three new TES materials concepts have been invested and evaluated: building materials in which solid-state phase-change materials have been incorporated; a nearly room temperature solid/liquid phase-change material based upon a hydrate of trimethylol ethan; and a means to use the natural supercooling of salt hydrate phase-change materials for efficient long-term thermal energy storage. FY 1987 activities included research on a promising

[1]Funded by the Office of Energy Storage.

mixture of neopentyl-glycol and pentaerythritol. Also, the physical mechanisms by which certain SERI-invested, proprietary devices nucleated the recrystallization of supercooled phase change materials were investigated. (This project is funded by the Office of Energy Storage.)

Keywords: Organics, Transformation, Low Temperature Service

160. Advanced Phase-Change Materials and Systems for Solar-Passive Heating and Cooling of Residential Buildings — FY 1987 $75,000

DOE Contact: R. 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 project is funded by the Office of Energy Storage.)

Keywords: Transformation, Low Temperature Service

161. Desiccant Materials/Dehumidifier Geometries Research — FY 1987 $311,000

DOE Contact: J. Goldsmith, (202) 586-8779
SERI Contact: A. Pesaran, (303) 231-7636

This project involves: (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) investigating 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 1987 activities included the collection of: (1) 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 (2) information on the effect of residential pollutants on silica gel capacity and how to characterize such effects for different pollutants.

Keywords: Polymers, Organics, Surface Phenomena, Desiccants

162. Advanced Desiccant Materials Research — FY 1987 $150,000

DOE Contact: J. Goldsmith, (202) 586-8779
SERI Contact: A. Czanderna, (303) 231-1240

This project involves determining how the desired sorption performance of advanced desiccant materials can be predicted by understanding the role of their surface phenomena and materials modifications. The technological objective is to identify a next generation, low-cost material with which solar radiation or heat from another low-cost energy source is used for regenerating the water vapor sorption activity of the desiccant. In FY 1987 a quartz crystal microbalance (QCM) was used to measure the sorption performance of 22 polymeric material identified as potential candidates.

Keywords: Polymers, Surface Phenomena, Desiccants

163. Open-Cycle Absorption Solar Cooling — FY 1987 $209,000

DOE Contact: J. 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, Absorbents

164. Solar Cooling Research Facility — FY 1987 $ 0

DOE Contact: J. Goldsmith, (202) 586-8779
Florida Solar Energy Center Contact: S. Chandra, (305) 783-0300

The purpose of this project is to establish a comprehensive experimental and analytical capability for the study and advancement of solar cooling technologies applicable to hot, humid climates. Research will be concentrated in four areas: (1) moisture research and analysis; (2) radiant barrier systems, (3) enthalpy exchange systems; and (4) integrated systems research. The recent increase in population in hot, humid regions of the United States has significantly increased the energy demand for air conditioning in these climates, resulting in the need for research on solar cooling and dehumidification technologies. Activities will include the identification of the utility and application of desiccant materials and the development of innovative materials and systems.

Keywords: Low Temperature Service, Desiccants, Absorption

165. Materials with Enhanced Transport Properties for High Performance Desiccant Systems — FY 1987 $15,000

DOE Contact: J. Goldsmith, (202) 586-8779
Illinois Institute of Technology Contact: Z. Lavan, (312) 567-3189

The objective of this project is to conduct desiccant analysis and materials research in enhanced heat and mass diffusion rates. These materials employ small particles bound into an expanded matrix, or felt, in order to provide improved volumetric efficiency. This is especially important for passive systems, which require a substantial mass of active desiccant distributed over a relatively small area. Solid desiccant systems are of great interest to the solar industry as a method for converting solar thermal energy into cooling for buildings. This technology suffers major problems, principally related to the limited heat and mass transfer rates of the desiccant materials. This work will aid in the development of improved understanding of the transfer mechanism. Accomplishments in FY 1987 include the fabrication of first generation desiccant felts and demonstration of cold bed absorption.

Keywords: Low Temperature Service, Desiccants

166. Evaluation of Photochromic Plastics — FY 1987 $47,000

DOE Contact: M. M. Jenior, (202) 586-2998
American Optical Corporation Contact: N. Chu, (617) 765-9711

Research 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 inactivated 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.

Keywords: Low Temperature Service, Polymers, Coatings and Films

167. Daylighting Enhancement — FY 1987 $100,000

DOE Contact: M. M. Jenior, (202) 586-2998
LBL Contact: Steven Selkowitz, (415) 486-5064

The objectives of this activity are to identify, develop, and characterize light guide materials and systems for collecting and transmitting sunlight 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 1987 light guide research included scale model and full scale tests of hollow light guide sections incorporating high reflectance materials. The performance of various geometric cross-sections was evaluated. Methods to collect the light using tracking and stationary concentrators efficiently was also investigated.

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

168. Silver/Polymer Reflector Research — FY 1987 $808,000

DOE Contact: Frank Wilkins, (202) 586-1684
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 of more (within a 4-mrad cone angle). Useful film lives of 5 years of 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 polymers or polymers modified by laboratory procedures to meet performance requirements. Research is also being conducted to understand degradation mechanisms of candidate polymer/silver combinations in simulated solar environments.

Research is also being conducted on optically transmitting and structural polymer materials for solar thermal technology applications. The problems being investigated are: identification, testing, and evaluation of polymeric stabilizers to improve the durability of

polymers in solar thermal applications; and identification, testing, and evaluation of these additives that can act as ultraviolet (UV) absorbers and/or quenchers of excitation energy in polymers.

Keywords: Polymers, Coatings and Films, Surface Characterization and Treatment, Corrosion, Radiation Effects, Reflectors, UV Degradation

Materials Properties, Behavior, Characterization, or Testing

169. High Temperature Materials — FY 1987 $185,000

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

The aim of this research is to obtain information needed to select the best materials for use in the direct absorption receiver, as well as information needed to evaluate other receiver concepts.

Research on molten salts, which may be used as the working fluid in new central receiver concepts, is being carried out. In the direct absorber receiver solar energy is directly transferred to the flowing salt. To maximize the efficiency, absorbing materials are added to the normally transparent salts. Work is underway to establish the stability limits of metal oxide powders in molten nitrate salts, and to establish the compatibility of these mixtures with alloys which are candidates for piping and containment elements.

There is a continuing effort to identify and define failure modes of metal tubes that have been subjected to high solar flux, high temperature, and thermal cycling. To establish the durability of ceramic and metallic parts, continuous tests of components under solar conditions are carried out.

Keywords: Ceramics, Thermal Fluids, Alloys, Corrosion, Radiation Effects

170. High Flux Effects on Materials — FY 1987 $645,000

DOE Contact: Frank Wilkins, (202) 586-1684
SERI Contact: Daniel M. Blake, (303) 231-1222

Research on the beneficial effects of high intensity solar flux on materials is being conducted; particular investigations include surface alloying, thin-film deposition of metals and ceramics on suitable substrates, and the enhancement of the mechanical properties of carbon fibers and carbon-carbon composites.

Quantitative correlations between high intensity flux (over 1,000 suns) and degradation of materials are also being determined, and materials to reduce the degradation effects of high intensity radiation are also under investigation.

Keywords: Surface Alloying, Carbon Fibers, Surface Modification, Radiative Degradation

171. Composite Materials for Concentrators — FY 1987 $182,000

DOE Contact: Frank Wilkins, (202) 586-1684
SERI Contact: L. Marty Murphy, (303) 231-1050

The objective of this research (being conducted by the University of Arizona and Science Applications, Inc.) is to determine the feasibility of designing and building durable, low cost heliostats fabricated from advanced composite materials.

One of the major goals of the Solar Thermal Research Program is to show the technical feasibility of innovative durable, low cost concentrators.

Three conceptual designs for stretched membrane heliostats are under investigation:

- o laminated wood ring with double polymer membranes,
- o graphite fiber-reinforced wooden core ring with double polymer membranes, and
- o open weave graphite fiber "fishnet" membrane to support thin membrane reflector panels mounted on a frame.

The conceptual designs are being subjected to a computer-based structural analysis to predict their stress-strain behavior. Scale models are to be fabricated for each of the three conceptual designs and subjected to various mechanical tests (e.g., plane bending stiffness, torsional stiffness, etc.).

The expected results of the research is the conceptual design for a durable, lightweight, and potentially low cost stretched membrane heliostat fabricated from composite materials.

Keywords: Polymer Membrane, Stretched Membrane, Composite Materials, Heliostat

172. Radiant Transport and Optical Properties of Materials

FY 1987
$165,000

DOE Contact: Frank Wilkins, (202) 586-1684
SERI Contact: John Webb, (303) 231-1430

The radiative, dielectric, and optical properties of molten nitrate salts, molten salt blackeners, ceramics and metals, particles, and bulk materials are to be determined experimentally. Some of this research is for the design and development of the Direct Absorption Receiver (DAR).

Keywords: 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

173. Amorphous Silicon for Solar Cells — FY 1987 $10,500,000

DOE Contact: Morton B. Prince, (202) 586-1725
SERI Contact: Ed Sabisky, (303) 231-1483

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

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

174. Polycrystalline Thin Film Materials for Solar Cells — FY 1987 $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

175. Deposition of III-V Semiconductors for High-Efficiency Solar Cells — FY 1987 $2,000,000

DOE Contact: Morton B. Prince, (202) 586-1725
SERI Contact: John Benner, (303) 231-1396
SNLA Contact: Dan Arvizu, (505) 846-0387

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

176. Materials and Device Characterization — FY 1987 $2,900,000

DOE Contact: Morton B. Prince, (202) 586-1725
SERI Contact: Larry Kazmerski, (303) 231-1115

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

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

Device or Component Fabrication, Behavior or Testing

177. High-Efficiency Crystal Silicon Solar Cells — FY 1987 $2,000,000

DOE Contact: Morton B. Prince, (202) 586-1725
SERI Contact: John Benner, (303) 231-1396
SNLA Contact: Dan Arvizu, (505) 846-0387

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 TECHNOLOGY

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

178. High Temperature Elastomers for Dynamic Sealing Applications — FY 1987 $100,000

DOE Contact: R. LaSala, (202) 896-4198
BNL Contact: L. E. Kukacka, (516) 282-3065

This project performs 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 do not currently exist, and a successful development could substantially reduce drilling and completion costs. The effects of compositional changes on the properties of the elastomer are being determined, and the formulation optimized to yield the specific sealing requirements. Prototype and full-scale testing is performed. Achieving the goal will result in significant improvements in the cost and reliability of geothermal components.

Keywords: Organics, Material Degradation, Stress, Drilling, Seals and Bearings

179. Geothermal Waste Utilization and Disposal — FY 1987 $25,000

DOE Contact: G. J. Hooper, (202) 896-1146
BNL Contact: L. E. Kukacka, (516) 282-3065

This program involves 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 involves the selection of encapsulating or concentrating materials, and the fabrication and evaluation of waste forms. A successful program will result in significant improvements in the economic and environmental aspects of geothermal energy.

Keywords: Cements, Polymers, Bonding Agents, Material Degradation, Bulk Characterization, Waste Management

180. Materials for Non-Metallic Heat Exchangers — FY 1987 $75,000

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. 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

181. Biochemical Concentration and Removal of Toxic Components from Geothermal Wastes — FY 1987 $165,000

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

182. Corrosion Resistant Elastomeric Liners for Well Casing — FY 1987 $52,000

DOE Contact: R. LaSala, (202) 896-4198
BNL Contact: L. E. Kukacka, (516) 282-3065

This program investigates the effectiveness of Y-267 EPDM elastomers as corrosion resistant liners on carbon steel well casing. Currently, casing corrosion is a major problem at many geothermal sites, and although the use of high chrome steels and nickel alloys extend casing life considerably, they cost 6 to 15 times as much as carbon steel. The R&D consists of the identification and evaluation of high temperature chemical bonding agents, development of lining methods, and performance of field corrosion tests on prototype sections. If successful, the cost of geothermal wells will be considerably reduced.

Keywords: Bonding Agents, Organics, Corrosion, Joining, Material Degradation, Casting

183. Advanced High Temperature Geothermal Well Cements — FY 1987 $125,000

DOE Contact: R. LaSala, (202) 896-4198
BNL Contact: L. E. Kukacka, (516) 282-3065

Lightweight (< 1.2 g/cm^3) chemically and thermal resistant well cements are needed to reduce the potential for lost circulation problems during well completion operations. Materials designed for temperatures $>300^\circ$C will be needed as higher temperature resources are developed. Cements resistant to brines containing high concentrations of CO_2 at temperatures $>150^\circ$C are also needed. Emphasis should be 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

184. Corrosion in Binary Geothermal Systems — FY 1987 $48,000

DOE Contact: R. LaSala, (202) 896-4198
BNL Contact: D. van Rooyen, (516) 282-4050

This program yields corrosion data from laboratory and 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 operating plants and in a laboratory test loop in which the levels of water, oxygen and salt can be varied. When completed, the programs 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

185. Metallic Liners for Well Casing — FY 1987 $10,000

DOE Contact: R. LaSala, (202) 896-4198
BNL Contact: D. van Rooyen, (516) 282-4050

Corrosion of conventional well casing is a major problem in geothermal systems, and the use of high chrome steels and nickel alloys is uneconomical. Therefore, the use of clad metallic systems is being investigated. The work consists of the selection and laboratory evaluation of potentially useful cladding systems. If successful, the cost of geothermal wells will be considerably reduced.

Keywords: Alloys, Coatings, Metals, Corrosion, Diffusion, Fatigue

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 currently 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 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 1987 (DOE/ER-0348 dated September 1987). 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, Bahavior, Characterization or Testing

186. Bounds on Dynamic Plastic Deformation — FY 1987 $123,000

DOE Contact: Oscar P. Manley, (301) 353-5822
Argonne National Laboratory Contact: C. K. Youngdahl, (312) 972-6149

In many applications where load is transmitted to the structure through a fluid, details of the load history and spatial distribution affect significantly the final plastic deformation. The objective of this project 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, but will be extended to include strain hardening and elastic effects if the work to determine load parameters is successful.

Keywords: Plastic Deformation

187. Diffusion, Fluid Flow, and Sound Propagation in Disordered Media — FY 1987 $65,000

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 will be calculated. The project has only just begun, but a molecular dynamics simulation of lattice vibrations (sound) on disordered lattices is running. While the program was being tested, almost accidentally, a clear manifestation of the unusual localization phenomenon in two dimensions was discovered and is now being analyzed; this phenomenon is most interesting theoretically. Lattice vibrations in several disordered systems, and the other transport problems listed, will be investigated as the project develops.

Keywords: Disordered Media, Statistical Mechanics

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

FY 1987
$90,000

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 coincidence technique. A small measurement volume is defined by two independent lens/sensing systems. When a particle is present in the measurement lens/sensing systems. When a particle is present in the measurement volume, a signal will be observed and recorded simultaneously by each sensing system. Once a signal is recorded, the particle temperature may be deduced. The uncertainty in this temperature determination will be due to lack of information concerning the particle size, shape, and emissivity; and due to the presence of an emitting, absorbing, and scattering medium.

The program consists of three phases: In Phase I (FY 85) individual particles were electrodynamically suspended, then heated by a laser beam. The particle temperatures and emissivities were measured. Results to date indicate that optical property data for the parent material are adequate for estimation of particle emissivity. In Phase II (FY 86) the in-flight coincidence technique was developed. This effort included the development of both analog and digital signal processing techniques. Phase III will apply, and modify as necessary, these techniques to measure particle temperatures in a high temperature plasma. This phase of the program will address the problems associated with the presence of an emitting, absorbing, and scattering atmosphere.

This project is one of six projects comprising a collaborative research program with the Massachusetts Institute of Technology.

Keywords: Plasma Processing, Particle/Plasma Interaction

189. Experimental Measurement of the Plasma/Particle Interaction

FY 1987
$328,000

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, 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, the development of 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

190. Integrated Sensor/Model Development for Automated Welding — FY 1987 $496,000

DOE Contact: Oscar P. Manley, (301) 353-5822
Idaho National Engineering Laboratory Contacts: H. B. Smartt, (208) 526-8333, J. A. Johnson, (208) 526-9021, J. O. Bolstad, (208) 526-1753

The objectives of this research are: (1) to develop a model of the gas metal arc welding process suitable for real-time process control, (2) to develop an optical sensing capability to provide critical weld bead geometry data, and (3) to develop an untrasonic sensing capability to directly sense weld bead side-wall fusion and penetration. 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. Although iterative numerical solution techniques are requires, finite difference/finite element methods are not used. A computer controlled welding machine has been built and used to demonstrate the ability to independently control the heat and mass input to the weld, using the above model in combination with an adaptive feedback control scheme. This work is being extended to allow real-time, optimized control of pulsed current welding to be achieved.

A pulsed laser enhanced, gated electro-optical sensor has been developed which suppresses most of the welding arc light, providing an image of the electrode wire, weld pool, and surrounding base metal which is suitable for image processing. Image processing techniques are being developed to obtain quantitative information from the above images regarding the weld pool geometry and position.

Direct sensing of the weld pool solid/liquid interface location is being developed using conventional pulse-echo ultrasonic transducers. Signal analysis/pattern recognition techniques are being developed for automated measurements. Signal generation by use of laser pulses directed on the weld pool surface is also being studied.

Keywords: Welding, Ultrasonic Sensing, Optical Sensing

191. Nondestructive Characterization of Fracture Dynamics and Crack Growth FY 1987
$193,000

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.

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 ray-tracing model, an ultrasonic transducer, operating in the pulse-eco mode is assumed to be equivalent to a large number of spherical sources spread uniformly over the face of the transducer. The total field in the region of a crack is calculated as the sum of the fields from all these sources. The reflected and diffracted fields fromthe crack are calculated from the incident field from the transducer and a model of the field-crack interaction. These fields are then traced back to the transducer face and the integrated field across the face is determined.

In the finite difference model, a source of acoustic emission (AE) 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.

The dynamic crack growth measurements have used ultrasonics techniques to measure the properties of a growing crack. An advanced AE detection system is being developed which will be capable of detecting and digitizing AE signals at much higher frequencies than in convential systems. This will allow improved resolution in detecting the locations of the sources of emissions and in discriminating between types of sources.

This program is coordinated with the Elastic-Plastic Fracture Analysis program at INEL and the Modeling and Analysis of Surface Cracks at Massachusetts Institute of Technology.

Keywords: Nondestructive Evaluation, Fracture

192. Boiling of Aqueous Polymer Solutions FY 1987
$67,000

DOE Contact: Oscar P. Manley, (301) 353-5822
University of Illinois at Chicago Contact: J. P. Hartnett, (312) 996-4490

The goal of this research is to study the pool boiling behavior of aqueous polymer solutions, both purely viscous and viscoelastic with the objective of providing accurate boiling measurements using well-defined fluids. Detailed measurements of the transport and rheological properties of the test fluids are being carried out prior to and following the experiments. It has been determined that the chemistry (i.e., changes in the polymer

structure as a result of increases in operating temperature level, interactions with the materials of the test section, etc.) plays a major role. Consequently, careful monitoring of the rheology is critical if the boiling results are to be meaningful. The direct measurements of the boiling heat flux and surface and fluid temperatures will be supplemented by photograhic studies to provide additional insight into the boiling process.

Measurements of free convection heat transfer from horizontal platinum wires to surrounding purely viscous and viscoelastic non-Newtonian fluids have been carried out prior to the boiling studies. For free convention to purely viscous non-newtonian fluids at Rayleigh numbers of the order of 10^{-2} to 1 it is found that the Nusselt number decreases with decreasing power law index whereas a high Rayleigh number $Ra >> 1$, the Nusselt number increases with decreasing power law index. In the case of free convention to voscoelastic fluids the heat transfer measurements are in agreement with values predicted for Newtonian fluids provided that the zero shear rate viscosity is used for the viscoelastic fluid viscosity.

Keywords: Boiling, Polymers

193. Plasma Reduction of Metallic Oxide Particles — FY 1987 $76,000

DOE Contact: Oscar P. Manley, (301) 353-5822
MIT Contacts: J. F. Eliott, (617) 253-3305, J. Szekely, (617) 253-3236, R. E. Spjut, (617) 253-0252

The objective of this research is to characterize the reduction to metal of oxide particles injected into the tail flame of an arc plasma. At the present time, it is not known if a significant degree of reaction occurs in flight, or if such reduction processes require a molten bath and, hence, a transferred arc plasma. The experimental method involves injecting mixtures of carbon and metallic oxide particles, in the size range of 20 to 100 microns, into an arc plasma just beyond the point of initial generation and sampling downstream at various distances with a sample, water-cooled suction cup. The particles thus removed from the plasma may be examined by microscopy and electron microanalysis to determine the extent of reduction.

Another important aspect of this work is to determine the rate of heat transfer between the plasma and injected solid particles. In a preliminary set of experiments, solid particles of varying thermophysical properties will be injected into the plasma and then collected. By sectioning and analyzing these particles it will be possible to establish the extent to which melting has in fact occurred. These experimental measurements will be critically compared with the theoretical predictions.

The new 50ks furnace has been installed and placed in operation. It can be operated in either the non-transferred arc or transferred arc mode. The system is equipped with automatically controlled devices for feeding powders into the plasma flame. Initial work has been begun on the physical and chemical modifications of simple oxide particles and composite carbon-oxide particles that have passed through the plasma flame.

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

194. High-Temperature Gas-Particle Reactions — FY 1987 $230,000

DOE Contact: Oscar P. Manley, (301) 353-5822
MIT Contacts: J. F. Eliott, 617-253-3305, R. E. Spjut, (617) 253-3305

The objective of the research program is to examine the physiocochemical behavior of individual inorganic particles in conditions simulating those to which particles are exposed in arc plasmas. In the experimental arrangement, a particle is suspended by the field in an electrostatic balance and it is heated in a laser beam. Manipulation of the charge on the particle and precise measurement of the strength of the field permits determination of the weight of the particle before and after the heating and cooling of the particle in the experiment. The composition of the gas in the reaction chamber is controlled, and the temperature of the particle can be measured and controlled with a time resolution as short as one or two milliseconds.

Experiments are in progress to determine the rate of volatilization of alumina and silica particles in various gas compositions, and the kinetics of reactions in composite carbon-alumina and carbon-silica particles.

This work is closely coordinated with the other plasma processing programs in the Department of Materials Science and Engineering at MIT and with the experimental program on plasma processing at the Idaho National Engineering Laboratory.

Keywords: Plasma/Particle Interaction

195. Mathematical Modeling of Transport Phenomena in Plasma Systems — FY 1987 $102,000

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 electromagnetic force field, the velocity field, temperature field and chemical composition of plasma flames, together with their interaction with solid particles.

To date, computed results have been obtained describing the flow field, the temperatures and the composition of a non-transferred arc with swirl, with annular and sideways injected gas streams.

It has been shown that swirl plays a profound effect in modifying both the flow and the entertainment of the secondary and tertiary streams. These calculations should form the basis of the rational design of plasma reactors.

The theoretical predictions are being compared to measurements conducted at the Idaho National Engineering Laboratory.

Keywords: Plasma Systems, Transport Properties

196. In-Process Control of Residual Stresses and Distortion in Automatic Welding

FY 1987
$87,000

DOE Contact: Oscar P. Manley, (301) 353-5822
MIT Contact: Koichi Masubuchi, (617) 253-6820

The objective of this research program is to develop the technology of in-process control of residual stresses and distortion in automatic welding. The program consists of the following three 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 3: Plans for future advancement of the technology of in-process control of residual stresses and distortion.

The effort thus far covers primarily Phases 1 and 2. The program has been carried out smoothly as originally proposed.

Keywords: Automatic Welding, Control

197. Multivariable Control of the Gas-Metal Arc Welding Process

FY 1987
$102,000

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 begun this work at two extremes, one starting from a specific two-variable problem in GMAW for which models and measurements exist, and the other from a more basic, but idealized perspective. The former will allow us to quickly identify where gaps in our knowledge of the process and the characterization of the measurements exist, and allow us to perform initial experiments within the first year of the project. The latter will begin building a comprehensive framework for the solution of the complete control problem, defined as independent regulation of all relevant outputs while rejecting a significant range of system disturbances.

This project is coordinated with the experimental work at Idaho National Engineering Laboratory.

Keywords: Welding, Control

198. Modeling of GMA Weld Pool Geometry and Metal Transfer — FY 1987 $88,000

DOE Contact: Oscar P. Manley, (301) 353-5822
MIT Contact: William Unkel, (617) 253-2193

Realtime control of weld parameters such as weld pool geometry can reduce welding flaws and therefore increase the productivity of producing welded structures. One important component to achieving online control is a physically-based model of the welding process. For a complex process such as welding, models play several roles including:

(a) interpreting noisy and often indirect measurement data;
(b) identifying process modifications that make multivariable control easier; and
(c) providing a component of the actual control algorithm.

Previous modeling efforts have concentrated on the Gas Tungsten Arc Welding (GTAW) process and have laid the groundwork for the present work on the Gas Metal Arc Welding (GMAW) process.

The principal goal of the present work is to develop physically based, but computationally simple models for the GMAW stiuation and to use these models to identify process modifications to allow a more effective multivariable control system to be implemented. Those models will be confirmed by comparison with experimental data and will also be considered for use in online interpretation of sensor datas.

This research is coordinated with the experimental work at Idaho National Engineering Laboratory.

Keywords: Welding, Control

199. Modeling and Analysis of Surface Cracks — FY 1987 $200,000

DOE Contact: Oscar P. Manley, (301) 353-5822
MIT Contacts: David M. Parks, (617) 253-1630

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. Exploratory experiments are also being undertaken to probe effects of asymmetry of loading, prior plastic strain history, and other factors on subsequent ductile fracture. Load biaxiality effects have been simulated for axial tension and internal pressure loading on pipes containing a circumferential crack. Accepted solutions for J derived for tension alone can underestimate fully plastic biaxial J-values by up to an order of magnitude.

Recent developments have results in marked improvement in agreement between calculations and experimental data obtained in a parallel effort at INEL.

Keywords: Fracture

200. Thermal Plasma Processing of Materials — FY 1987 $142,000

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 scalling and transmission electron microscopy, x-ray and electron diffraction, and measurements of the trnsition temperature for superconducting compounds.

Keywords: Plasma Processing, Plasma Diagnostics

201. Transport Properties of Disordered Porous Media from the Microstructure

FY 1987
$90,000

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

202. Effects of Crack Geometry and Near-Crack Materials Behavior on Scattering of Ultrasonic Waves for QNDE Applications

FY 1987
$65,000

DOE Contact: Oscar P. Manley, (301) 353-5822
Northwestern University Contact: J. D. Achenbach, (312) 491-5527

Among the methods of quantitative non-destructive evaluation of structural elements, the method based on scattering of ultrasonic (elastic) waves by flaws is particularly useful. 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 have also provided invaluable aid in the interpretation of scattering data for the inverse problem. In recent work, numerical results have been obtained by the finite difference method (flaws near surfaces) and by the boundary element method (distribution of voids). The usual mathematical modeling of ultrasonic wave scattering by cracks is being extended to account for several typical characteristics of fatigue and stress-corrosion cracks, and the environment of such cracks. Work in in progress on scattering by a cloud of microcracks and/or a plastic zone, which surrounds a crack tip. Further parametric

studies are expected to display the masking of characteristic "crack-like" features of the scattered field by a spectrum of signals due to deviations from idealized crack geometries and idealized material behavior.

Keywords: Nondestructive Evaluation, QNDE

203. Inelastic Deformation and Damage at High Temperature — FY 1987 $120,000

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 interation 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 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.

At the temperature of interest (presumably 550°C or 600°C) tests will be conducted to ascertain whether aging and recovery are significant. Exploratory experiments and tests intended for identifying material functions of the theory will be performed. They include biaxial, high temperature low-cycle fatigue and ratcheting experiments. These test results and data from the literature are needed to find material constants and functions of the theory. Test results not used in determining the material properties provide for a check of the predictive capability of the theory.

Keywords: Fracture, Damage

204. Energy Changes in Transforming Solids FY 1987 $ 0

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. During the past year we have examined material forces associated with solids containing a specified distribution of dislocations and disclinations. Furthermore, a remarkably simple formula has been derived for calculating the hoop stress distribution along the boundary of a circular cavity in an infinite sheet containing arbitrary sources of internal stresses; the calculation can be made without solving an elastic boundary value problem. As several specific examples show, this formula is most useful for calculating energy release rates. Work on generalizing this approach to cavities of arbitrary shape is currently in progress.

Keywords: Stress Analysis, Materials Science

205. Nondestructive Testing FY 1987 $115,000

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 1-8 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 ina 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 use to measure film thicknesses and profiles.

We are now developing a new acoustic transducer operating in air which utilized a 1000 A thick pellicle of boron nitride as the detector of acoustic waves in the air. The deflection of the surface is measured by highly sensitive optical phase measurement of

an optical beam reflected from the pellicle. The system is as sensitive as our previous acoustic transducer, but has the advantage that it can be operated over a bandwidth from a few Hz to several MHz.

Keywords: Nondestructive Evaluation, Acoustic Sensors

206. Effective Elastic Properties of Cracked Solids — FY 1987 $107,000

DOE Contact: Oscar P. Manley, (301) 353-5822
Tufts University Contact: Mark Kachanov, (617) 628-5000, ext. 2821

Effective elastic properties of solids with cracks will be investigated on the basis of the new approach to many cracks problems developed recently by the author. The results will be sensitive to mutual positions of cracks within the representative volume and will be applicable up to quite high crack densities.

Keywords: Fracture, Elasticity

207. Elastic-Plastic Fracture Analysis Emphasis on Surface Flaws — FY 1987 $365,000

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 data on the lower shelf (K_{Ic}), transition zone (J_{Ic}, J-R curves, etc.), and on the upper shelf (J_{Ic}, J-R curves, etc.). Results from the lower shelf and transition region are being used to predict failure conditions for specimens containing surface flaws. Predictions are then compared with experimental test data. These tests have been supplemented by data generated from Ti-15-3 heat treated to develop a plastic zone size of nominally 0.1 mm. 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 for comparison with analytical models. Laser interferometry and infrared thermography techniques will be used to evaluate and quantify the deformation in the crack region.

Keywords: Fracture, Ferrous Metals including Steels

208. Continuous Damage Theory FY 1987 $44,000

DOE Contact: Oscar P. Manley, (301) 353-5822
University of Illinois Contact: D. Krajcinovic, (312) 996-7000

The research conducted during the past year was focused on two seemingly disparate tasks; establishment of a common mathematical basis for the phenomenological models and formulation of a micromechanically based continuum damage model. As it turned out the two tasks had a lot in common. Using the effective field approximation it was possible to derive the compliance tensor for an elastic solid weakened by an ensemble of microcracks.

Once the essential structure of the analytical model was established it was possible to demonstrate that the so called scalar, second and fourth order tensor models are only the truncations of the general model. Moreover, the phenomenological model developed during the work on this project proves to be directly related to the micromechanical one. In other words, the proposed phenomenological model also contains the scalar, second and fourth order tensor models as special cases.

The so called Taylor approximation was used to simplify the analyses using the micromechanical model. The results in replicating the experimental trends are very encouraging.

The current plans are to further develop the formulated models with an ultimate objective of the combined brittle-dectile phenomena.

Keywords: Ferrous Metals icluding Steels, Fracture, Fatigue, Creep

209. Loss Characteristics of Cord-Rubber Composites FY 1987 $73,000

DOE Contact: Oscar P. Manley, (301) 353-5822
University of Michigan Contact: S. K. Clark, (313) 764-4256

The research is divided roughly into two phases, the first being completion of data acquisition on the loss characteristics of cord-rubber composites under both uniaxial and multiaxial stress states. This effort will utilize information currently available as well as measurements made here. The effects of prestrain, frequency, strain amplitude, and temperature will be included in the assessment of the viscoelastic properties of these materials.

The major activity during the latter part of the work will be analysis and measurement of the rolling loss of a relatively simple pneumatic tire. The tire geometry will be essentially cylindrical in form, similar to the type of tire used in vehicles transversing soft or marshy terrain. These are essentially cylindrical rollers, but with end closures making it possible to inflate them. Analysis will be carried out using the visco-elastic material properties previously obtained, as well as finite element codes suitable for this type of problem. Comparison of calculated and measured rolling resistance values

will give valuable insight into the types of finite element models best suited for this computation, and should give confidence to the tire industry in its efforts to apply finite element techniques to the calculation of tire operating properties.

Keywords: Composites

210. Effects of Crack Geometry and Near-Crack Material Behavior on Scattering of Ultrasonic Waves for QNDE Applications — FY 1987 $65,000

DOE Contact: Oscar P. Manley, (301) 353-5822
Northwestern University Contact: J. D. Achenbach, (312) 491-5527

This project is concerned with applications 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. The usual mathematical modeling of ultrasonic wave scattering by cracks is adjusted to account for several typical characteristics of fatigue and stress-corrosion cracks, and the environment of such cracks. Effects due to crack-face roughness, crack-closure and crack-face interactions are considered, as well as global anisotropy. Local anisotropy and inhomogeneity due to near-tip voids, and the effect of a zone of plastic deformation near a crack tip will also be investigated. Parametrical studies are expected to display the masking of characteristic "crack-like" features of the scattered field by a spectrum of signals due to deviations from an idealized crack geometry and idealized material behavior. Progress has been made on the effects of crack-face interactions and global anisotropy.

Keywords: Ferrous and Non-Ferrous Metals, Fracture, NDE

211. Multiviewing Tranducer System — FY 1987 $241,000

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 demonstrate a composite, multiviewing ultrasonic transducer system suitable for detecting, characterizing, and reconstructing flaws in structural materials for flaw sizing. Development of this transducer utilizes a combination of recent advances in ultrasonic scattering and inversion theories with new concepts in transducer configurations and excitation methods. Automated data acquisition has been developed using seven transducer elements multiplexed for both pulse-echo and pitch-catch modes. The reconstruction protocol fits the acquired data to an "equivalent" ellipsoid of general shape (3 axes, 3 angles), a shape that is compatible with a fracture mechanics description of growing flaws and thus suitable for failure prediction. In the effort to improve the reconstruction reliability with a limited aperture, a multi-angle signal amplitude contour technique was developed which instructed the automated system to acquire data with the most favorable angular configuration. This technique has dramatically improved the reconstruction reliability for flaws oriented at a difficult tilt angle for the reconstruction. In addition, artificial intelligence may be incorporated to

determine the shape and angular configuration of the flaw from the signal amplitude contours and the full reconstruction may be constrained by such predetermined information for greater stability and reliability. New techniques have also been developed for generating unipolar stress pulses in both pulse-echo and pitch-catch modes. These pulses show significantly broader bandwidths than do the usual ultrasonic pulses, a feature that is necessary in the application of inversion algorithms for flaw sizing. They are also important in the measurement of gradients of material properties. A new transducer system has also been designed using these advances that will extend reconstruction capabilities to include 2-D computed tomographic and 3-D ultrasonic reconstructions.

Division of Advanced Energy Projects

212. Aerodynamic Focusing of Particles and Heavy Molecules — FY 1987 $73,026

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, Wf_6, etc.) diluted in gaseous H_2 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 lijmit 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 I_2 molecules seeded in high-speed jets of H_2 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

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

213. Semiconductor Radiation Detector Technology — FY 1987 $398,000

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

214. Development of Silicon Avalanche Internal Gain Radiation Detection Structures — FY 1987 $260,000

DOE Contact: G. Goldstein, (301) 353-534, FTS 233-5348
University of Southern California Contact: G. Huth, (213) 822-9184

The project objectives are to attain the highest possible values of useful impact ionization ("avalanche") internal gain in solid-state silicon radiation detection structures and to study its uniformity on the micrometer spatial level. Interest in radiation detector technology is based on the breakthrough in silicon single crystal technology represented by neutron transmutation doping (NTD). The applications objective is the first practical, room temperature operable, solid-state substitute for the vacuum photomultiplier tube.

Potentially useful applications include: (1) a solid-state detector for low-energy beta emitters such as tritium, and (2) arrays in very high speed (sub-nanosecond) optical data acquisition applications involving fiber optics for DOE weapons test-related projects, and in optical imaging-with-gain concepts that have fundamental implications.

Keywords: Semiconductors, Radiation Effects, Ion Implantation, Instrumentation or Technique Development

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 6 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 2 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, 1985 (DOE/ER-0181/2), Abstracts of Phase II Awards, 1984 (DOE/ER-0209), and Abstracts of Phase II Awards, 1985 (DOE/ER-0209/1). 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 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 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

215. Fuel Process Development — FY 1987 $790,000

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 have very low defective particle yields.

Keywords: Fuels, Ceramics, Sintering, Coatings, Chemical Vapor Deposition

Materials Properties, Behavior, Characterization or Testing

216. Fuel Materials Development — FY 1987 $515,000

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, testing, and evaluation of irradiation experiments, performance of post-irradiation fission product release tests, 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

217. Fuel Development and Testing — FY 1987 $1,065,000

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 primarily on the low enriched uranium-oxycarbide/thorium-oxide fuel system, with limited work on advanced fuels. 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

218. Graphite Development — FY 1987 $65,000

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

219. Graphite Development and Testing — FY 1987 $390,000

DOE Contact: J. E. Fox, (301) 353-3985
ORNL Contact: W. P. Eatherly, (615) 574-5220

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

220. Metals Technology Development — FY 1987 $195,000

DOE Contact: J. E. Fox, (301) 353-3985
GA Technologies Contact: W. R. Johnson, (619) 455-2905

This work includes testing activities to characterize and qualify the metallic materials selected for applications in the near-term steam cycle HTGR system. Tasks involve evaluations of the effects of extended high temperature exposure in simulated helium environments on structural integrity and work to identify the database required for code qualifications. Principal alloys include 2 1/2 Cr-1 Mo steel and Alloy 800H.

Keywords: Alloys, Strength, Corrosion, Joining, Microstructure, High Temperature Service

221. Structural Materials Development — FY 1987 $380,000

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.

Keywords: Alloys, Strength, Corrosion, Joining, Microstructure, High Temperature Service

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 develop acceptable technologies for the treatment and immobilization of nuclear fuel cycle and special types of radioactive waste.

Materials Preparation, Synthesis, Deposition, Growth or Forming

222. Technical Support to West Valley Demonstration Project — FY 1987 $4,100,000

DOE Contact: E. Maestas, (716) 942-4314
PNL Contact: R. A. Brouns, (509) 376-0731

Provide technical assistance in supernatant treatment and borosilicate glass formulation for West Valley Demonstration Project waste.

Keywords: Radioactive Waste Host

Materials Properties, Behavior, Characterization or Testing

223. Materials Characterization Center Testing of West Valley Formulation Glass — FY 1987 $525,000

DOE Contact: H. F. Walter, (301) 353-5510
PNL Contact: M. Kreiter, (509) 375-2666

Evaluate, using various MCC test methods, samples of glass having the expected composition of West Valley borosilicate glass incorporating high-level waste.

Keywords: Radioactive Waste Host

224. Test Development and Testing of West Valley Reference Formulation Glass FY 1987 $1,100,000

DOE Contact: E. Maestas, (716) 942-4314
CUA Contact: P. B. Macedo, (202) 635-5327

Vitreous State Laboratory, Catholic University of America (CUA), is developing borosilicate glass waste form test methods and is testing nonradioactive reference West Valley Demonstration Project waste formulation glass.

Keywords: Radioactive Waste Host

225. Process and Product Quality Optimization for West Valley Waste Form FY 1987 $465,000

DOE Contact: E. Maestas, (716) 942-4314
AU Contact: L. D. Pye, (607) 871-2432

Alfred University (AU) is contributing to maximizing the range of conditions around the optimum which will produce acceptable quality borosilicate glass waste form product and to methods for control of product quality during routine manufacture of the West Valley Demonstration Project waste form.

Keywords: Radioactive Waste Host

Device or Component Fabrication, Behavior or Testing

226. Special Waste Form Lysimeter for Arid Regions FY 1987 $200,000

DOE Contact: M. W. Shupe, (208) 526-1288
EG&G Idaho Contact: D. Halford, (208) 526-2163

Conduct waste form leaching tests in a field facility in order to determine typical source terms generated by commercial solidified low-level waste in an arid climate, identify the chemical and physical processes that control the concentrations of radionuclides in the surrounding soil, and determine methods for representing the source term boundary conditions for transport models.

Keywords: Radioactive Waste Host

227. Special Waste Form Lysimeter for Humid Regions FY 1987 $200,000

DOE Contact: M. W. Shupe, (208) 526-1288
EG&G Idaho Contact: D. Halford, (208) 526-2163

Conduct waste form leaching tests in a field facility in order to determine typical source terms generated by commercial solidified low-level waste in a humid climate, identify the chemical and physical processes that control the concentration of

radionuclides in the surrounding soil, and compare radionuclide emigration from solidifed commercial low-level waste in order to evaluate the benefits of solidification.

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 positon. 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, not withstanding the provisions of Section 3617 of the Revised Statutes (31 USC 484). The sum appropriated is reduced as uranium enrichment revenues are received during a fiscal year so as to result in a net fiscal year appropriation of $0. Total obligations for all uranium enrichment activities in FY 1987 was $1549 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 1987 was $8,785,000. 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 plant operate on the principle that lighter weight gaseous isotopes have slightly higher average velocities and thus can be made to diffuse through a porous barrier more rapidly than heavier species. Two streams can be created, one enriched in the lighter isotope and one depleted. Because enrichment for a single cycle, or stage, is very small, a cascade of stages is required. For example, a plant constructed for producing 4 percent assay U-235 would contain about 1200 stages. Although many other methods for enrichment are still being investigated and another production technique is being used in parts of Europe, diffusion plants today still provide more than 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

228. Gaseous Diffusion: Barrier Quality — FY 1987 $2,150,000

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

229. Gaseous Diffusion: Materials and Chemistry Support — FY 1987 $2,515,000

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

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 1986, DOE selected AVLIS for further development and possible future deployment into the uranium enrichment enterprise. The primary emphasis for AVLIS in FY 1987 was to continue activities that will allow significant full-scale operational engineering demonstrations in the next few years. Available resources were focused on this goal and also on the operation of existing testbeds to conduct and evaluate key subsystems. The AVLIS contractor continued the operation of the first phase and procurement of the second phase of the Laser Demonstration Facility, which is a copper vapor laser pumped dye laser system. In addition, a one-half scale separator facility was operated in FY 1987 and planned for FY 1988 to demonstrate enrichment and provide component development and design data for a full scale separator. The AVLIS materials activities in FY 1987 were in support of the separator system and on uranium processing. 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 AVLIS into the nuclear fuel cycle.

230. AVLIS: Separator Materials — FY 1987 $3,220,000

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

231. AVLIS: Uranium Processing — FY 1987 $900,000

- o Design, fabrication and operation of uranium electrolysis cells for AVLIS feed. Bath chemistry, solubility and construction materials studies.
- o 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, Gaseous Diffusion, Uranium, Laser Isotope Separation, Atomic Vapor Laser Isotope Separation (AVLIS)

Office of Civilian Reactor Development

Division 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

232. Fuel Performance Demonstration — FY 1987 $4,846,000

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

233. Pyroprocess Development — FY 1987 $3,000,000

DOE Contact: David L. Hoff, (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

234. Fuel Safety Experiments and Analysis — FY 1987 $2,965,000

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 irradiation U-Pu-Zr fuels, and continue preparations for two PRF/TREAT tests.

Keywords: Reactor Safety, Actinides

235. Core Design Studies — FY 1987 $2,500,000

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

236. Fuel Cycle Studies — FY 1987 $2,000,000

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 Cycle

237. Design Methodology Development and Applications — FY 1987 $3,700,000

DOE Contact: John Lewellen, (301) 353-3684, FTS 233-3684
ANL Contact: D. C. Wade, (312) 972-4858, FTS 972-4858

This task encompasses the modification and validation of neutronics, thermal hydraulics, structural and seismic methods, and computer codes required for the safe design and operation of fast reactors utilizing metallic fuels. Included also is design and analysis support for the advanced reactor programs. Complete development of fluid structure interaction codes and validation. Continues investigations into feasibility of seismic isolation and the techniques for achieving isolation. Carries out the necessary development of methods of analysis accounting for all modes of motion. Pursues potential collaboration with the National Science Foundation in funding actual seismic experiments on Japanese buildings with and without isolation. Participates in the development with ETEC of a DOE Seismic Technology Development Plan. Continues to provide seismic design support to the advanced reactor program. Program conducts Phase I testing in Natural Convection Shutdown Heat Removal Test Facility (NSTF) and hydraulics tests of advanced design upper plenum internal structure. Develops and maintains an integrated, validated and broad scope set of reactor core design and safety analysis methods and state-of-the-art computer codes. Applies updated sloshing codes in evaluating seismic isolation technology for potential application to advanced reactor concepts.

Keywords: Seismology, Hydraulics, Reactor Design

238. Innovative Design Key Feature Test — FY 1987 $ 0

DOE Contact: C. Chester Bigelow, (301) 353-4299, FTS 233-4299
ANL Contact: Dean R. Pedersen, (312) 972-3335, FTS 972-3335

This task provides for the testing program required to validate key features of the advanced innovative reactor designs intended to enhance inherent safety and/or reduce costs. Included are such features as RVACS/RACS full segment testing and thermal hydraulic aspects of reactivity feedback mechanisms. The goals of the testing program are to validate the design features and analytic design tools, provide design data, verify performance predictions, aid in optimizing designs, and reduce conservatisms.

Keywords: Reactor Design, Hydraulics

239. Reactor Systems Component Development — FY 1987 $800,000

DOE Contact: Eli I. Goodman, (301) 353-2966, FTS 233-2966
ANL Contact: Richard W. Weeks, (312) 972-4931, FTS 972-4931

Continue reactor systems component development program including necessary testing of insulation for EM pumps and scale model thermal hydraulics testing of

advanced concepts. Program will conduct 1/5 scale PRISM and 1/10 scale SAFR reactor system thermal hydraulics tests, and preliminary life test of EM pump quarter length stator section.

Keywords: Hydraulics, Reactor Components

Structural Materials and Design Methodology

Materials, Properties, Behavior, Characterization and Testing

240. Structural Design/Life Assurance Technology — FY 1987 $400,000

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, Welding, Creep

241. Modified 9 Cr-1 Mo Steel Design Properties — FY 1987 $400,000

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

242. Nondestructive Testing Technology for Heat Exchangers

FY 1987
$40,000

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

243. Nuclear Systems Materials Handbook

FY 1987
$72,000

DOE Contact: C. Chester Bigelow, (301) 353-4299, FTS 233-4200
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.

Keywords: Mechanical Properties, Creep, Fatigue

244. Materials Survey

FY 1987
$ 0

DOE Contact: David L. Hoof, (301) 353-2964, FTS 233-2964
ORNL Contact: P. Rittenhouse, (615) 574-5103, FTS 233-5103

Conduct review of materials needs and applications in support of liquid metal reactors (e.g., fuel cladding, ducts, control systems, pressure boundaries) and match with potential emerging new materials and developments. Compile nuclear island materials needs and problems with particular emphasis on PRISM and SAFR. Review of foreign and domestic materials developments as they relate to needs.

Keywords: Nuclear Reactor Materials

245. Absorber and Reflector Procurement — FY 1987 $ 0

DOE Contact: Andrew Van Echo, (301) 353-3930, FTS 233-3930
WHC Contact: Robert Leggett, (509) 376-2505, FTS 444-2505

Continue the procurement of materials and alloys to fabricate hardware for the manufacturer of FFTF reflector and control rod assemblies to improve the reliability, enhance the safety, and extend the effective full power days (EFPD) in the reactor to reduce operating costs. Support shall include the development of the capability to allow HT-9 and Dispersion Strengthened Ferritic (DSF) alloys to extend the performance potential of LMR core components (direct support to existing DSF fabrications and international commitments). Establish material properties of interest for LMR applications (direct support to Series III fuel design). Provide support to designers and analysts of innovative LMRs. Initiate procurement of replacement radial reflector components. Conduct PIE on in-reactor creep behavior and irradiation effects on mechanical properties of ferritic alloys to high exposure in MOTA-1E. Determine mechanical properties of dispersion strengthened ferritic (DSF) clad tubing.

Keywords: Control Rods, Mechanical Properties, Ferrous Metals

246. MOTA Fabrication and Operation — FY 1987 $ 0

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 HT-9 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-1E operations report. Complete fabrication of MOTA-1F test train and its installation into the test vehicle.

Keywords: Irradiation, Environmental Testing

247. Absorber Development — FY 1987 $300,000

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 conducting PIE on ADVAB-1A and ADVAB-2 and

providing analytical support to extend FFTF absorber lifetime to 900 Effective Full Power Days (EFPD). Provide final report on B4C absorbers. Issue updates for design codes (CONRD, CRPBOW).

Keywords: Control Rods, Nuclear Absorbers

248. FFTF Metal Core — FY 1987 $1,400,000

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 the transition of the FFTF from an oxide-fuel core to a binary metal fuel core. These activities include acquisition of metal fuel safety analysis codes; continuation of the Final Safety Analysis Report Event Analysis; multi-year metal fuel program plan support; initiation of FFTF metal fuel irradiations; and transient testing in TREAT. Initiate preliminary design for Series III metal fuel for FFTF. Fabricate first full HT-9 clad FFTF binary metal driver fuel test assembly, at nominal Series III fuel conditions (MFF-2).

Keywords: Fuel Rods, Nonferrous Metals

249. Core Demonstration Experiment (CDE) — FY 1987 $2,000,000

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. Initiate TREAT tests of CDE lead fuel pins. Conduct PIE on pins from ACO-1 and FO-2 lead tests. Analyze the transient and steady-state test results. Fabricate two low power CDE assemblies for irradiation, draft Cycle 9 CDE report, evaluate data for justifying continued irradiation of CDE to goal exposure (900 EFPD) and beyond (1,200 EFPD) based on steady-state and transient data. Initiate PIE of ACO-1 and FO-2 pins. Initiate PIE of CDE transient tested pins.

Keywords: Fuel Rods, Nonferrous Metals

250. FFTF Assembly Operations — FY 1987 $3,765,000

DOE Contact: Robert G. Lange, (301) 353-5338, FTS 5338
WHC Contact: LeRoi H. Rice, (509) 376-4080, FTS 444-4080

Fabricate metal and plutonium-oxide test series fuel pins for FFTF fuel assemblies. Continue Phase I activities under the DOE/PNC Fuels and Materials agreement. Initiate draft plans to begin binary metal fuel pin fabrication upon receipt of metal fuel slugs

from Argonne National Laboratory-West. Fabricate three FFTF metal fuel test assemblies in accordance with the FFTF Metal Fuel Program Plan; fabricate five FFTF Plutonium-Oxide (PO) series fuel test assemblies.

Keywords: Actinides, Fuel Rods

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

251. Development of Improved Thermoelectric Materials for Space Nuclear Power Systems — FY 1987 $550,000

DOE Contact: W. J. Barnett, (301) 353-3097, FTS 233-3097
General Electric Co. 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 X 10^{-3}°C^{-1} over the temperature range of 300-1000°C.

Studies conducted in 1987 have shown that an ultra fine grain structure, while quite effective in reducing thermal conductivity, only yields a modest, typically 10 to 18 percent, improvement in figure of merit. Future efforts shall be focused on elucidating the beneficial effects of gallium phosphide additions.

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: Semiconductors, Consolidation of Powder, Solidification-Rapid, Structure, Thermoelectric

252. Development of an Improved Process for the Manufacture of DOP-26 Iridium Alloy Blanks FY 1987 $750,000

DOE Contact: W. J. Barnett, (301) 353-3097, FTS 233-3097
ORNL Contact: R. L. Heestand, (615) 574-4352, FTS 624-4352

An iridium alloy, DOP-26 (i.e., Ir-O.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).

Scale-up to a nominal 2" diameter x 8 kg. consumable arc melt extrusion billet size has been successfully demonstrated with anticipated high product yields. Product qualification has proceeded successfully through cup fabrication and weldability trials including clad vent set (CVS) closure welds. Fabrication of urania simulant fuel clad impact test hardware was initiated. Both scale-up studies and product qualification tests shall be continued in FY 1988.

Keywords: Non-ferrous Metals, Extrusion, High Temperature Service

253. Carbon Bonded Carbon Fiber Insulation Manufacturing Process Development and Product Characterization FY 1987 $500,000

DOE Contact: W. J. Barnett, (301) 353-3097, FTS 233-3097
ORNL Contact: W. P. Eatherly, (615) 574-5220, FTS 624-5220

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.

Replacement rayon fiber and binder/activator materials have been screened. Material selections were made, specifications were prepared and procurement of production quantities of raw materials was initiated.

Process control and inspection simplification cost reduction studies were pursued. During FY 1988 effort shall be focused on process optimization, inspection simplification and product qualification.

Keywords: Insulators/Thermal, High Temperature Service, Fibers

Device or Component Fabriction, Behavior or Testing

254. Nondestructive Testing Methods Development and Application to Thermoelectric Materials and Devices FY 1987 $160,000

DOE Contact: W. J. Barnett, (301) 353-3097, FTS 233-3097
ORNL Contact: R. W. McClung, (615) 574-4466

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 bands, and the post-test diagnostic evaluation of multicouples.

Keywords: Nondestructive Testing, Thermoelectric

Material Properties, Behavior, Characterization or Testing

255. Characterization of State-of-the-Art Thermoelectric Device/Materials and Exploratory Studies of Rare Earth Sulfide Thermoelectric Materials FY 1987 $350,000

DOE Contact: W. J. Barnett, (301) 353-3097, FTS 233-3097
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 thermoelectric properties of rare earth chalcogenides are being studied. Fabrication techniques are being developed. Particular attention is being directed toward rare earth ternary sulfides. This phase of the program was significantly reduced in FY 1987.

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: Semiconductors, Thermoelectrics

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 $65 million in FY 1987 including over $35 million as the cost for irradiation testing in the Advanced Test Reactor. The DOE contact is Robert H. Steele, (703) 557-5565.

OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT

Office of Storage and Transportation Systems

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.

256. Development of Criteria for Nuclear Spent Fuel Storage in Air — FY 1987 $733,000

DOE Contact: D. E. Shelor, (202) 586-2836
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: Spent Nuclear Fuel, UO_2 Oxidation, Interim Dry Storage, Fuel Degradation

257. Development of Zircaloy Deformation and Creep Rupture Models for Predicting Cladding Behavior During Interim Dry Storage — FY 1987 $67,000

DOE Contact: D. E. Shelor, (202) 586-2836
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 will be put to mainframe and popular PC formats. Documentation of the program will be prepared and published.

Keywords: Cladding Rupture, Spent Nuclear Fuel, Zircaloy Cladding

258. PWR and BWR Spent Fuel Assembly Crud Composition, Characterization, and Effects on Operations — FY 1987 $19,000

DOE Contact: D. E. Shelor, (202) 586-2836
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 to fuel rod removal were monitored during the disassembly operations, qualitative observations were made and a videotape prepared.

In FY 1987 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.

Keywords: Disassemble, Fuel Rod Removal, Crud

Office of Civilian Radioactive Waste Management/Nevada Nuclear Waste Storage Investigations Project (OCRWM/NNWSI)

The primary goal of the OCRWM/NNWSI 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. Many of the activities described in the FY 1986 Annual Report continued into FY 1987 but were terminated in mid-FY 1988.

259. Waste Package Environment — FY 1987 $945,000

DOE Contact: C. P. Gertz, (702) 295-8920
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

260. Waste Form Testing — FY 1987 $2,745,000

DOE Contact: C. P. Gertz, (702) 295-8920
LLNL Contact: David Short, (415) 422-1287

Develop a fabrication and emplacement process for waste package packing which will ensure that the packing will meet its post-closure performance requirement to limit water flow around the waste package to that necessary to ensure mass transport is dominated by diffusion.

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

261. Metal Barrier Testing — FY 1987 $1,321,000

DOE Contact: C. P. Gertz, (702) 295-8920
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

262. Other Engineered Barrier Waste Package Components — FY 1987 $137,000

DOE Contact: C. P. Gertz, (702) 295-8920
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

263. Integrated Testing — FY 1987 $1,298,000

DOE Contact: C. P. Gertz, (702) 295-8920
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.

264. Waste Package: Performance Assessment — FY 1987 $638,000

DOE Contact: C. P. Gertz, (702) 295-8920
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

265. Research on Geochemical Modeling of Radionuclide Interaction with a Fractured Rock Matrix — FY 1987 $915,000

DOE Contact: C. P. Gertz, (702) 295-8920
LLNL Contact: David Short, (415) 422-1287

Further develop the geochemical modeling code EQ3/6 for use in long-term predictions of radionuclide release from a nuclear waste repository.

Keywords: Goechemical Modeling, Computer Modeling, Rock-Water-Waste Interaction

266. Waste Package: Design, Fabrication and Prototype Testing — FY 1987 $1,168,000

DOE Contact: C. P. Gertz, (702) 295-8920
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

267. Waste Package Environment Field Tests — FY 1987 $252,000

DOE Contact: C. P. Gertz, (702) 295-8920
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 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.

268. Microstructure Investigation of Nodular Cast Iron — FY 1987 $25,000

DOE Contact: F. Falci, FTS 233-5466
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

269. Composition Investigation of Nodular Cast Iron — FY 1987 $25,000

DOE Contact: F. Falci, FTS 233-5466
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

270. Generate Material Property Database for Nodular Cast Iron — FY 1987 $140,000

DOE Contact: F. Falci, FTS 233-5466
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

271. Investigate the Feasibility of Using Depleted Uranium as a Structural Component in Cask Construction — FY 1987 $5,000

DOE Contact: F. Falci, FTS 233-5466
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

272. Evaluate Current NDE Methods for Applicability to Thick Section Nodular Cast Iron

FY 1987
$130,000

DOE Contact: F. Falci, FTS 233-5466
SNL Contact: K. B. Sorenson, (505) 844-5360

Sandia has contracted with the National Bureau of Standards 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

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, while continuing progress toward development of final waste disposal strategies at Hanford and 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. Alternatives evaluated in the Hanford Defense Waste ES include: geological disposal, in-place stabilization and disposal, continued storage, and a reference alternative which incorporates elements of the first two disposal alternatives.

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

273. Waste Form Qualification — FY 1987 $4,000

DOE Contact: Ken Chacey, (301) 353-4970 and Marv Furman, (509) 376-7072
Westinghouse Hanford Company Contact: Dave Turner, (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)

274. Immobilization/Volume Reduction/In-place Stabilization — FY 1987 $4,500

DOE Contact: Ken Chacey, (301) 353-4970 and Marv Furman, (509) 376-7062
Westinghouse Hanford Company Contact: Dave Turner, (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

Inertial Fusion Division

Applied research and development oriented toward producing controlled thermonuclear fusion reactions in a laboratory environment for military and energy applications.

Device or Component Fabrication, Behavior or Testing

275. Target Fabrication — FY 1987 $1,500,000

DOE Contact: Carl B. Hilland, (301) 353-3687
LANL Contact: Dave Duchane, (505) 667-9893
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

276. Laser Materials and Optical Components — FY 1987 $1,500,000

DOE Contact: Carl B. Hilland, (301) 353-3687
LLNL Contact: E. Storm, (415) 422-0400
KMS Fusion, Inc. Contact: Jon Larsen, (313) 769-8500
University of Rochester Contact: R. McCrory, (716) 275-5286

This project is concerned with developing Nd:glass amplifier discs and optical components for kilojoule-class laser systems. The optical components include lenses, frequency-conversion crystals, anti-reflective coatings, and mirrors.

Keywords: Inertial Fusion, Coatings and Films

Weapons Research Division

Sandia National Laboratories - Albuquerque

Solid State Sciences Directorate, 1100

Ion Implantation and Radiation Physics Research Department, 1110

Materials Properties, Behavior, Characterization or Testing

277. Ion Implantation Studies for Friction and Wear — FY 1987 $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 stainless 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 stainless 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

278. Silicon-Based Radiation Hardened Microelectronics — FY 1987 $770,000

DOE Contact: A. E. Evans, (301) 353-3098, FTS 233-3098
SNL (Contract No. DE-AC04-76DP00789) Contacts: H. J. Stein, (505) 844-6279; K. L. Brower, (505) 844-6131 and J. A. Knapp, (505) 844-2305

Optical, electrical and compositional measurements, in conjunction with electron paramagnetic resonance, Rutherford backscattering/channeling, and related techniques are used to determine the fundamental defect structures and materials properties required for radiation-hardened Si-based microelectronics. Recent studies have concentrated on amorphous silicon nitride, which is the charge storage medium for radiation-hard nonvolatile semiconductor memories; defects in SiO_2 and at the Si-SiO_2 interface, which markedly affect the radiation tolerance of MOS devices, and the formation of buried dielectric layers which may be essential for next generation radiation hard microelectronics. Relationships between the materials composition, chemical bonding, and defect configurations and the electrical performance are evaluated to permit long-term prediction of the performance of devices in a radiation environment and to develop new structures with particular properties.

Keywords: Microelectronics, Radiation Hardened, Silicon Nitride, Silicon, Silicon Dioxide, Defects

279. New Concepts in Microsensors FY 1987 $650,000

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 optical emission using principles of semiconductor device operation and fabrication, surface acoustic wave propation, and optical properties of solids. Microsensors based on the properties of semiconductor surfaces include a radiation-sensing field-effect transistor (RADFET), which operates by the trapping of radiation-produced holes in the silicon dioxide gate dielectric of the FET, and chemical sensors which operate by inducing charged layers at the metal-silicon dioxide interface in response to the chemical species. Surface acoustic waves have been exploited to make new sensors for various vapors, surface layers, and the viscosity of liquids. Optical and magnetic field detectors based on the properties of new materials, like semi-magnetic semiconductors and strained layer superlattices, are being developed for high frequency response field and infrared signal detection applications in the 5-12um wavelength range.

Keywords: Microsensors, Microcircuitry

Laser and Physical Chemistry, 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

280. Tungsten Deposition FY 1987 $350,000

DOE Contact: A. E. Evans, (301) 353-3098, FTS 233-3098
SNL Contact: Ken Greenberg, (505) 844-1243

Deposition of tungsten on a variety of materials using an abnormal glow discharge. Deposited thin films adhere well to all materials studied and have IC-device-quality conductivity.

Keywords: Nonferrous Metals, Refractory Metals, Plasma Synthesis, Films

281. Laser-Based Aluminum Etching — FY 1987 $200,000

DOE Contact: A. E. Evans, (301) 353-3098, FTS 233-3098
SNL Contact: Wayne Johnson, (505) 844-8782

Developed a laser-based system to etch aluminum interconnects on high-density ICs without damaging nearby circuit elements and to deposit new networks of polysilicon and/or tungsten interconnects on ICs. System is useful for IC design error corrections and customization.

Keywords: Nonferrous Metals, Laser Etching, Integrated Circuit Fabrication

282. Gas Phase Studies — FY 1987 $200,000

DOE Contact: A. E. Evans, (301) 353-3098, FTS 233-3098
SNL Contact: Ken Greenberg, (505) 844-1243

Gas phase studies of species densities in plasma etch reactors for the purpose of model validation.

Keywords: Plasma, Synthesis

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; and (2) 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, modification and control of surface properties, the early stages of oxidation and corrosion, adhesion of metals to polymers, and the mechanism of operation of metal-insulator-semiconductor (MIS) electronic gas sensors.

Materials Properties, Behavior, Characterization, or Testing

283. Shock Chemistry — FY 1987 $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-activated thermal batteries are being studied to determine the mechanisms and materials parameters which influence electrical output. The work also provides insights about the nature of the shock process itself. A revolutionary time-resolved dynamic stress gauge using the piezoelectric polymer PVF_2 is being developed for laboratory, field testing and

component diagnostics application. The mechanism for the operation of the gauge is being investigated.

Keywords: Organic Solids, Inorganic Solids, Molecular Structure, Shock

284. Initiation of Granular Explosives — FY 1987 $350,000

DOE Contact: A. E. Evans, (301) 353-3098
Sandia Contact: R. E. Setchell, (505) 844-5459

Experimental and theoretical efforts are being directed at developing a fundamental understanding of the mechanisms involved in the shock wave initiation and growth to detonation of heterogeneous granular explosives. Materials of current interest include hexanitrostilbene and PBX 9404.

Keywords: Shock Waves, Granular Explosives

285. Surface Science — FY 1987 $400,000

DOE Contact: A. E. Evans, (301) 353-3098
SNLA Contact: D. W. Goodman, (505) 844-5435

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, 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.

Keywords: Surface Physics, Field Ion Microscopy, Auger Electron Microscopy, UV Photoemission Spectroscopy

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, semiconductor physics (theory and experiment) and materials science in a coordinated effort. 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 switching.

Materials Preparation, Synthesis, Deposition, Growth or Forming

286. Materials Growth by Molecular Beam Epitaxy (MBE) — FY 1987 $500,000

DOE Contact: A. E. Evans, (301) 353-3098, FTS 233-3098
Sandia Contact: L. R. Dawson, (505) 846-3451

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

287. Materials Growth by MOCVD — FY 1987 $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

288. Strained Layer Superlattices for IR Detectors — FY 1987 $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 um range. These IR materials are being grown by both MBE and MOCVD techniques and evaluated by electrical and optical techniques.

Keywords: Strained-Layer Superlattices, Infrared Detectors

289. Novel Processing Technology for Semiconductor Technologies

FY 1987
$500,000

DOE Contact: A. E. Evans, (301) 353-3098, FTS 233-3098
Sandia Contact: D. S. Ginley, (505) 844-8863.

This program involves studies of new technologies for formation of diffusion barriers for improved epitaxial growth, novel metallurgies for Shottky barrier and Ohmic contact formation, and development of new metallurgical techniques for deposition of reactive alloys.

Keywords: Semiconductor Devices

290. Materials Processing for Sensors

FY 1987
$300,000

DOE Contact: A. E. Evans, (301) 353-3098, FTS 233-3098
SNL Contacts: D. S. Ginley, (505) 844-8863, R. J. Baughman, (505) 844-6337

High quality semimagnetic semiconductors are grown for magnetic field sensors, processing technologies are developed for fabricating fiber-optic based strain and chemical sensors, and thin dielectric and organic films for chemical sensors.

Keywords: Magnetic Field Sensors, Strain Sensors, Chemical Sensors

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

291. Superconductivity

FY 1987
$300,000

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. Heat capacity studies to elucidate the mechanism of superconductivity. Development of theoretical models of high temperature

superconductivity. Development of new processing technologies for ceramic superconductors.

Keywords: Superconductivity, Ceramics

292. Semiconductors — FY 1987 $300,000

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

293. Surface Science — FY 1987 $450,000

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

294. Disordered Materials — FY 1987 $450,000

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 Forming

295. Dyed Antireflective Photoresist Material — FY 1987 $150,000

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

296. Sulfonated Aromatic Polysulfones — FY 1987 $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.

Keywords: Polymers, Coatings and Films, Batteries

297. Carbon Foams — FY 987 $150,000

DOE Contact: A. E. Evans, (301) 353-3098, FTS 233-3098
SNL Contacts: R. L. Clough, (505) 844-3492

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 Testing

298. Radiation Hardened Dielectrics — FY 1987 $150,000

DOE Contact: A. E. Evans, (301) 353-3098, FTS 233-3098
SNL Contacts: R. L. Clough, (505) 844-3492; S. R. Kurtz, (505) 844-5436 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. Emphasis is placed on material preparation, testing, and the study of charge carrier transport and generation mechanisms. X-ray and electron induced photoconductivity measurements, optical and magnetic measurements, and chemical analysis techniques are utilized in this work. 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. Future studies will involve alternate dopants and thicker films.

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 Properties, Behavior, Characterization or Testing

299. Polysilanes, Photoresists, Photoconductors, and Non-Charring Dielectrics FY 1987 $125,000

DOE Contact: A. E. Evans, (301) 353-3098, FTS 233-3098
SNL Contacts: J. M. Zeigler, (505) 844-0324; P. Walsh, (505) 844-8547; R. G. Kepler, (505) 844-7520; K. Schweizer, (505) 846-7536

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. Emphasis is being placed on understanding 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. Meltable, crosslinkable polysilanes are being developed for that application.

Keywords: Insulators/Dielectrics-Polymeric, Photoresistant

Materials Preparation, Synthesis, Deposition, Growth or Forming

300. Mechanistic Studies of Polysilane Synthesis — FY 1987 $70,000

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. This work has led to improved synthesis procedures which are currently being patented.

Keywords: Polymers, Predictive Behavior Modeling

301. Chemistry of Plasma Etching and Deposition Processes — FY 1987 $110,000

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 films.

Keywords: Plasma Etching, Plasma Deposition

Materials Structure and Composition

302. Materials Structure, Dynamics, and Property Studies by Multinuclear Pulsed NMR Spectroscopy FY 1987 $70,000

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 ^{1}H spectroscopy of liquids was used to determine the molecular weight and stereochemistry of precursors used in the preparation of encapsulants and foams. The chemical structures of newly synthesized explosives were also analyzed. Both liquid and solid state spectroscopy are being applied to the study of degradation pathways and products in organic materials. Imaging techniques have been used to characterize liquid foams and will be adapted to solid foams.

Keywords: Polymers, Organics, Coatings, Films

303. Studies of Adhesion at the Molecular Level by Surface Science Techniques FY 1987 $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

The mechanism of polymer-polymer and polymer-metal adhesion is being determined by a combination of surface sensitive techniques including ESD, PSD, XPS, and Auger spectroscopies. The studies have direct relevance to questions of delamination of copper from printed circuit boards and bonding of metals to various substrates, including PTFE. Results to date indicate that atmospheric moisture contributes to delamination of copper from printed circuit boards by reacting with the Cu O_x bonding surface to produce poorly bonding Cu-OH functionality. Work is continuing to identify the mechanism of bonding of epoxy and polyimide to the CuO_x surface with a goal of developing process conditions which reduce the copper delamination.

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

304. Microporous Foam Development — FY 1987 $150,000

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 have discovered a new way to produce carbon foams of low density and small cell size. The process involves the production of polyacrylonitrile (PAN) by a solution-gelation technique followed by CO_2 solvent extraction. The resulting PAN foam is then carbonized by exposure to elevated temperatures. These foams are of potential use in several weapons applications.

Keywords: Foams, Carbon Foams, Polymeric Precursor Route, Weapons

305. Development of Removable Encapsulants — FY 1987 $150,000

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. The polymer is then infused with a blowing agent such as freon or pentane. The coated beads can simply be poured into an electronic subassembly to be encapsulated. When the unit is heated above the glass transition temperature of the polymer, the blowing agent generates a foam which then fuses the glass microballoons together. This new process is versatile: in principle, any thermoplastic polymer can be used. Furthermore, since the resultant encapsulant is mostly silica, the thermal expansion coefficient is low providing a better match to the electronic components. Removal of the encapsulant for rework is easily achieved by solvent treatment.

Keywords: Polymers, Glass, Encapsulants

Materials Properties, Behavior, Characterization or Testing

306. Mechanical Properties of Encapsulants — FY 1987 $20,000

DOE Contact: A. E. Evans, (301) 353-3098, FTS 233-3098
SNL Contact: D. Adolf, (505) 844-4773

The bulk modulus of polymeric encapsulants is essential for predicting internal stresses from thermal cycling. Up to now, only estimated values of the bulk modulus have been used since it is a difficult quantity to evaluate. Recently we have demonstrated that the bulk modulus can be obtained by using the tri-axial testing facility.

Preliminary measurements indicate significant departures from previous estimates of the bulk modulus for polymeric encapsulants.

Keywords: Polymeric Encapsulants, Organic, Tests, Bulk Modulus

307. The Strength of Kevlar Narrow Fabrics — FY 1987 $70,000

DOE Contact: A. E. Evans, (301) 353-3098, FTS 233-3098
SNL Contact: R. H. Ericksen, (505) 844-8333

The tensile strength of dry Kevlar narrow fabrics is reduced 10-30 percent after wet compression relative to the strength of samples compressed dry. This phenomenon is peculiar to the fabric; individual yarn strength is not changed. The influence of variables important for parachute applications was studied and tests to determine the fabric deformation mechanisms are underway.

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

308. High Electric Field Varistors — FY 1987 $100,000

DOE Contact: A. E. Evans, (301) 353-3098, FTS 233-3098
SNL Contacts: R. G. Kepler, (505) 844-7520 and G. E. Pike, (505) 844-7562

Measurements of defects associated with the addition of transition metals into ZnO. These are made tractable by starting with ultrapure ZnO produced by a solution chemistry technique. Although the ground states of the transition metals are one to two eV below the conduction band edge, several shallow defects have been found from admittance spectroscopy which affect the formation of potential barriers at grain boundaries.

Keywords: ZnO, Varistor, Transition Metal

309. Hydrogen Effects in Silicon — FY 1987 $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 as a complex and passivate it as an acceptor. 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

310. Rapid Thermal Processing of Gate Oxides — FY 1987 $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 SiO_2 layers are required for new generations of microelectronics. Silicon has been oxidized to a thickness of 20 nm and characterized for various electrical properties. The effect of X-rays in producing radiation defects is tested using capacitance-voltage techniques. The dielectric breakdown strength is tested using Fowler-Nordheim current measurements.

Keywords: Rapid Thermal Oxidation, Silicon, Radiation Hardness

Materials Characterization Department, 1820

Department 1820 performs chemical, 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

311. Development of Automated Methods for Chemical Analysis — FY 1987 $200,000

DOE Contact: A. E. Evans, (301) 353-3098, FTS 233-3098
SNL Contact: S. H. Weissman, (505) 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. Since 1985, development of a new inductively coupled plasma atomic emission spectroscopy (ICP-AES) system and improved digestion methods using microwave ovens have enabled studies on tracing of elements in aerosols generated in simulated nuclear reactor accidents and in analysis of glass and electrolytes being developed for use in new batteries.

Keywords: Instrumentation and Technique Development, Chemical Analysis

Electron Optics and X-Ray Analysis Division, 1822

Materials Preparation, Synthesis, Deposition, Growth or Forming

312. Thermomechanical Treatment of U Alloys — FY 1987 $40,000

DOE Contact: A. E. Evans, (301) 353-3098, FTS 233-3098
SNL Contact: K. H. Eckelmeyer, (505) 844-7775

Strengthening mechanisms are being investigated in U-Ti and U-Nb alloys with the goals of simplifying processing procedures and increasing strength-ductility combinations. It has been found that decreasing Ti content from the conventional O.75 percent to 0.60 percent results in a factor of 3 decrease in the quench rate required to suppress diffusional decomposition of the gamma-phase and get age-hardenable martensite, thus enabling processing of thicker parts and minimizing quenching-induced residual stresses. A deformation strengthening mechanism has also been developed whereby parts of any thickness can be processed to yield strengths as high as 125 ksi without the need for quenching. In addition, a combined solid solution-deformation strengthening approach has been developed which permits yield strengths as high as 165 ksi to be obtained with reductions-in-area in excess of 45 percent. Work is continuing to determine the natures of the wide variety of phase transformations which occur during these treatments and how these transformations and their resultant microstructures influence toughness.

Keywords: U-Alloys, Strengthening Mechanisms, Thermomechanical Processing

Instrumentation and Facilities

313. Advanced Methods for Electron Optical, X-Ray and Image Analysis — FY 1987 $200,000

DOE Contact: A. E. Evans, (301) 353-3098, FTS 233-3098
SNL 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. The components of a microstructural image analysis system (including a light microscope, a scanning electron microscope, several image analyzers, and a central file server) have been purchased and are now operational. Programs involving statistical characterization of the geometries and chemistries of particles and microstructural features as small as 1um are now underway, and our capabilities are expanding as additional software is written. In addition, an automated analytical electron microscope has been purchased and installed. Future work on this instrument will involve automatic logging of specimen locations and automated tilting of samples for unequivocal compound identification.

Keywords: Automation, Electron Optics, Transmission Electron Microscopy, Instrumentation 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

314. Advanced Methods for Surface and Optical Analysis — FY 1987 $700,000

DOE Contact: A. E. Evans, (301) 353-3098, FTS 233-3098
SNL Contact: J. A. Borders, (505) 844-8855, FTS 844-8855

The development of new facilities, methods and data analysis techniques for surface and optical analysis is continuing. A gas chromatograph and a microscope have been interfaced to Fourier transform infrared spectrometer, which will increase our capabilities for the identification of complex chemical mixtures and compliment the Raman microprobe for the analysis of contaminants. A micro-focusing ion source has been added to the multi-technique surface analysis facility, which will enable secondary ion mass spectroscopy to be performed at much higher lateral resolutions than was

previously attainable. We have purchased an additional high resolution scanning Auger microprobe which is contributing to an increase of the amount of analytical work that is performed and is decreasing the turnaround time for service analysis. False color Auger imaging has been added to the old Auger microprobe. This has improved our analysis capabilities and the clarity with which data can be presented to our customers.

Keywords: Gas Chromatograph, Fourier Transform Infrared Spectrometer, Raman Microprobe, Secondary Ion Mass Spectroscopy, Scanning Auger Microprobe, False Color Imaging

Thermophysical Properties Division, 1824

The mission of Division 1824 is the measurement and analysis of thermal and optical properties of engineering materials in support of Sandia's weapons and energy programs. Capabilities include thermal conductivity and diffusivity measurements, calorimetry, densitometry, dilatometry, optical reflectance, optical emittance, and ellipsometry.

Instrumentation and Facilities

315. Design and Fabrication of a Multi-Source X-Ray Gauge — FY 1987 $80,000

DOE Contact: A. E. Evans, (301) 353-3098, FTS 233-3098
SNL Contact: W. D. Drotning, (505) 844-7934

A technique has been developed for chemical analysis based on the attenuation of two radioisotopic X-ray energy beams (dual energy X-ray gauging). Single source X-ray gauging has previously been used to provide rapid nondestructive quantitative chemical analysis of materials containing a single X-ray absorber. With dual energy gauging, the capability is being expanded to include measurements on materials with two different X-ray absorbers. Our device employs X-rays from selected radioisotopes with a single channel analysis system in order to obtain the best performance. We have demonstrated agreement to better than 3 percent with standard (destructive) chemical analysis methods. System performance will be optimized and selective tests will be performed to determine system accuracy and repeatability.

Keywords: Instrumentation Development, X-Rays, Chemical Analysis

316. Infrared Reflectometer Development — FY 1987 $50,000

DOE Contact: A. E. Evans, (301) 353-3098, FTS 233-3098
SNL Contact: H. L. Tardy, (505) 846-6548

The infrared reflectometer development project has progressed to the system test and evaluation phase, involving measurements on materials from DOE weapons and energy programs. As an example, the degradation of Pyromark black absorbing paint is being studied. This paint is used in high-temperature solar absorbers but the solar

absorptance of the paint has been found to decrease after exposure to high temperatures and solar fluxes. The infrared spectral absorptance is being measured as a function of exposure time in order to determine the degradation mechanism.

Keywords: Infrared Reflectometer, Reflectance Emittance

317. Flash Thermal Diffusivity Measurements of Multilayer Samples — FY 1987 $50,000

DOE Contact: A. E. Evans, (301) 353-3098, FTS 233-3098
SNL Contacts: J. N. Sweet, (505) 844-3343 and E. P. Roth, (505) 844-7934

New data analysis methods are being developed for determining the thermal diffusivity and/or thermal resistance of one layer of a multilayer stack from flash thermal diffusivity measurements. The basis of the method is the application of nonlinear least-squares techniques to transient time vs. temperature data. The software under development has been tested on a number of standard test samples and has been used to measure the thermal diffusivity of pressed powder explosives. Future work will be devoted to evaluation of the software for use in measurements on thin coatings such as paints and sprayed materials.

Keywords: Instrumentation and Technique Development

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.

Coating Technology Division, 1831

The Coating Technology Division conducts basic and applied research in two areas: (1) coatings and (2) optical diagnostics for processes. Coating research is currently being conducted in the areas of plasma deposition, chemical vapor deposition, electrophoretic deposition, and sputtering. In addition, this division provides support for design engineers in the specification of processes and transfer of technology involving coatings.
Coating Technology Division, 1831

Materials Preparation, Synthesis, Deposition, Growth or Forming

318. Plasma Deposition of Amorphous Metal Alloys — FY 1987 $70,000

DOE Contact: A. E. Evans, (301) 353-3098, FTS 233-3098
SNL Contact: A. K. Hays, (505) 844-9996

A technique is being developed to deposit amorphous metal alloys using a radio frequency discharge. Amorphous metals can be formulated that have outstanding strength, corrosion resistance, and abrasion resistance. Their use in industrial applications has been limited by the techniques presently employed to obtain them (rapid-solidification, sputtering, etc.). Present studies include the plasma-deposition of amorphous Ni-P-C films from $Ni(CO)_4$ and PH_3 in a H_2 carrier gas. Future work will include the development of a technique to deposit amorphous metal alloys using plasma-enhanced chemical vapor deposition.

Keywords: Coatings and Films, Metallic Glasses, Plasma Synthesis, Radio Frequency Synthesis

319. Electrophoretically-Deposited Coatings — FY 1987 $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

320. Near-Net-Shape Processing of Nickel-Based Alloys — FY 1987 $150,000

DOE Contact: A. E. Evans, (301) 353-3098, FTS 233-3098
SNL Contacts: A. K. Hays, (505) 844-9996 and A. W. Mullendore, (505) 844-6833

Near-net-shape processing allows for reductions in cost, time, and raw material usage in metallurgical processing. A technique is being developed to produce nickel-based alloys from the chemical vapor deposition of $Ni(CO)_4$ and selected metalloid

hydrides. Future work will include the characterization of these alloys with respect to mechanical properties and microstructure.

Keywords: Ferrous Metals including Steels, Coatings and Films, Chemical Vapor Deposition

321. High Temperature Semiconductors — FY 1987 $80,000

DOE Contact: A. E. Evans, (301) 353-3098, FTS 233-3098
SNL Contacts: A. K. Hays, (505) 844-9996 and A. W. Mullendore, (505) 844-6833

Present microelectronics using silicon or germanium have limited use temperatures due to the fact that these materials are intrinsic conductors at temperatures above 500°C. Boron-based compounds have been suggested for use as high temperature semiconductors. Present studies include the growth of single crystals of B_4C using chemical vapor deposition. Future work will be directed towards the development of a technique for growing boron phosphide crystals suitable for device fabrication.

Keywords: Coatings and Films, Semiconductors, Chemical Vapor Deposition

Materials Properties, Behavior, Characterization or Testing

322. Optical Diagnostics for Materials Processing — FY 1987 $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 of species present in the atmosphere during standard 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 interlectrode gaps of VAR furnaces. Future plans include developing optical diagnostics for chemical vapor deposition.

Keywords: Optical Diagnostics, Welding, Vacuum Arc Remelting

Device or Component Fabrication, Behavior or Testing

323. Development of Materials for Magnetic Fusion Reactors — FY 1987 $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 beryllium

limiter assembly was designed, fabricated and delivered to the ISX-B Tokomac experiment at Oak Ridge National Laboratory. Performance has met design expectations. Secondly, 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

Physical Metallurgy Division, 1832

The mission of the Physical Metallurgy Division 1832 is to provide the characterization and understanding of the 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 capabilities are part of this division, and extensive use is made of the analytical capabilities at Sandia.

Materials Properties, Behavior, Characterization or Testing

324. Toughness of Ductile Alloys — FY 1987 $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: Ferrous Metals, Fracture, Predictive Behavioral Modeling

325. Properties of Ni-B Alloys — FY 1987 $50,000

DOE Contact: A. E. Evans, (301) 353-3098, FTS 233-3098
SNL Contact: A. N. Campbell, (505) 844-7452

The mechanical response of Ni-B alloys produced by chemical vapor deposition (CVD) is being characterized. Microstructural examination is being performed to explain and model the deformation process for this material.

Keywords: Alloys, Chemical Vapor Deposition, Microstructure, Deformation, Metals

326. Analytical Electron Microscopy of Engineering Alloys — FY 1987 $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. This has been applied to uranium alloys (where the high Z values create problems) and in stainless steel weldments. These quantitative measurements allow diffusion properties to be measured and, in turn, the kinetics of such metallurgical phenomena as precipitation to be determined.

Keywords: Ferrous and Non-Ferrous Metals, Joining and Welding, Transformation, Electron Beam Methods, Weapons

327. Friction and Wear of Modified Surfaces — FY 1987 $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: Ferrous and Non-Ferrous Metals, Erosion/Wear/ Tribology, Ion Implantation, Weapons

328. Alloy Deformation Response and Constitutive Modeling — FY 1987 $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: Ferrous Metals, Creep, Fatigue, Nuclear Reactors, Predictive Behavioral Modeling, Weapons

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

329. Vacuum Arc Remelting — FY 1987 $60,000

DOE Contact: A. E. Evans, (301) 353-3098, FTS 233-3098
SNL Contact: F. J. Zanner, (505) 844-7073

Both fluid flow and 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. Future work will include spectrographic studies to characterize the plasma.

Keywords: Ferrous and Non-Ferrous Metals, Conventional Solidification

Device or Component Fabrication, Behavior or Testing

330. Aluminum Laser Welding — FY 1987 $40,000

DOE Contact: A. E. Evans, (301) 353-3098, FTS 233-3098
SNL Contact: M. J. Cieslak, (505) 846-7500

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 and is dependent on the development of improved laser systems.

Keywords: Non-Ferrous Metals, Joining/Welding, Conventional Solidification

331. Copper Brazing to Carbon — FY 1987 $20,000

DOE Contact: A. E. Evans, (301) 353-3098, FTS 233-3098
SNL Contact: F. M. Hosking, (505) 844-8401

Assembly of copper flexible circuits often requires sequential joining processes and/or rework. To produce joints that resist damage during subsequent soldering or de-soldering operations, a study of the mechanical properties of solid-state welds of copper produced with indium or indium-silver alloy interlayers has been evaluated. Mechanical tests and fractographic analysis indicate that this process produces high-quality joints. The resistance to thermal damage is increased by raising process temperatures so that indium is diffused into the base metal.

Keywords: Non-Ferrous Metals, Joining/Welding, Fracture

332. Dissimilar Metal Welds — FY 1987 $200,000

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

Weapon components typically include several alloys that must be welded to one another. As high-performance alloys are incorporated into new designs, significant welding problems are encountered. Studies have been initiated to define the solidification mechanics in complex alloy systems with the goal of avoiding compatibility problems, particularly hot-cracking. Studies involving CO laser welding of high-alloy martensitic steels to martensitic stainless steels have been completed. Additional studies are in progress involving pulsed Nd:YAG laser welding of Kovar to a number of ferrous and nickel-based alloys. Future studies will emphasize the welding compatibility of precipitation strengthened nickel-based alloys.

Keywords: Ferrous and Non-Ferrous, Joining/Welding, Solidification-Conventional

333. Welding of Nickel-Based Alloys — FY 1987 $225,000

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. Also, future work will include solidification studies in the Ni-Cr-Mo system.

Keywords: Non-Ferrous Metals, Joining/Welding, Conventional Solidification

334. Plasma Arc Welding — FY 1987 $175,000

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 design specification has been developed for a variable-polarity plasma-arc welding power supply. Future studies will evaluate cathodic cleaning, welding efficiency, and arc stability as a function of the current-voltage characteristics.

Keywords: Non-Ferrous Metals, Joining/Welding, Conventional Solidification

335. Laser Welding — FY 1987 $175,000

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. Future work will continue to emphasize beam-plume interactions and will include the development of a weld pool reflectivity test.

Keywords: Lasers, Joining/Welding, Process Modeling

Surface and Interface Technology Division, 1834

The Surface Metallurgy Division 1834 is concerned with the influence of surface and near-surface regions to 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

336. Deposition of Amorphous Materials With a Dual Beam Ion System — FY 1987 $80,000

DOE Contact: A. E. Evans, (301) 353-3098, FTS 233-3098
SNL Contact: J. K. G. Panitz, (505) 844-8604

Amorphous films can reduce friction, wear, and corrosion susceptibility. A dual beam system has been developed to sputter-deposit amorphous film material onto selected substrates with concurrent ion bombardment with inert and reactive gas ions (hydrogen and argon have been used). Preliminary coatings have been deposited, and system parameters have been defined. The mechanical properties are dependent on the conditions of deposition of the sputter-deposited amorphous material, specifically hardness. Future work will emphasize the development of hard, wear-resistant coatings for mechanical applications.

Keywords: Metallic Glass, Erosion/Wear/Tribology, Coatings and Films

Materials Properties, Behavior, Characterization or Testing

337. Modification of Mechanical Properties by Ion Implantation — FY 1987 $35,000

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 and which function in inert atmospheres 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 austenitic and martensitic stainless steels and permits self-mating wear couples, 304 rubbing on 304 stainless steel, for example. Future work will emphasize the implantation of other elements and will attempt to optimize the chemical composition for maximum wear performance.

Keywords: Ion Implantation, Coatings and Films, Erosion/Wear/Tribology, Structure, Surface

Device or Component Fabrication, Behavior or Testing

338. Development of Materials for Magnetic Fusion Reactors — FY 1987 $200,000

DOE Contact: A. E. Evans, (301) 353-3098, FTS 233-3098
SNL Contacts: M. F. Smith, (505) 846-4270; J. B. Whitley, (505) 844-5353; J. M. McDonald, (505) 846-7735

Materials used in magnetically confined fusion energy devices experience severe environments. Two materials have been developed for these applications. A beryllium limiter assembly was designed, fabricated, delivered to the ISX-B tokamak experiment at Oak Ridge National Laboratory. Performance has met design expectations. Secondly, 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

339. Plasma Cleaning Studies — FY 1987 $65,000

DOE Contact: A. E. Evans, (301) 353-3098 , FTS 233-3098
SNL Contacts: R. R. Sowell, (505) 844-1038

Fluorocarbon plasmas have been used to remove metal oxide films from the surface of Inconel 718 that are formed during an S-glass-to-Inconel metal sealing process.

Keywords: Surface, Welding, Joining, Plasmasynthesis, Metals, Ferrous

Instrumentation and Facilities

340. Ion Beam Reactive Deposition System — FY 1987 $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 depend on stoichiometry, temperature of deposition, system pressure, and ionization state. A system has been constructed for reproducible reactive ion beam deposition of compound films; the system can control stoichiometries, energy input of each ion/atom/molecule, gas phase composition, and deposition rates. The system will be used to study mechanisms of compound film formation in addition to friction and wear responses of films for wear parts. Future

studies will involve deposition of TiN, but eventually this method will be used to study complex film deposition of compounds not readily obtainable by current deposition methods.

Keywords: Coatings and Films, Erosion/Wear/Tribology, Surface

341. In-Situ Friction, Wear, and Electrical Contact Resistance Systems FY 1987 $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. The surface composition is easily masked by exposure to ambient conditions between testing and analysis. A device has been assembled in a scanning Auger analytical system to complete oscillatory or unidirectional sliding friction experiments while monitoring 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. Future modifications will allow kinetic friction coefficients to be measured in-situ.

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. The department also supports the Laboratories through the study of metallurgical corrosion and oxidation. Electrochemistry constitutes a major element of these studies. Initiative is taken to stimulate advanced weapons and energy related concepts by providing new materials and developing 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

342. Ceramic Processing — FY 1987 $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 Treatment

Materials Properties, Behavior, Characterization or Testing

343. Fracture of Ceramics — FY 1987 $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

Inorganic Materials Chemistry Division, 1846

Division 1846 has responsibility for relating the chemical properties of inorganic materials to their application in a variety of Sandia weapons, energy, and reactor safety programs. The division has programs in the chemical preparation of glasses and ceramics including sol-gel chemistry of glasses for coatings and monolithic structure and electroactive ceramic powders, precipitation of ion exchangeable transition metal oxides

for catalysts, thin-film capacitors, and solution stabilization to yield homogeneous, monodispersed structural and electronic ceramics. The division also has programs to study the properties and survivability of inorganic materials in reactive environments, e.g., solvent (aqueous, acidic and basic, corrosive) dissolution of inorganic glasses, ionic conductivity of high temperature electrolytes, and the physical and chemical properties, especially thermal stability, of inorganic materials at high temperature.

Materials Preparation, Synthesis, Deposition, Growth or Forming

344. Glass and Glass-Ceramic Development — FY 1987 $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 lithium silicate glass ceramic which is being used to make hermetic seals to Inconel alloys for actuator headers. A family of phosphate-based glasses is being used to form seals to Al, Cu, and stainless steels. Previously we developed a new glass which 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 now have developed a new glass with a 10-year life and have begun using it on a pilot scale. 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

Corrosion Division, 1847

Division 1847 personnel perform research to understand and control the corrosion and oxidation of metals, and they also characterize gas-metal reactions involving species such as hydrogen and ammonia. Corrosion research is directed toward: (a) developing new and improved materials; (b) defining boundaries for applying existing materials; and (c) performing failure analyses. Emphasis is on understanding the mechanistic nature of corrosion processes. The division maintains expertise in the areas of corrosion by aqueous and non-aqueous electrolytes; corrosion by gases; stress corrosion cracking; gas-metal interactions including scattering, adsorption, and desorption; and electrodeposition.

Materials Properties, Behavior, Characterization or Testing

345. Corrosion — FY 1987 $1,150,000

DOE Contact: A. E. Evans, (301) 353-3098, FTS 233-3098
SNL Contacts: R. B. Diegle, (505) 846-3450 and 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

Sandia National Laboratories - Livermore

Materials Preparation, Synthesis, Deposition, Growth or Forming

346. Powder Metallurgy — FY 1987 $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; J. W. Zindel, (415) 294-2051

The installation of an inert gas atomizer, a spark erosion system, a melt spinner for the production of fine metal powders has further expanded our powder metallurgy capabilities. Emphasis is being placed on the effect of processing parameters on material characteristics and on the development of alloy systems utilizing rapid solidification processing. Studies on spark erosion are emphasizing the effect of processing parameters on powder size distribution, surface morphologies, and production rates of micron-size particles.

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 solidifi-

cation processing facilities will also be utilized to produce powders for matrix composites. Extensive powder characterization and handling capabilities have been developed including automation imaging analysis.

Keywords: Alloys, Rapid Solidification, Metals, Near-Net-Shape Processing, Shock Wave Compaction

347. Advanced Electrodeposition Studies — FY 1987 $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.

Keywords: Metals, Electrodeposition, Electroforming, Mechanical Properties, Chromium

348. Metal Forming — FY 1987 $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

Fundamental understanding of nonelastic deformation processes is being developed through crystal plasticity modeling and experimentation. This work focuses upon large-strain phenomena and anisotropy which are important in metal forming and failure processes. Experimental and model results are applied directly to process development and to metal forming problems through the Interagency Metal Forming Working Group (established under this program). Recent work has revealed a new understanding of microstructure texture evolution and anisotropy. In particular, strain-rate sensitivity has been found to influence texture evolution in shear. This result impacts how yield surfaces, anisotropy, and material rotations are represented in phenomenological models for finite element analysis. Large-strain experiments examining axial effects during shear have been compared with both physical model and phenomenological model predictions for the purpose of improving our ability to predict failure due to strain localization. The fundamental understanding developed in this work is being expressed in constitutive relations which can be incorporated into multi-dimensional finite-element codes.

Keywords: Ferrous and Nonferrous Metals, Fatigue, Fracture, Near-Net-Shape Forming

349. Advanced Organic Materials — FY 1987 $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

350. Particulate Technology — FY 1987 $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

351. Tritium Getter Technology — FY 1987 $50,000

DOE Contact: A. E. Evans, (301) 353-3098, FTS 233-3098
SNL Contacts: D. L. Lindner, (415) 294-3306 and D. A. Nissen, (514) 294-2767

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 are examining the potential 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 (phenyletynly) benzene has shown that when mixed with appropriate catalysis, it can quickly getter tritium (as it does hydrogen). Aging studies of the tritiated getter demonstrate that no gaseous tritided species are evolved over extended periods of time.

Keywords: Hydrogen Getters, Organic

352. Molded Desiccant Foam — FY 1987 $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, Dessicants

353. Plasma Processing — FY 1987 $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

354. Helium-Induced Crack Growth in Metals and Alloys — FY 1987 $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 J. E. Costa, (415) 294-2352

The effect of helium on the low-temperature mechanical properties of fcc metals is being investigated experimentally. Tritium decay is used to introduce helium into metals without inducing radiation damage into the metal. A variety of experimental techniques are employed to study the resultant tritium and helium effects, including transmission electron microscopy, autoradiography, tritium imaging, and thermal desorption spectroscopy. Mechanical properties of materials containing helium are studied in an effort to understand the plastic flow and fracture of metals as functions of helium concentration and distribution within the solid. The chemical similarity of tritium to hydrogen makes these techniques relevant to a wide variety of technologies. Slow crack growth experiments at ultra-high hydrogen pressures are also being conducted to determine the effects of mechanical processing, microstructure, and welding on the resistance of advanced materials to hydrogen-induced cracking. The observed effects of hydrogen on crack growth kinetics and thresholds are being used to identify mechanisms and evaluate models of hydrogen embrittlement. Theoretical analysis based on the Embedded Atom Method developed at Sandia have begun to elucidate the role of helium in altering microstructures and mechanical properties of the alloys.

Keywords: Ferrous Metals, Non-Ferrous Metals, Crystal Defects/Grain Boundaries, Fracture

355. Joining Science and Technology — FY 1987 $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. Spingarn, (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/Welding, NDE, Microstructure, Metals, Transformation, Solidification, Modeling

356. Composites: Characterization and Joining — FY 1987 $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. Spingarn, (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. Condensible volatile materials in resins considered for space applications are being identified. Coatings for composite materials are under investigation to enhance stability for special design needs (e.g., mirrors). 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/Welding, Fibers, Corrosion, Coatings

357. Compatibility, Corrosion, and Cleaning of Materials — FY 1987 $75,000

DOE Contact: A. E. Evans, (301) 353-3098, FTS 233-3098
SNL Contacts: L. R. Thorne, (415) 294-2636; 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

358. Tritium-Metal Interaction — FY 1987 $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 experimental 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 ≤ 10 um spatial resolution.

Keywords: Ferrous Metals, Non-Ferrous Metals, Surfaces, Defects/Grain Boundaries, Tritium

359. Measurement of Multilayer Thin Film Structures — FY 1987 $50,000

DOE Contact: A. E. Evans, (301) 353-3098, FTS 233-3098
SNL Contacts: 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 or Technique Development, Films

Instrumentation and Facilities

360. New Spectroscopy — FY 1987 $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

361. Tritium Facility Upgrade for Materials Characterization and Testing — FY 1987 $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

Continuing materials research in the Tritium Research Laboratory has prompted the need for new analytical techniques and equipment and the upgrading of existing experimental test equipment. New capabilities being developed include a quantitative ^3He mass spectrometer for characterizing helium build-in levels resulting from tritium decay. A high-pressure T_2 thermal charging and quench facility is being built which, in conjunction with a dissolution/scintillation-counting apparatus, will allow for the precise measurement of tritium solubility as a function of temperature and pressure. Mechanical test capabilities have been upgraded by the addition of a computer-interfaced servohydraulic test frame. A modern scanning electron microscope with light-element analysis capability has been installed to provide for fractographic analysis of failed materials.

Nuclear magnetic resonance is being developed for tritium and helium-3 analysis of powdered materials exposed to tritium environments. The capability will provide information on metal-tritide phases and helium trap characteristics as well as quantitative determinations of isotope concentrations. Since the technique is nondestructive, materials will be examined with time to determine their aging behavior. Sophisticated NMR techniques will be explored for investigating, for example, metal lattice strain near helium-filled defects and surface/interface states of hydrogen-metal systems.

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 .1C 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 quadrapole mass spectrometer permits a degree of sample preparation and characterization prior to PCT study.

Keywords: Spectrometer, Tritium Charging, Mechanical Testing, Scanning Electron Microscopy

Lawrence Livermore National Laboratory

Materials Preparation, Synthesis, Deposition, Growth or Forming

362. Ion Beam Modification of Materials — FY 1987 $230,000

DOE Contact: A. E. Evans, (301) 353-3098, FTS 233-3098
LLNL Contact: R. G. Musket, (415) 422-0483, FTS 532-0483

It has been shown that aluminum ion implantation combined with selective oxidation reduced the permeation of tritium through 304L stainless steel by more than a factor of 20 at temperatures below 200°C. Ultra-high-dose implantations of aluminum into beryllium near room temperature leads to several interesting phenomena, including precipitation of aluminum with precipitate growth affected by radiation-enhanced diffusion. Chemical effects were found for the implantation of oxygen into iron previously implanted with aluminum, and these effects resulted in highly Al_2O_3-rich layers inside the iron. The layers formed by ion implantation, which are often unique, can sometimes be predicted, and can dramatically change the response of the material to various environments.

Keywords: Ferrous Metals, Metals: Non-Ferrous, Hydrogen Attack, Ion Implantation, Surface

363. Formation of Metastable Surface Alloys — FY 1987 $180,000

DOE Contact: A. E. Evans, (301) 353-3098, FTS 233-3098
LLNL Contact: E. N. Kaufmann, (415) 543-2640, FTS 543-2640

Four alloy systems are being studied using electron-beam surface modification: Cu-Zr, Cr-Ta, U-Cr and U-Mo systems. The Cu-Zr system is a binary metallic-glass forming system, the study of which extends our initial work on a quaternary glass in the previous fiscal year. The Cr-Ta and U-Cr systems are studied as part of our high temperature alloys and stainless uranium surface-alloys. For the Cu-Zr alloy, the critical cooling rate for glass formation is determined as 10^6 C/s. The rate-limiting mechanism is the nucleation rather than the growth of crystalline phases. The nucleation of the $CuZr_2$ phase is more difficult than that of the CuZr phase. For the Cr-Ta alloy, fine cellular microstructures develop on the modified surfaces. The cell size decreases with solidification rate. At very rapid rate (>2 m/s), the cellular morphology converts into a planar morphology. Fine dispersions of second phase particles also exist in front of the solidification boundary. For the U-Cr and U-Mo alloys studied, the formation of metastable phases with extended solubility of Cr and Mo up to 20 atomic % in uranium have been achieved.

Keywords: Metals: Non-Ferrous, Electron Beam Methods, Surface

364. Synthesis Project (Explosives) — FY 1987 $120,000

DOE Contact: A. E. Evans, (301) 353-3098, FTS 233-3098
LLNL Contact: C. L. Coon, (415) 422-6311, FTS 532-6311

We have established strict guidelines pertaining to energy, density, sensitivity, and stability to choose 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. We have also identified key reactions which require 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. The synthesis of Bicyclo-HMX and related compounds was studied extensively. The fully nitrated Bicyclo-HMX fused-ring systems were synthesized for the first time and have been demonstrated to be stable materials. These materials contain the fused 5-,5-, 5-,6-, and 5-,7- ring systems plus one added substituent and represent a class of materials not previously available. The pathway to these materials was made possible by our development of a new nitrolyzing system consisting of N_2O_5, HNO_3, and trifluoroacetic anhydride. This unique system is also adaptable for use on the synthesis of a wide range of energetic materials. We were also successful in synthesizing the keto analog of homo-Bicyclo-HMX, a target material on the present program. This material is currently undergoing characterization.

Keywords: Explosives, Chemical Synthesis, Weapons

365. Synthesis and Reactivity of Transition Metal Fluorocarbon Complexes FY 1987 $104,000

DOE Contact: A. E. Evans, (301) 353-3098, FTS 233-3098
LLNL Contact: R. D. Sanner, (415) 423-3875, FTS 543-3875

We have focused on the trifluoromethyl group (CF_3) as a potential ligand since it holds the greatest promise for yielding stable, volatile products. We have developed new synthetic routes utilizing either CF_3I or $Cd(CF_3)_2 \cdot DME$ as the trifluoromethyl source. Our choices for transition metals have been guided by relevance to Laboratory programs although our synthetic procedures may be applied to any transition metal. We have discovered a method to photochemically generate CF_3 radicals with high quantum efficiency using rhenium carbonyl. We have prepared several new gold alkyls and fluoroalkyls and have begun a comparative study of these new complexes. In addition, we have prepared stable gold complexes with the novel ligand hexafluoroacetylacetonate and note an increase in volatility compared to the analogous acetylacetonate compounds. Finally, we have synthesized iridium complexes using trifluorophosphine (PF_3) as a ligand. The use of the trifluoromethyl ligand allows us to prepare stable transition metal compounds with fairly high vapor pressures. We have devised general synthetic routes to trifluoromethyl transition metal complexes and examined the use of hexafluoro-acetylacetonate as a ligand to impart both stability and volatility.

Keywords: Fluorocarbons, Composites, Metals: Non-Ferrous Metals

366. Advanced Ceramics Synthesis and Processing FY 1987 $157,000

DOE Contact: A. E. Evans, (301) 353-3098, FTS 233-3098
LLNL Contact: J. B. Holt, (415) 422-8003, FTS 532-8003

Since the chemical reaction to form B_4C from the two elements is weak exothermally, a thermite-type combustion reaction, as shown by the following equation, was chosen to synthesize submicron powders.

$$2\ B_2O_3 + 6\ Mg + C \rightarrow B_4C + 6\ Mg\ O \qquad (1)$$

Once the mixed reactant powders are ignited, the combustion reaction proceeds spontaneously without the need for further external energy. The MgO is leached from the combustion products with HC1, leaving behind an ultra-fine-grained B_4C powder. We have demonstrated that a submicron (~0.5U) powder can be synthesized by the combustion reaction as presented in equation (1). The reaction occurs very rapidly, within seconds, relying entirely on chemical energy to raise the temperature. The average particle size of the B_4C product is strongly influenced by the particle size of the carbon powder and to a lesser degree, by the combustion temperature. The higher temperature promotes large grain sizes and increases the amount of agglomeration. The development of a new process for the production of submicron B_4C powder, based on solid combustion

reactions, could be a major factor in making decisions regarding the use of B_4C in weapons applications. Up to this time the high cost of production has greatly restricted any large-scale utilization of B_4C parts.

Keywords: Ceramics, Combustion Synthesis, Weapons

367. Sputtering (Plutonium Alloys) — FY 1987 $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/cm^2-s, which allow deposition rates as high as 400Å/s, can simultaneously be bombarded by ionized or neutral noble gas atoms at fluxes up to 1×10^{17} atoms/cm^2-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 atomic size mismatch and changes in Pu 5-f bonding influence the formation of amorphous and metastable phases. The synthesis of amorphous and metastable Pu alloy compositions by triode sputtering has provided valuable insight on the electronic structure of Pu in different alloy systems. The unique controllable features of the triode sputtering process has provided opportunities to synthesize new materials not possible by other techniques.

Keywords: Sputtering, Actinides

368. Kinetic Models (Hydrogen, Methane Oxidation) — FY 1987 $15,000

DOE Contact: A. E. Evans, (301) 353-3098, FTS 233-3098
LLNL Contact: J. R. Creighton, (415) 423-7949, FTS 543-7949

The approach is to analyze numerical solutions of detailed chemical kinetics models of the reaction systems studied. The models consist of sets of reaction steps generally corresponding to reactions occurring in a single collision, with corresponding rate constants. These varied in complexity from 3 reversible reactions involving 3 species for ozone decomposition to 85 reaction steps involving 26 species for methane oxidation. The analysis consists mainly of looking for steady states which couple species concentrations, causing them to track one another. This yields simplified, but phenomenologically correct models. These steady states also reduce the number of degrees of freedom on the path to equilibrium. The behavior of chemically reacting systems near equilibrium has been known, in a linear approximation, since the time of Onsger. This appears to be the first treatment of the entire path to equilibrium and does not require a linearizing approximation.

Keywords: Hydrogen, Organic Gases, Oxidation Predictive Behavior Modeling

369. An Investigation of Multifilamentary NbN Superconductors — FY 1987 $180,000

DOE Contact: A. E. Evans, (301) 353-3098, FTS 233-3098
LLNL Contact: L. Summers, (415) 423-6574, FTS 543-6574

The objective is to develop new methods of fabricating superconductors into shapes suitable for fusion energy magnets. Superconductors such as NbN have excellent strain and radiation-tolerance properties, but have not been formed in useful geometries. The approach is to use a combination of physical vapor deposition and liquid metal infiltration to fabricate multifilamentary NbN that is stabilized with copper or aluminum. We conducted experiments to identify critical parameters for the uniform partial vapor deposition of superconducting NbN on small (10-um) ceramic filaments. The process has been extended to the fabrication of 30-m-long graphite tows that contain 3000 filaments per bundle. Liquid metal infiltration with aluminum stabilizers has proven successful. The superconductor appears unaffected by the introduction of molten aluminum. Electrical characterization of the composite is underway.

Keywords: Superconductors, Vapor Deposition, Fibers

370. Grinding Glass in the Ductile Regime — FY 1987 $140,000

DOE Contact: A. E. Evans, (301) 353-3098, FTS 233-3098
LLNL Contact: K. L. Blaedel, (415) 422-0290, FTS 532-0483

Bound abrasive grinding of glass may result in material removal in a brittle or ductile fashion. The objective of this project is to develop a bound abrasive grinding process by which an optic may be made sufficiently smooth that only 0.5 to 2 um of material needs to be polished away. A further objective is to understand the conditions that determine the transition between brittle and ductile material removal mechanisms. We have adapted a newly constructed lathe, the CBN machine, for use as a ductile grinder. Although its roller ways make it unsuitable for actual use as a grinder, the CBN machine's thermally controlled environment, cutting fluid handling system, the repeatability suit it for development of the material removal process. To this machine we have mounted an LLNL-designed and constructed air bearing grinding head. We are currently working to improve thermal control of the machine; poor thermal control has made controlling the depth of cut of the grinding wheel very difficult. To date, we have sporadically produced ductile grinding in fused silica and Zerodur but have not been able to produce such surfaces over large areas or on demand. We have made progress toward perfecting techniques of balancing the wheel, monitoring its condition, and sensing its location acoustically.

Keywords: Glass Ceramics and/or Non-Metallic Glasses, Grinding, Surface

371. A Basic Study of the Single-Point Cutting Process — FY 1987 $410,000

DOE Contact: A. E. Evans, (301) 353-3098, FTS 233-3098
LLNL Contact: R. Donaldson, (415) 422-1916, FTS 532-1916

The overall objective is to obtain a fundamental understanding of the single-point cutting process, which will improve the cutting accuracy and ultimate surface finish achievable with a broad range of engineering materials. The approach is to combine the fundamentals of precision engineering with an understanding of materials science to create a series of cutting experiments and then to compare the results of these experiments with finite-element code analyses. Current efforts are focused on two areas. One is the diamond turning of silicon for optical mirrors, where tool wear and surface damage are significant factors. The cutting fluid used has been found to change these factors by orders of magnitude. The second effort is aimed at determining the smallest attainable depth of cut for a well-made diamond tool. Copper chips have been produced with a nominal depth of cut of 30 Å (about 10 atomic spacings), which challenges the resolution of our scanning-electron microscope equipment.

Keywords: Glass, Metals, Surface, Machining

Materials Structure and Composition

372. Theory of Polar Fluid Structure and Dynamics — FY 1987 $49,000

DOE Contact: A. E. Evans, (301) 353-3098, FTS 233-3098
LLNL Contact: D. Calef, (415) 422-7797, FTS 532-7797

Theoretical models for structure and dynamics of polar fluids can be achieved by modifying existing integral equation theories to include both the short and long range forces present in polar molecules. The resulting structures can be used in dynamic calculations, either to construct model potential surfaces, or by use of "analytical continuation" methods. The existing literature, on both the methods of calculating the structures and using them in resulting dynamics, have been reviewed. A promising approach is being discussed, as are extensions to the dynamic methods.

Keywords: Fluids, Predictive Behavior Modeling

373. Structures of Actinide-Hydrogen Compounds and Solutions at High Pressures — FY 1987 $150,000

DOE Contact: A. E. Evans, (301) 353-3098, FTS 233-3098
LLNL Contact: R. H. Condit, (415) 422-8729, FTS 532-8729

Small specimens are compressed in a diamond anvil cell press at pressures up to 40 GPa (400 kbars), X-ray diffraction measurements are used to identify the crystal structures which form at these pressures, and the volume compression induced by pressure is derived. Measurements have been carried out in a sample of $PuH_{2.5}$ with the finding

at 20 GPa of a phase transformation from the simple (normal pressure) fluorite structure to a complex structure which we have not yet identified. This work will gain meaning in the context of measurements on hydrides of various H/Pu ratios where the f-electron overlap should be influenced by the stoichiometry. It will also extend into work on solutions of hydrogen in plutonium metal.

Keywords: Actinides, Hydrides, Structure, High Pressures

374. Actinide Thermochemistry — FY 1987 $120,000

DOE Contact: A. E. Evans, (301) 353-3098, FTS 233-3098
LLNL Contact: M. G. Adamson, (415) 523-2024, FTS 543-2024

Three extant general-purpose chemical equilibrium computer codes will be assessed with respect to suitability for application to "simple" actinide alloy systems and complex multiphase actinide systems that also contain alloy phases. After selection of a suitable code, thermodynamic solution models will be developed for important non-stoichiometric compound phases and alloy phases that commonly occur in actinide processing equilibria, and a thermochemical data base for Pu compounds and alloys will be compiled. The programs selected are FACT (on-line system at McGill University) and SOLGAXMIX (PC-operable, stand-alone program). The technical significance of completing development of the general purpose thermochemical model is great. There are potentially large pay-offs for any program interested in the preparation, enrichment, or recovery of plutonium metal or alloys.

Keywords: Actinides, Chemistry, Predictive Behavior Modeling

Materials Properties, Behavior, Characterization or Testing

375. The Influence of Cooling Rate on the Microstructure of Duplex Austenitic-Ferritic Stainless Steel — FY 1987 $65,000

DOE Contact: A. E. Evans, (301) 353-3098, FTS 233-3098
LLNL Contact: J. W. Elmer, (415) 423-8235, FTS 432-8235

A series of seven high-purity stainless steel alloys have been electron-beam surface-melted at cooling rates which vary from 5×10^2 °C/s^{-1} to 8×10^6 °C/s^{-1}. The microstructure of these surface melts is being studied to determine the primary solidification mode, ferrite content, ferrite morphology, dendrite arm spacing and micro-chemical compositions of the ferrite and austenite phases. These observations will be combined with thermodynamic information and kinetic studies to develop a model which will predict the microstructural changes with cooling rate and composition.

Keywords: Metals: Ferrous, Fatigue, Joining/Welding, Structure Solidification

376. The Role of Interfaces in Metallic-Layered Thin Films — FY 1987 $70,000

DOE Contact: A. E. Evans, (301) 353-3098, FTS 233-3098
LLNL Contact: A. F. Jankowski, (415) 423-2519, FTS 543-2519

The approach for this program includes: (1) modeling efforts emphasizing the role of interfaces in the realms of phase stability and elastic behavior; (2) procurement of facilities for the production of multilayer thin films; (3) conducting physical measurements of mechanical properties; and (4) characterization of these multilayer microstructures by X-ray analysis and electron microscopy.

Keywords: Coatings and Films, Structure, Predictive Behavior Modeling

377. Capillary Structures (in Foams) — FY 1987 $190,000

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

378. Pretransformation Behavior in Alloys — FY 1987 $90,000

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

379. Polymer Modeling — FY 1987 $100,000

DOE Contact: A. E. Evans, (301) 353-3098, FTS 233-3098
LLNL Contact: R. Cook, (415) 422-6993, FTS 532-6993

Purely on the basis of molecular parameters, we have been able to predict the flexibility characteristics of polyisocyanate polymers, and determine the molecular origin of the flexibility. We have successfully studied the dynamics and energy storage of polymer chains in a bulk sample subjected to deformation forces. We have shown how the deformation energy becomes concentrated in the bond angles and lengths when conformational freedom is suppressed. We have developed a model of bulk polymeric materials that includes the feature of polymer chain conformational motion. Computer simulation studies of stress-strain behavior using the model reproduce the essential features of the experimental data on real polymeric materials.

Keywords: Polymers, Structure, Predictive Behavior Modeling

380. Nuclear Spin Polarization — FY 1987 $200,000

DOE Contact: A. E. Evans, (301) 353-3098, FTS 233-3098
LLNL Contact: P. C. Souers, (415) 422-1302, FTS 532-1302

During this fiscal year the following results were achieved: Longitudinal triton relaxation has been studied from 3 to 10°K and found to follow the "heat capacity theory." Radiation reduces the relaxation time from 0.08 to 1.3 s. Another order of magnitude should be achievable with enriched molecular DT. The e.s.r. equipment is now coming on the air after two years of construction. We have e.s.r. test signals at 4°K. Negotiations between LLNL and CERN have begun in order to use their polarization system. We have constructed the first model of dynamic cooling.

Keywords: Hydrogen Isotopes, Radiation Effects, Laser Fusion, Magnetic Fusion

381. Plutonium Martensitic Transformation Plasticity — FY 1987 $100,000

DOE Contact: A. E. Evans, (301) 353-3098, FTS 233-3098
LLNL Contact: P. H. Adler, (415) 423-4417, FTS 543-4417

We determined that despite the very large volume change, the $\delta \leftrightarrow \alpha$ transformation could be martensitic. We then used a computer program to predict the crystallographic energetic and interfacial features of this transformation. The $\delta \leftrightarrow \alpha$ transformation in Pu alloys can be martensitic despite the ~20 percent volume change. Calculated free energy functions show a strong linear dependence over a large temperature range prior to obtaining a zero slope near 0°K as required by the third law of thermodynamics. This means that, in order to achieve the observed isothermal kinetic behavior, the critical

driving force to obtain a given constant transformation rate, $\Delta G_{crit}(f)$, must be non-linear in temperature. This is borne out by an observed non-linear dependence of the activation energy, Q, at large driving forces, ΔG.

Keywords: Actinides, Structure, Transformation

382. Theory of Deflagration at High Pressures — FY 1987 $140,000

DOE Contact: A. E. Evans, (301) 353-3098, FTS 233-3098
LLNL Contact: D. Calef, (415) 422-7797, FTS 532-7797

We have employed the methods of modern statistical mechanics to develop expressions for the rates of chemical processes and transport processes for high temperature conditions. Calculations on the pressure dependence of the structure and reactivity of small molecules (N_2, H_2O, CH_3OH) have been made. Investigations on thermal transport are in progress. Calculations reveal the fascinating complexity of molecular systems indicates we are approaching the capability of handling systems of applied interest.

Keywords: Energetic Materials, Reactions, Predictive Behavior Modeling

383. High Pressure-High Temperature Raman Spectroscopy of Energetic Materials — FY 1987 $130,000

DOE Contact: A. E. Evans, (301) 353-3098, FTS 233-3098
LLNL Contact: M. S. Costantino, (415) 422-6923, FTS 532-6923

Two non-linear Raman spectroscopies, stimulated Raman gain (SRG) and coherent anti-Stokes Raman spectroscopy (CARS), are examined for their relative potential for obtaining portions of the Raman spectrum of nitromethane, HMX, and other explosives in a heated diamond anvil cell (DAC) at pressures to 40 GPa and temperatures to 1300 K. The shifts, widths, and intensities of the scattered lines in the Raman spectrum are measured using a single laser pulse that has a time resolution of about 10 nanoseconds. A pulsed Raman spectroscopy facility has been fully developed. CARS was determined to be a much more sensitive technique for these purposes than SRG. Single shot CARS spectrum of nitromethane was obtained in a DAC with a signal to noise ratio of about 10, demonstrating the feasibility of the experimental approach. The ability to explode nitromethane in the DAC with a laser pulse, without damaging the cell, has been developed. This is the first reported CS spectrum in a diamond anvil cell. Because of the very general nature of this spectroscopic technique, the clear opportunity now exists for the first time to study directly the fundamental reactive and structural modifications that energetic molecules undergo at pressures and temperatures near those in a detonation.

Keywords: Energetic Materials, Reactions, Instrument or Technique Development, Predictive Behavior Modeling, Weapons

384. Hot Spot Microdynamics/High Explosives R&D — FY 1987 $140,000

DOE Contact: A. E. Evans, (301) 353-3098, FTS 233-3098
LLNL Contact: R. Simpson, (415) 423-0379, FTS 543-0379

The approach has been to use multichannel visible radiometry for the determination of temperature and extent of reaction in an energetic material as a function of time. Desired hydrodynamic conditions were generated, in general, with thin flyers accelerated by an electrically exploded foil to velocities of 1-9 mm/usec. Piezoelectric transducers together with an optical isolation system were used to monitor flyer velocities and shock positions. Synchronization of the optical and electrical signals can be made to under 10 nsec. All of the instrumentation developed achieved the desired specifications. Successful EOS measurements were made on an insensitive form of TATB at pressures greater than 20 GPa. A JWL EOS was found to fit the data at high pressures. The material was also found to be insensitive to 35 GPa. Temperature measurements were made on TATB, PETN, and TNT. Theoretical thermodynamic calculations using the JCZ3 EOS were in agreement with the PETN data. In addition, delayed initiation studies on PETN were carried out. Evidence was found that for densities greater than 97 percent theoretical maximum there may be a detonation induction time as long as 100 nsec. The instrumentation and techniques developed in this program have enabled the routine evaluation of phenomena associated with the initiation and propagation of explosives. Dynamic temperature measurements serve as a necessary basis for the development of EOS models which take into account temperature effects. The comparisons made between experiment and theory in this study have clearly demonstrated the inability of existing EOS which are based on macroscopic measurement to properly account for the reaction chemistry.

Keywords: Energetic Materials, Reactions, Instrument or Technique Development, Weapons

385. Roles of Post-Yield Properties and Physical Aging in the Fracture of Highly-Crosslinked Networks — FY 1987 $90,000

DOE Contact: A. E. Evans, (301) 353-3098, FTS 233-3098
LLNL Contact: J. D. LeMay, (415) 423-3599, FTS 543-3599

Recently observed structure-fracture relationships in usually brittle, highly-crosslinked epoxy polymers were proposed to be due to the unique properties of the material in the highly constrained plastic zone localized at the crack tip. The microscopic size of the plastic zone at the crack tip inhibits direct characterization of the material within; therefore, experimental evaluation is limited to the testing of bulk specimens. A technique for inducing the post-yield condition and large strains in bulk glassy polymers in tensile testing under high hydrostatic pressure. When highly-crosslinked epoxy specimens were tested in tension under large hydrostatic pressures, they became exceptionally ductile, easily entered the post-yield regime of their stress-strain response, and could be deformed to unusually large strains. The resulting deformed polymer displayed unique thermal, physical, and mechanical properties. The thermal and physical

properties of the deformed glassy polymer indicated that the strain energy of deformation was not due only to changes in molecular configuration. The non-configurational contribution to the strain energy might explain the paradox of why both glassy and elastomeric fracture in epoxy networks exhibit identical structure-fracture relationships.

Keywords: Polymers, Structure, Predictive Behavior Modeling, Physical Properties

386. Studies of Material Properties at High Temperatures — FY 1987 $72,000

DOE Contact: A. E. Evans, (301) 353-3098, FTS 233-3098
LLNL Contact: O. H. Krikorian, (415) 422-8076, FTS 532-8076

The approach for this study was to apply solid-state theory, solution theory, and thermodynamics, together with (1) parameters such as atomization energy and microhardness to explain thermal expansivity behavior, (2) solution and migration mechanisms to explain solubility and diffusivity behavior, and (3) proposed solute species combined with regular solution theory to identify chemical species in liquid metal solutions. Phosphides were identified as likely the best containment materials for liquid metals. Accurate ($\pm 10\%$) methods for thermal expansivity prediction were extended to phosphides, sulfides, and selenides. A definitive paper was completed on solubilities and diffusivities of H_2O and H_2 in Li_2O. Li_2 was identified as an important liquid-phase species in the Li-LiH system. Accurate property prediction and evaluations can be made for high temperature materials by applying a combination of theory and correlation methods. Results found should be of significant scientific benefit as well as provide a good basis for development of advanced materials for Laboratory programs such as nuclear weapons, fusion reactors, and nuclear waste processing.

Keywords: Refractory Ceramics, High Temperatures, Structure, Prediction Behavior Modeling, Weapons, Fusion, Radioactive Waste Host

387. Catalytic Properties of Actinide Compounds — FY 1987 $174,000

DOE Contact: A. E. Evans, (301) 353-3098, FTS 233-3098
LLNL Contact: C. A. Colmenares, (415) 422-6352, FTS 532-6352

X-ray and ultraviolet photoelectron spectroscopies, XPS and UPS respectively, are being used to study the reactivity of U and actinide intermetallics (UFe_2, UNi_2, UNi_5, UMn_2, $NpCo_2$) with O_2, CO, CO_2, CH_4, and C_2H_4 because these compounds are exposed to air in their use, CO is hydrogenated to alcohols and hydrocarbons in one of our model reactions (Fischer-Tropsch process) and CO_2 is one of the products from this reaction. ThO_2 and doped-ThO_2 are being tested as catalysts for the hydrogenation of CO to alcohols and hydrocarbons in a high-pressure differential flow reactor. The photoemission data on uranium, UFe, UNi_5 and $NpCo_2$ has produced a good understanding of the behavior of these materials in oxidizing atmospheres and advanced our knowledge in the

following areas: mechanism of oxidation of actinide metals and alloys, behavior of uranium in storage in CO and CO_2 atmospheres, and reactivity and electronic structure of these materials.

Keywords: Actinides, Structure, Surface, Catalysis, Predictive Behavior Modeling

388. Computer Molecular Dynamics — FY 1987 $100,000

DOE Contact: A. E. Evans, (301) 353-3098, FTS 233-3098
LLNL Contact: A. M. Karo, (415) 422-7800, FTS 532-7800

Computer molecular dynamics (CMD) involves the numerical solution of Newton's Second Law equations of motion for all the interacting atoms and molecules in the simulation, thereby providing a detailed time history of the coordinates and velocities of each of the particles. The state-of-the-art molecular dynamics codes that we have developed permit a detailed investigation to be carried out for particle-surface dynamics, down to the subpicosecond nanometer regime. The surface configuration, composition, and temperature can be varied arbitrarily. Initial states of the atomic and molecular particles can be randomly selected or given starting values. Statistical analyses of the final states of the particles and their post-collision paths are automatically executed by the code. Clarification of the volume and surface for negative ion generation requires an understanding of the mechanisms that affect the concentrations of atoms and vibrationally excited molecules in plasma and wall interactions. This knowledge provides a basis for neutral beam and source designers for extrapolation to high-power systems.

Keywords: Plasmas, Magnetic Fusion, Inertial Fusion, Reaction Vessel, Surface

389. Dislocation Microstructure of Aluminum Deformed to Large Steady-State Creep Strains — FY 1987 $140,000

DOE Contact: A. E. Evans, (301) 353-3098, FTS 233-3098
LLNL Contact: M. E. Kassner, (415) 423-2329, FTS 543-2329

The dislocation feature associated with the rate-controlling process for creep was examined by performing large-strain deformation experiments of aluminum at elevated temperature to various strains within the primary, but especially the steady-state regime, using unique mechanical testing capabilities at Stanford University. The dislocation microstructure at the various strain levels is examined in the transmission electron microscope. The rate-controlling process for creep in aluminum clearly shows that it is independent of the spacing of dislocations that compose subgrain boundaries (or subgrain misorientation angle). The cause of large-strain softening has been unambiguously determined as resulting from a texture by a series of experiments and analysis. The large-strain ambient-temperature deformation of silver has been characterized for the first time in terms of a steady-state equation that includes an activation energy that appears to be close to that of dislocation-pipe diffusion.

Keywords: Metals: Non-Ferrous, High-Temperature Behavior, Creep

390. In Situ Reversed Deformation Experiments — FY 1987 $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

391. Hyperfine Studies and Radiation Effects — FY 1987 $110,000

DOE Contact: A. E. Evans, (301) 353-3098, FTS 233-3098
LLNL Contact: C. E. Violet, (415) 422-7728, FTS 532-7728

Using Mössbauer spectroscopy and a diamond anvil press, the melting point will be determined from the Fe^{57} Mössbauer spectra. The diamond anvil press with heaters will apply pressure up to 250 kb and increase temperatures up to ~700°C. $Nd_2Fe_{14}B$ magnets samples have been exposed to 14 MeV neutrons at the RTNS-II for fluences of $\sim 10^{17}$ n's/cm^2. The Fe^{57} Mössbauer spectra of these irradiated samples will be analyzed and compared to the spectra of unirradiated samples to study the effects of 14 MeV neutron damage on a microscopic scale.

Keywords: Metals, Radiation Effects, Instrumentation or Technique Development

392. Actinide Phase Diagrams — FY 1987 $30,000

DOE Contact: A. E. Evans, (301) 353-3098, FTS 233-3098
LLNL Contact: M. E. Kassner, (415) 423-2329, FTS 543-2329

There are several aspects to the evaluation. There is the usual assessment of the reliability of the experiments of different investigations that determine the phase boundaries. Whenever possible, however, attempts will be made to carry out a

thermodynamic assessment and modeling of the phase boundaries. This may allow more accurate and realistic assessment of the phase boundaries and the relative phase stabilities. The Pu-Ga binary is the most important of the six assigned systems and was completed during FY 1986. The evaluation of the Pu-A, Al-Th, Al-Np and Al-Am have been completed this fiscal year.

Keywords: Actinides, Phase Diagrams

393. Modeling and Experimental Measurement of Residual Stress — FY 1987 $170,000

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

394. Numerical Modeling of Crack Growth and Plastic Deformation Material Model — FY 1987 $192,000

DOE Contact: A. E. Evans, (301) 353-3098, FTS 233-3098
LLNL Contact: R. A. Riddle, (415) 523-7541, FTS 543-7541

The "global" J Integral failure criterion is being correlated with a "local" failure criterion, which postulates a "damage process zone" at the crack tip. Crack growth initiates when a weighted function of effective plastic strain reaches a critical value in the damage process zone. We implemented this local failure criterion in NIKE2D for tie-break slidelines. By correlating global and local failure criteria, one can predict fracture toughness from microstructural variables like grain size and second phase particle distributions. We will develop the ability to use finite-element analysis to predict failure in components due to crack growth and plastic deformation. We will develop appropriate analytical techniques for characterizing the state of stress at a crack tip, experimental methods for determining the constitutive and crack growth resistance properties, and statistics for determining the inherent defect population for D38 uranium, HY130 and HP 9-4-0.20 steels, and glass materials. We have obtained the precise form of the modified J Integral to account for thermal stresses and strains and are implementing it in NIKE2D. Finite element analyses of the dynamic tear and compact tension specimens have shown

that assuming a constant effective plastic strain to failure along a tie-break slideline leads to a positively sloped J vs. crack-growth curve, as typically occurs in materials testing. From fracture toughness testing of D38 uranium, we determined that the amount of carbon in the microstructure has a large effect in decreasing material fracture toughness at low temperature.

Keywords: Crack Growth, Deformation Predictive Behavior Modeling, Metals: Non-Ferrous, Ferrous, Glass/Glass Ceramics

395. A Study of Residual Stress for Epoxy-Resin Composites — FY 1987 $305,000

DOE Contact: A. E. Evans, (301) 353-3098, FTS 233-3098
LLNL Contact: W. Feng, (415) 422-8701, FTS 532-8701

We have developed a mathematical model that simulates the elastic behavior of composite materials. The composite simulated in the model is composed of graduated sizes of long cylinders embedded in a continuous matrix system. Using the thermal mechanical properties of the fiber and matrix, the model calculates the residual strains of a composite caused by curing. Also as part of our analytical work, we developed a relationship between the curvatures and the residual strains of a flat laminate before curing. In the experimental work, we designed and built an apparatus for determining the curvatures of a shell. With the apparatus, the curvatures determined analytically can be verified experimentally. We have determined the thermal viscoelastic properties of a matrix, including the relaxation function of F263 epoxy from 0.1 s to 1,000,000 y for a reference temperature of 150°C. The temperature considered in the relaxation function can be shifted within a range between room temperature and the glass transition temperature.

Keywords: Composites, Encapsulants, Predictive Behavior Modeling

396. High Temperature Metal Alloy Radiant Property Measurements in Conjunction with Advanced Surface Spectroscopy — FY 1987 $80,000

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 or Technique Development

397. Evaluation of a Thermo-Plastic Material Model — FY 1987 $126,000

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 research is to measure the thermomechanical response of 304L stainless steel and uranium in well-controlled homogeneous uniaxial tests. The validity of range of applicability of the thermo-plastic materials models will then be assessed. A basis will then exist for proposing new models that account for observed discrepancies. The materials for this study have been processed and characterized. We have designed and constructed a unique experimental apparatus that uses a laser to measure the longitudinal and transverse strains in a test sample. With it we have begun a series of experiments to evaluate the material model under both isothermal and transient conditions. A finite element model of the test sample has been complete.

Keywords: Metals: Ferrous, Actinides, Instrumentation Technique Development, Predictive Behavior Modeling

398. Strength of Composite Materials — FY 1987 $50,000

DOE Contact: A. E. Evans, (301) 353-3098, FTS 233-3098
LLNL Contact: S. E. Groves, (415) 422-1331, FTS 532-1331

The objective of this development project was to significantly improve our ability to accurately predict the strength of composite materials, both experimentally and theoretically. The primary goals were (1) review the existing failure criterion, (2) develop a new failure criterion, and (3) design a biaxial test apparatus for generating failure surfaces for composites. The major effort was concerned with developing the biaxial test apparatus which included design and fabrication of a set of tension-torsion-internal pressurization grips and a biaxial extensometer for simultaneous measurement of the axial and torsional displacements. This apparatus was not commercially available. The biaxial test apparatus was not completely finished under the funding of the development project; however, FY 1988 ME research funds have provided funds for the completion of the apparatus. This apparatus was not tested during the project; nevertheless it is completed and ready for use in generating the necessary failure surfaces for evaluation of the failure criteria. Several existing failure criteria have been reviewed and a new failure criterion was proposed which was written in terms of the Cauchy finite strain invariants for a transversely isotropic medium. This new failure criterion was successfully applied to predict the failure of a mechanical part.

Keywords: Composites, Predictive Behavior Modeling, Mechanical Properties, Instrumentation or Technique Development

399. Integrated Engineering Applications Software (IDEAS) Project — FY 1987 $100,000

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 or Technique Development

400. High Strain Rate Tensile Testing — FY 1987 $127,000

DOE Contact: A. E. Evans, (301) 353-3098, FTS 233-3098
LLNL Contact: D. H. Lassila, (415) 423-9537, FTS 543-9537

New analysis techniques have been developed for the tensile Hopkinson bar test to determine stress-strain behavior of materials at high strain rates. The new techniques center on the use of high-elongation post-yield strain gages to measure dynamic strain. High-speed digitizers are used to record transient strain gage signals of about 200uS duration to obtain stress vs. time histories. These histories are then phased to produce a stress-strain record. Tests performed on 316 stainless steel demonstrate the utility of the developed techniques and indicate that the tensile Hopkinson bar results are consistent with compression tests.

Keywords: Metals: Ferrous, Instrumentation or Technique Development

Instrumentation and Facilities

401. Shockwave Fiber Optics Probe — FY 1987 $150,000

DOE Contact: A. E. Evans, (301) 353-3098, FTS 233-3098
LLNL Contact: G. Haugen, (415) 422-7779, FTS 532-7779

An ultra-fast ruby pressure sensor is under development to measure the profile of shock waves. It has been shown that the ruby response can be increased by a factor of 1000 and still retain a significant signal level, however, the loss in the optical fiber and scatter originating in the fiber deteriorate the S/N. Feasibility study of the optical properties of various doped crystals eliminated the transition metals and many of the lanthanide as candidates. Ce^{+3}, Sm^{+2}, and Pr^{+3} ions were the only activators with appropriate optical properties. Ce^{+3} was eliminated because of the poor transmission

properties of the optical fiber. Sm^{+2} was eliminated because of its low quenching temperature. Pr^{+3} still has promise and is being explored.

Keywords: Instrumentation or Technique Development, Mechanical

402. Laser Induced Chemistry — FY 1987 $238,000

DOE Contact: A. E. Evans, (301) 353-3098, FTS 233-3098
LLNL Contact: C. Stevens, (415) 422-6208, FTS 532-6208

We have identified two approaches to the control of chemical reactions through laser excitation. In one approach, a visible laser excites a specific X-H bond (X = C, N, or O) in a polyatomic molecule to a highly excited vibrational state (v = 5, 6, or 7). This step is followed by a second laser that further excites the "primed" bond to a dissociative electronic state before the localized stretching motion dissipates into the rest of the molecule. In the second approach we are exploring reactions where bond selectivity can be achieved in a one-step laser excitation process. This approach examines reactions that have transition states closely associated with the extension of a single X-H bond and reaction barriers surmountable by vibrational energy placed into a high overtone of the X-H bond. We have completed construction and testing of the facility, flexible enough to address basic studies in laser chemistry and extend the art of measurement science. An ideal candidate for demonstrating bond-selective chemistry is the 2-step photodissociation of CD_3H. A theoretical calculation shows that the reaction

$$CD_3H \xrightarrow[1]{hv} CD_3\text{-}H^+ \xrightarrow{hv} CD_3 + H$$

has a high likelihood of exhibiting bond selectivity. We have photodissociated both CH_31 and CD_31 with one laser and detected CH_3 and CD_3 by multiphoton ionization time-of-flight mass spectrometry at the levels expected in the 2-step photodissociation of CD_3H.

Keywords: Instrumentation or Technique Development, Laser-Induced Chemistry

403. Synchrotron Radiation Studies — FY 1987 $345,000

DOE Contact: A. E. Evans, (301) 353-3098, FTS 233-3098
LLNL Contact: J. Kinney, (415) 423-1126, FTS 543-1126

High-energy electron storage rings at Stanford (SPEAR) and Hamburg (DORIS) were utilized. A high-resolution, thermoelectrically cooled CCD imaging array camera was developed for detecting the intense X-ray beams. A high resolution phosphor was developed for optimizing counting statistics. A data acquisition/processing system was assembled with the software necessary to perform on-line reconstructions and to conduct advanced image processing. It is possible to perform chemically specific tomography on small samples with a spatial resolution of 5um. Furthermore, the ability to perform truly three dimensional reconstructions allows for the study of interconnected structures in ways

never before possible. With improvements in the X-ray optics and detector efficiency, it will be possible to push the resolution to better than 1um. This will open up many applications in materials and biological sciences. The ability to perform non-destructive, chemical-state mapping with high resolution will significantly impact our ability to characterize microstructures. This has been demonstrated in tomographic examinations of a laser fusion micro-balloon and a low density foam sample in a series of experiments performed at SSRL this past April.

Keywords: Instrumentation or Technique Development, Microstructure, Inertial Fusion, Foams

404. Scanning Tunneling Microscope — FY 1987 $150,000

DOE Contact: A. E. Evans, (301) 353-3098, FTS 233-3098
LLNL Contact: W. Siekhaus, (415) 422-6884, FTS 532-6884

Scanning tunneling microscopes were constructed at Lawrence Berkeley Laboratory. Operation in air was tested by observing the surface of graphite. Atomic resolution was obtained in the topographic mode (constant tunnel current) and in the current mode, where the surface is scanned at high speed and the average tip-sample distance has kept constant. Atomic resolution has also been achieved for the same surface coated with a few um of silicone oil. A second complete STM system has been assembled for work in ultra-high vacuum. An ion-pumped UHV chamber equipped with capability for low-energy electron diffraction, Auger spectroscopy, and quadropole mass analysis has been set up to receive the UHV STM mounted on a flange. STM can be carried out on surfaces covered by fluids as well as under UHV conditions. In the latter case, the surface under study can be viewed by other surface probes without exposure to the atmosphere.

Keywords: Instrumentation or Technique Development, Surface, Structure

405. Study of Solid Deformation Processes Using a Novel Calorimetric Technique — FY 1987 $80,000

DOE Contact: A. E. Evans, (301) 353-3098, FTS 233-3098
LLNL Contact: R. E. Lyon, (415) 423-8323, FTS 543-8323

A new principle of measuring heat from calorimetric signals (1) forms the basis for designing and constructing a gas pressure deformation calorimeter to simultaneously measure the heat and work of uniaxial solid deformation. The change in internal energy of the material is obtained directly according to the first law of thermodynamics, yielding a total energy balance for the deformation process. The calorimeter, which was made operational during FY 1986, has been calibrated at 298°K using both steady-state and transient electrical heating. The dynamic response of the calorimeter to an imposed heating history has been determined, allowing for an analytical deconvolution of the pressure signal to obtain the total heat, instantaneous heat and instantaneous heat flow for an arbitrary thermal process. A new isothermal theory of large reversible deformation

of compressible materials has been completed. The derivation originates from simple physical hypotheses while retaining fully nonlinear kinematics to arrive at a three-dimensional constitutive equation requiring only two physical property constants.

Keywords: Instrumentation or Technique Development, Deformation, NDE

406. Scanning Tunneling Microscopy (STM) as a Detector — FY 1987 $90,000

DOE Contact: A. E. Evans, (301) 353-3098, FTS 233-3098
LLNL Contact: W. Siekhaus, (415) 422-6884, FTS 532-6884

The objective of this program is to use STM to detect submicrometer-sized flaws in nonconducting optical components. These flaws have been impossible to detect with conventional nondestructive evaluation methods. Initial experiments concentrated on using ultraviolet light to excite electrons into the conduction band. These excited electrons give rise to the tunneling effect, which is caused by electrons passing between two surfaces in very close proximity. A voltage applied between the surface catches and accelerates some electrons toward the opposite surface, thus generating a tunneling current used by the STM. Our experiments were successful with doped materials that had band gaps to 2.3 eV (the limit of available lasers) but were discontinued because of the development of Atomic Force Microscopy (AFM). AFM uses atomic forces (rather than tunneling) to do topographic imaging of conducting and insulating materials. We have designed an AFM based on capacitance gauging of a thin membrane (the capacitance gauge and thin membrane technologies are both borrowed from other LLNL programs). This design can simultaneously perform AFM and STM and uses existing servosystems, such as those in the acoustic microscope or Large Optic Diamond Turning Machine, to detect flaws on insulating optics.

Keywords: Optical Components, Instrumentation or Technique Development, Defects, NDE

407. Research in Quantitative Ultrasonic Nondestructive Evaluation — FY 1987 $247,000

DOE Contact: A. E. Evans, (301) 353-3098, FTS 233-3098
LLNL Contact: G. A. Clark, (415) 423-9759, FTS 543-9759

The objective of this research is to develop experimental, theoretical, and signal-processing tools to remove distortion from signals and to improve our ability to interpret data acquired with the ultrasonic test bed and the acoustic microscope. In addition to processing signals from controlled experiments, we have successfully processed signals produced during measurement of layer parameters and joints in parts used for LLNL programs. These include adhesive thickness measurements, W83 weapon welds, S-1 computer chip bonds, and the weld underbead for the W79 weapon. We are developing algorithms that use wave-propagation models to estimate layer parameters (thicknesses and reflection coefficients). We have successfully produced preliminary impulsive sound field measurements with a hardware signal synthesizer and a deconvolution algorithm.

Our technology transfer efforts have led to computationally efficient computer programs that implement signal processing algorithms on fast processors.

Keywords: Instrumentation or Technique Development, NDE, Ultrasonics

408. Research in Computerized Tomographic Imaging — FY 1987 $100,000

DOE Contact: A. E. Evans, (301) 353-3098, FTS 233-3098
LLNL Contact: J. Brase, (415) 422-6992, FTS 532-6992

Overall objectives are to obtain an understanding of three-dimensional imaging techniques in industrial situations; to develop systems capable of producing quantitative, high-resolution CT images; and to establish techniques for the use of a priori knowledge about the object under study to improve inspection accuracy and speed. We have developed two research systems; first, a video-based system or VCAT, is complete and has demonstrated the ability to produce images with 100-um spatial resolutions. With VCAT, we have developed image deconvolution and three-dimensional data-display techniques. The second, a pencil beam system (PBCAT), can make spectral measurements at each data point. Its design is complete, and implementation is underway. This system will allow us to make extremely accurate attenuation measurements and to perform elemental imaging.

Keywords: Instrumentation or Technique Development, NDE, Computerized Tomography

409. Contour Measurement with Capacitance Sensor — FY 1987 $115,000

DOE Contact: A. E. Evans, (301) 353-3098, FTS 233-3098
LLNL Contact: S. Patterson, (415) 422-6133, FTS 532-6133

The objective of this research is to develop a technique for making rapid, highly accurate, non-contact measurements of the contour of a conductive workpiece surface. We deconvolve the measured signal to determine the workpiece geometry. We will enhance lateral resolution by reducing probe size and by requiring low-noise measurement of small capacitances. We have improved the sensitivity of our instruments by reducing the noise level and increasing the rejection of parasitic capacitances that arise in measurements. We have also modeled the electric field between the sensor and workpiece; knowledge of the field is necessary to deconvolve the workpiece contour information from the measurement data. Results show that precision of the computer code is inadequate and that the code will have to be modified. Work has started on a two-dimensional experimental setup; we are currently fabricating good step artifacts.

Keywords: Instrumentation or Technique Development, Contour Measurement, Capacitance

410. Tritium Facility Upgrade — FY 1987 ($1,500,000)[1]

DOE Contact: A. E. Evans, (301) 353-3098, FTS 233-3098
LLNL Contact: G. M. Morris, (415) 423-1770, FTS 543-1770

The $700K of FY 1985 funding and the $2,500K of FY 1986 funding has been authorized for the design, construction, and major equipment procurements. In FY 1987, $1,500K was authorized to continue with the office addition construction and activation, special facilities major procurements, fabrication and installation. An additional $3,100K was approved to complete the special facilities: Vacuum Effluent Recovery System (VERS) and the Secondarily Contained Tritium System (SCOTS). This will complete the entire project.

Keywords: Facilities, Tritium

411. Dedication of the Weapons Materials Research and Development Facility — FY 1987 ($28,300,000)[1]

DOE Contact: A. E. Evans, (301) 353-3098, FTS 233-3098
LLNL Contact: M. G. Adamson, (415) 423-2024, FTS 543-2024

Groundbreaking ceremonies for the $28.3M Weapons Materials Research and Development Facility were held in 1983; construction was completed in August 1986; the building was dedicated August 21, 1987. The facility's 90,377 total square feet includes a laboratory wing of 28,385 sq. ft., a basement of 18,010 sq. ft., and an office wing of 43,982 sq. ft. The office wing has space for 120 occupants and houses the Associate Director for Chemistry and Materials Science and his staff, the C&MS Materials Division Leader and his staff, members of the C&MS Materials Division, the C&MS Condensed Matter and Analytical Sciences Division, and members of the Mechanical Engineering, Electronics Engineering, and Hazards Control Departments.

Eleven laboratory areas supporting the Weapons Program and having applications to programs in lasers and energy as well, are located in the west wing of building 235. In this facility, teams of materials scientists, chemists, physicists, and engineers maintain state-of-the-art capabilities and conduct research and development on a new generation of materials.

Keywords: Facilities, Materials Science: General

[1]Line-Item Construction Project: not included in subtotal or total.

Los Alamos National Laboratory

Materials Preparation, Synthesis, Deposition, Growth or Forming

412. Actinide Alloy Development — FY 1987 $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) 667-2556, FTS 843-2556

The aim of this project is the development of new alloys of plutonium. Research involves casting, thermomechanical working, sputtering, 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

413. Plutonium Oxide Reduction — FY 1987 $150,000

DOE Contact: A. E. Evans, (301) 353-3098, FTS 233-3098
LANL (Contract No. W-7405-ENG-36) Contact: D. Peterson, (505) 667-5181, FTS 843-5181

The thermodynamics of interactions among the components used in the direct-oxide reduction of plutonium are determined along with the relevant phase relations.

Keywords: Radioactive Materials, Plutonium, Thermodynamics, Phase Diagrams

414. Plutonium Oxide Removal — FY 1987 $150,000

DOE Contact: G. Bennett, (301) 353-3197, FTS 233-3197
LANL (Contract No. W-7405-ENG-36) Contact: P. Kleinschmidt, (505) 667-6945, FTS 843-6945

The thermodynamics of plutonium oxide and iridium are determined to provide the data required to identify ways of removing residual plutonium contamination from iridium.

Keywords: Radioactive Materials, Plutonium, Thermodynamics, Phase Diagrams

415. Replacement Noble-Metal Alloys FY 1987 $150,000

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

416. Powder Preparation by Plasma Chemical Synthesis FY 1987 $270,000

DOE Contact: A. E. Evans, (301) 353-3098, FTS 233-3098
LANL (Contract No. W-7405-ENG-36) Contact: G. J. Vogt, (505) 667-5813, FTS 843-5813

Thermal plasma chemical synthesis is being investigated for the heterogeneous preparation of submicron, high-purity powders of ceramics, metals, alloys, and metal-ceramic composites.

Keywords: Alloys, Ceramics, Metals, Composites, Thermal Plasma Synthesis

417. Synthesis of SiC Whisker - $MoSi_2$ Matrix Composites for Elevated Temperature Applications FY 1987 $50,000

DOE Contact: J. Eberhardt, (202) 586-5377
LANL (Contract No. W-7405-ENG-36) Contact: F. Gac, (505) 667-5126, FTS 843-5216

The objective of the present program is to improve the mechanical performance of $MoSi_2$ by incorporating SiC whiskers to serve as reinforcement members. The whisker reinforcement should serve two purposes: (1) toughen the material at lower temperatures where the matrix is brittle and (2) strengthen the material at higher temperatures where the matrix is ductile.

Keywords: Ceramics, Composites, Whiskers

418. Whisker Reinforced Structural Ceramics FY 1987 $225,000

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

This task is concerned with producing reinforcing materials for structural ceramics such as SiC and Si_3N24 which are being evaluated by the Fossil Energy Materials Program (FEMP) for such applications as high temperature heat exchanger systems, coal

gasification hardware and gas turbine components. Our basic approach is to use the technology developed at Los Alamos to grow long VLS SiC whiskers and use them in the development of staple yarns and subsequent woven cloth configurations. The use of yarns and cloths as directional reinforcement is expected to produce maximum strengthening and/or toughening for appropriately designed ceramic components. The main subtasks involved in this work are (1) growing of adequate quantities of high quality long whiskers for the textile work while continuing to improve the process of 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

419. Low Density Metal "Smokes" — FY 1987 $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

Low density metal smokes are produced by a modified vacuum deposition process. These materials can be collected on a substrate to yield a very small particle size, low-density form of the metal. For example, gold smokes have been produced at less than 1 percent of full-density gold. These materials have very little structural integrity, but are useful as a low density form of high-Z materials.

Keywords: Low Density, Smokes, Powder Fabrication

420. Ion-Beam Implantation — FY 1987 $200,000

DOE Contact: A. E. Evans, (301) 353-3098, FTS 233-3098
LANL (Contract No. W-7405-EN-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

421. Electroplating Low Atomic Number Materials — FY 1987 $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 will look at electroplating low-atomic-number metals (aluminum and beryllium)

by using non-aqueous plating baths. These new baths will include solvents and fused salts. Applications include weapons components and inertial confinement fusion (ICF) target fabrication.

Keywords: Electroplating, Aluminum, Beryllium, Coatings, Metals

422. Three New Conducting Polymers — FY 1987 $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

423. New Highly Conductive Doped Polyacetylene — FY 1987 $200,000

DOE Contact: A. E. Evans, (301) 353-3098, FTS 233-3098
LANL (Contract No. W-7405-ENG-36) Contact: D. V. Duchane, (505) 667-6887, FTS 843-6887

A 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

424. Liquid Crystal Polymer Development — FY 1987 $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

425. Surface Property Modified Plastic Components — FY 1987 $130,000

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

426. Low-Density, Microcellular Plastic Foams — FY 1987 $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

427. Target Coatings — FY 1987 $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

428. Physical Vapor Deposition and Surface Analysis — FY 1987 $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. Aluminum and rare earth oxides are ion plated 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 are fabricated.

Keywords: Coatings and Films, Physical Vapor Deposition, Sputtering, Ion Plating, Corrosion, Nondestructive Evaluation

429. Fluidized Bed Coatings — FY 1987 $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

430. Electrodeposition of Metallic Glasses — FY 1987 $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

431. Polymers and Adhesives — FY 1987 $866,000

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, Weapons

432. Tritiated Materials — FY 1987 $590,000

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

433. Salt Fabrication — FY 1987 $395,000

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

434. Slip Casting of Ceramics — FY 1987 $150,000

DOE Contact: A. E. Evans, (301) 353-3098, FTS 233-3098
LANL (Contract No. W-7405-ENG-36) Contact: F. D. Gac, (505) 667-5126, FTS 843-5126

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

435. Whisker Growth Technology — FY 1987 $120,000

DOE Contact: A. E. Evans, (301) 353-3098, FTS 233-3098
LANL (Contract No. W-7405-ENG-36) Contact: F. D. Gac, (505) 667-5126, FTS 843-5126

Silicon carbide whiskers are grown by a vapor-liquid-solid process which produces very long fibers. Research on this program is focusing on four areas: improving control over the process itself so as to obtain mono-sized whiskers of regular morphology; processing whiskers after growth to remove detritus and impurities, characterizing the whiskers and relating their properties to structural features; and growth of Si_3N_4 whiskers by the same process.

Keywords: Structural Ceramics, Whiskers

436. New Hot Processing Technology — FY 1987 $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

437. Glass and Ceramic Coatings — FY 1987 $10,000

DOE Contact: A. E. Evans, (301) 353-3098, FTS 233-3098
LANL (Contract No. W-7405-ENG-36) Contact: F. D. Gac, (505) 667-5126, FTS 843-5126

Vitreous enamels and general ceramic coatings are being developed to provide radiation-hardened, electrical-insulating components for accelerator technology. Research

involves synthesizing formulations to bond various metals, matching thermal expansion, and preserving electrical insulating qualities over very large areas.

Keywords: Enamels, Ceramic Coatings, Metals, Radiation Effects, High Temperature Service

438. Cold Pressing, Cold Isostatic Pressing and Sintering — FY 1987 $175,000

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

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, and metals such as copper. End uses include plutonium processing hardware and fluxes, simulated fuel pellets, high temperature resistant ceramics for nuclear reactors, and metal filters.

Keywords: Cold Pressing, Sintering, Ceramics, Metals

439. Plasma-Flame Spraying Technology — FY 1987 $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

440. Rapid Solidification Technology — FY 1987 $200,000

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

441. Superplastic Forming — FY 1987 $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

442. Microwave Sintering/Processing — FY 1987 $200,000

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, Microwaves, RF Heating

Materials Structure or Composition

443. Actinide Surface Properties — FY 1987 $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, Hydrogen Effects, Radioactive Materials

444. Neutron Diffraction of Pu and Pu Alloys — FY 1987 $160,000

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

445. Surface Studies — FY 1987 $500,000

DOE Contact: A. E. Evans, (301) 353-3098, FTS 233-3098
LANL (Contract No. W-7405-ENG-36) Contact: H. K. McDowell, (505) 667-4686, FTS 843-4686

Studies of surface structures and atomic and electronic properties of uranium alloys and intermetallics, UO_2 and ThO_2 single crystals, heavy fermion system, and palladium/hydrogen systems are underway in order to develop essential atomic-level understanding of surface properties of materials and physical and chemical processes. Problems being investigated are: surface modification, UPt_3 surface properties, and use of MeV ion beams to probe surface structure. Techniques used are: Low Energy Electron Diffraction (LEED), Auger and Loss Spectroscopies, Ion-Scattering Spectroscopy (ISS), Ultraviolet Photoelectron Spectroscopy (UPS), Synchrotron Radiation, and MeV-ion-beam scattering.

Keywords: Alloys, Ceramics, Microstructure, Surface Characterization and Treatment

Materials Properties, Behavior, Characterization or Testing

446. Mechanical Properties of Uranium — FY 1987 $60,000

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

Mechanical properties of U and uranium alloys at high strain rates are being evaluated. The effects of crystallographic texture on high rate (shock regime) uranium deformation are being determined.

Keywords: Alloys, Radioactive Materials, Microstructures, Strength

447. High Strain Rate Testing — FY 1987 $200,000

DOE Contact: A. E. Evans, (301) 353-3098, FTS 233-3098
LANL (Contract No. W-7405-ENG-36) Contact: P. S. Follansbee, (505) 667-8021, FTS 843-8021

Testing of metals at rates up to, but not including, the shock-wave regime is underway in order to elicit fundamental understanding of changes in mechanism as a function of deformation rate.

Keywords: High Strain Rate, Metals, Microstructure

448. Mechanical Properties of Plutonium and Its Alloys — FY 1987 $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 pretest and posttest microstructures of the materials using optical and electron microscopy and X-ray, electron and neutron diffraction.

Keywords: Alloys, Radioactive Materials, Microstructure, Strength, Transformation

449. Phase Transformations in Pu and Pu Alloys — FY 1987 $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, Transformation

450. Isobaric Expansion of Actinides — FY 1987 $300,000

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 P-V relationships in liquid actinide elements are determined by isobaric expansion measurements at high pressures. The facility developed for this work can be used to study other hazardous materials.

Keywords: Radioactive Materials, Plutonium Alloys, Thermal Expansion, Equation of State

451. Plutonium Shock Deformation — FY 1987 $350,000

DOE Contact: A. E. Evans, (301) 353-3098, FTS 3098
LANL (Contract No. W-7405-ENG-36) Contact: R. Gray, (505) 667-5452, FTS 843-5452

Plutonium 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

452. Dielectric Loss Measurements in Ceramics — FY 1987 $200,000

DOE Contact: M. Cohen, (301) 353-4253, FTS 233-4253
LANL (Contract No. W-7405-ENG-36): H. M. Frost (505) 667-1290, FTS 843-1290

Loss tangent and dielectric constant measurements in ceramics are made at very high frequencies to evaluate effects of neutron damage for magnetic fusion energy applications, and to study microwave sintering properties of ceramics.

Keywords: Dielectric Properties, Ceramics, Loss Tangent Measurements, Microwave Properties, Radiation Damage, Sintering, Fabrication

453. Plutonium Doping for Self-Irradiation Damage in Ceramics — FY 1987 $220,000

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

A short half-life plutonium isotope is added to titanate and silicate ceramics to induce self-irradiation damage. Conversion of the materials from a crystalline state to

the amorphous condition is studied to determine the atomic arrangements of these metastable structures.

Keywords: Isotope, Radiation Damage, Ceramics, Crystalline, Amorphous, Metastable State

454. Nondestructive Evaluation — FY 1987 $450,000

DOE Contact: A. E. Evans, (301) 353-3098, FTS 233-3098
LANL (Contract No. W-7405-ENG-36) Contact: A. Wilson, (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, Acoustic Emission

455. Powder Characterization — FY 1987 $90,000

DOE Contact: A. E. Evans, (301) 353-3098, FTS 233-3098
LANL (Contract No. W-7405-ENG-36) Contact: F. D. Gac, (505) 667-5126, FTS 843-5126

Processing of metal or ceramic powders critically depends on the characterization of the powder being used. This project characterizes starting powders, for example, RF plasma SiC, commercial powders of ThO_2, tungsten, copper, Si_3N_4, MgO and Al_2O_3. Properties determined include particle size and distribution, morphology, state of agglomeration, zeta potential, and surface area.

Keywords: Metal Powder, Ceramic Powder, Particle Size, Zeta Potential

Device or Component Fabrication or Testing

456. Radiochemistry Detector Coatings — FY 1987 $250,000

DOE Contact: A. E. Evans, (301) 353-3098, FTS 233-3098
LANL (Contract No. W-7405-ENG-36) Contact: D. V. Duchane, (505) 667-6887, FTS 843-6887

Physical vapor deposition of metallic and nonmetallic coatings is employed for preparation of radiochemical detectors.

Keywords: Coatings and Films, Physical Vapor Deposition, Radiochemical Detectors

457. Target Fabrication — FY 1987 $1,500,000

DOE Contact: C. B. Hilland, (301) 353-3687, FTS 233-3687
LANL (Contact No. W-7405-ENG-36) Contact: D. V. Duchane, (505) 667-6887, FTS 843-6887
KMS Fusion, Inc., Contact: Timothy Henderson, (313) 769-8500, ext. 302
LLNL Contact: W. Hatcher, (415) 422-1100

Hydrocarbon polymer (CH) is applied by plasma polymerization to glass microspheres to act as an ablator. These targets represent a unique fabrication capability that combines micromachining, plasma etching, and plasma polymerization. The targets are filled with a deuterium-tritium gas mixture during the process of making the glass microspheres. The targets are irradiated with a laser or particle beam to produce a fusion burn for various military and energy applications. Other techniques are classified.

Keywords: Inertial Fusion, Target Fabrication

458. Filament Winder — FY 1987 $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 843-5261

The Entec filament winder in MST-7 Plastics is a 4-axis computer-programmed machine with a winding envelope extneding 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

459. Polymeric Laser Rods — FY 1987 $100,000

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

460. High Energy Density Joining Process Development — FY 1987 $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

461. Arc Welding Process Development — FY 1987 $150,000

DOE Contact: A. E. Evans, (301) 353-3098, FTS 233-3098
LANL (Contract No. W-7405-ENG-36) Contact: H. Casey, (505) 667-4365, FTS 843-4365

Video monitoring and Varistraint testing have been established as techniques to investigate crack susceptibility of gas-tungsten-arc welds. Emphasis is directed toward dissimilar metal welds between 304L stainless steel and Inconel 625.

Keywords: Welding, Hot Cracks, Stainless Steel, Inconel, Varistraint, Video

462. Ceramic Technology — FY 1987 $60,000

DOE Contact: A. E. Evans, (301) 353-3098, FTS 233-3098
LANL (Contract No. W-7405-ENG-36) Contact: F. D. Gac, (505) 667-5126, FTS 843-5126

Castable ceramics are used to fabricate bodies for energy technologies. Typical materials are based on alumina or magnesia with a cement binder; parts fabricated include molds, crucibles, liners, and electrical insulators.

Keywords: Ceramics, Cements, Sintering, Refractory Liners

463. Solid State Bonding FY 1987
$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, 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

Advanced Research and Technology Development 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 resesarch; 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 programs supports workshops to identify research needs in all fossil energy technologies and manages selected training programs for faculty and students at Energy Technology Centers.

Materials Preparation, Synthesis, Deposition, Growth or Forming

464. Consolidation of Rapidly Solidified Aluminide Metal Powders FY 1987 $75,000

DOE Contact: E. E. Hoffman, (615) 576-0735; FTS 626-0735
Idaho National Engineering Laboratory (Contract No. DE-AC07-76ID01570) Contacts: J. E. Flinn, R. N. Wright, FTS 583-2627

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. Compositions of the aluminide powders will be based on Oak Ridge National Laboratory's assessment, and initially will involve Ni-80, Fe-10, Al-10, B-0.02 (all in wt. %), with and without microalloying additions, e.g., hafnium.

Keywords: Aluminides, Powders, Consolidation

465. Investigation of Electrospark Deposited Coatings for Protection of Materials in Advanced Steam Cycle Superheater Applications FY 1987 $50,000

DOE Contact: E. E. Hoffman, (615) 576-0735, FTS 626-0735
Hanford Engineering Development Laboratory (FTP/A 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

466. Short Fiber Reinforced Structural Ceramics FY 1987 $225,000

DOE Contact: E. E. Hoffman, (615) 576-0735; FTS 626-0735
LANL (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 whiskers and beta-phase silicon carbide 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

467. Fabrication of Fiber-Reinforced Composites by CVD Infiltration FY 1987 $187,000

DOE Contact: E. E. Hoffman, (615) 576-0735; FTS 626-0735
ORNL (Contract No. DE-AC05-84OR21400) Contacts: R. A. Lowden and D. P. Stinton, (615) 574-4559; FTS 624-4559

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 $\cdot$ $m^{1/2}$ 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 community. SiC fibers and matrices of SiC and Si_3N_4 have been identified as being most promising. Fiber dimensions, geometry, packing density, binder type and concentrations, and other processing variables have been evaluated experimentally.

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 CVD 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

CVD 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

468. Characterization of Fiber-CVD Matrix Interfacial Bonds — FY 1987 $125,000

DOE Contact: E. E. Hoffman, (615) 576-0735; FTS 626-0735
Oak Ridge National Laboratory (Contract No. DE-AC05-84OR21400) Contacts R. A. Lowden and D. P. Stinton, (615) 574-4559; FTS 624-4559

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 system. 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

469. Microwave Sintering of Sol-Gel Derived Ceramic Superconductors — FY 1987 $73,000

DOE Contact: E. E. Hoffman, (615) 576-0735; FTS 626-0735
Oak Ridge National Laboratory (Contract No. DE-AC05-84OR21400) 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 superconducting materials with major emphasis on the sol-gel synthesis and processing of these materials at INEL and microwave processing of these new ceramics at ORNL. The forms studied include tape and wire configurations in structures including a conductor such as copper, and monolithic ceramic shapes. The research is organized so as to utilize the skills and experience in INEL in sol-gel processing of ceramic oxides and the facilities and experience of ORNL in microwave processing of materials.

Keywords: Superconductors, Ceramics

470. Transfer of CVD Infiltration Technology to Industry — FY 1987 $50,000

DOE Contact: E. E. Hoffman, (615) 576-0735; FTS 626-0735
ORNL (Contract No. DE-AC05-84OR21400) Contact: T. M. Besmann, (615) 574-4551; FTS 624-4551

An innovative joint research and development program with Babcock & Wilcox Research Laboratories (B&W) will be conducted to transfer AR&TD-developed CVD infiltration technology to B&W. This effort is supported about 50 percent by the

AR&TD Fossil Energy Materials Program and 50 percent by B&W. Part of the work, including fabrication of dense fiber mats, will be conducted by B&W, Lynchburg, Virginia. The infiltration will be at ORNL with participation by B&W personnel.

Keywords: Composites, Fiber-Reinforced, Ceramics

471. Development of Advanced Fiber Reinforced Ceramics — FY 1987 $160,000

DOE Contact: 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

472. Development and Microstructural Evaluation of Austenitic Alloys — FY 1987 $100,000

DOE Contact: E. E. Hoffman, (615) 576-0735, FTS 626-0735
Oak Ridge National Laboratory (Contract No. DE-AC05-84OR21400) 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 to be 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.

Keywords: Steam Cycle, Materials, Mechanical Properties

Materials Properties, Behavior, Characterization or Testing

473. Mechanical Properties and Microstructural Stability of Advanced Steam Cycle Materials FY 1987 $140,000

DOE Contact: 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 steam cycle superheater alloys at temperatures ranging from 650-760°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

474. Transformation, Metallurgical Response and Behavior of the Weld Fusion and Heat Affected Zone in Cr-Mo Steels for Fossil Energy Applications FY 1987 $ 0[1]

DOE Contact: 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 is to develop fundamental information on the metallurgical behavior of the heat affected zone of welds in chromium-molybdenum alloys. This is being accomplished by: (1) documenting transformation 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

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[1]Prefunded in FY 1986.

475. Analysis of Hydrogen Attack on Pressure Vessel Steels — FY 1987 $ 0[1]

DOE Contact: 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

The initial objectives of the program have been achieved and physical models have been 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 have been predicted and appear to be reasonably consistent with available data. Additional work is needed to refine the analyses and confirm the adequacy of the basic thermodynamic information available in the literature. The model has been particularly useful in establishing the relative importance of microconstituents, deformation mechanisms, and fracure 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 is being 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

476. Investigation of the Weldability of Ductile Aluminides — FY 1987 $50,000

DOE Contact: 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 will be conducted as a PhD thesis project by a CSM student working at CSM and at ORNL.

Keywords: Joining Methods, Materials Characterization

477. Development of Iron and Nickel Aluminides — FY 1987 $160,000

DOE Contact: E. E. Hoffman, (615) 576-0735, FTS 626-0735
Oak Ridge National Laboratory (Contract No. DE-AC05-84OR21400) Contact: C. T. Liu, (615) 574-4459, DTS 624-4459

New, improved alloys are needed for components in severe environments for applications such as coal gasifiers, fluidized bed combustors, and fuel cells. The purpose of this task is to design and test materials that will use Al_2O_3 as the main protective layer to prevent sulfidation attack and that will possess good mechanical properties at high temperatures. Aluminides based on the pseudobinary systems Hi_3Al-Fe_3Al and NiAl-FeAl will form the basis for development of iron and nickel aluminides as structural materials could substantially improve the performance and reliability of advanced fossil energy conversion systems.

The approach of this task is to develop aluminides based on the pseudobinary system Ni_3Al-Fe_3Al. Iron will be macroalloyed to Ni_3Al for solid solution hardening at elevated temperatures and for corrosion resistance in sulfidizing environments. Boron and other elements will be employed for controlling the chemistry and cohesion of grain boundaries. The development of aluminides will also include the FeAl-NiAl system which contains 50 at. % Al for better oxidation and corrosion resistance.

Keywords: Strength, Intermetallics, Alloys

478. Joining of Advanced Aluminides — FY 1987 $75,000

DOE Contact: E. E. Hoffman, (615) 576-0735, FTS 626-0735
Idaho National Engineering Laboratory (Contract No. DE-AC07-76IDO1570) Contact: D. E. Clark, FTS 583-0746

The objective of this project is to investigate weldability problems limiting the use of aluminides in welded structures. This includes weldability effects of minor alloying elements, process and process variable effects, solidification mechanics, filler material development, and extension to heavier sections.

Keywords: Joining, Aluminides

479. Corrosion and Mechanical Properties of Alloys in FBC and Mixed-Gas Environments — FY 1987 $320,000

DOE Contact: 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 400-750°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 experimenotal 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 400-750°C in mixed-gas atmospheres using internally cooled tube specimens of selected commercial materials, (3) evaluate deposit-induced corrosion behavior of heat-exchanger and gas-turbine materials after exposure to multicomponent gas environments, and (4) develop corrosion rate expressions, based upon experimental data, for long-term extrapolation to component design lives.

The work being conducted under this project 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 850-1100°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

480. Investigation of Corrosion Mechanisms of Coal Combustion Products on Alloys and Coatings FY 1987 $80,000

DOE Contact: 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 is 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 will be model alloys selected for their ability to form single oxides of chromium, aluminum, and silicon. The temperature range of interest is 500-700°C and the test environments contain mixed oxidants (O_2, CO_2, SO_2, H_2S, and Cl_2). Specific objectives include 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) will be considered.

Keyword: Corrosion

481. Investigation of the Effects of Microalloy Constituents, Surface Treatment, and Oxidation Conditions on Development and Breakdown of Protective Oxide Scales FY 1987 $215,000

DOE Contact: E. E. Hoffman, (615) 576-0735; FTS 626-0735
Battelle Columbus Laboratories (Contract No. DE-AC05-84OR21400, Martin Marietta Energy Systems 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

482. Investigation of the Effects of Microalloy Constituents, Surface Treatment, and Oxidation Conditions on Development and Breakdown of Protective Oxide Scales

FY 1987
$215,000

DOE Contact: E. E. Hoffman, (615) 576-0735; FTS 626-0735
Case Western Reserve University (Contact No. DE-AC05-84OR21400, Martin Marietta Energy Systems 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 atmospheres containing high pS_2/pO_2 ratios. Iron based alloys, including Fe-25Cr and Fe-25Cr-20Ni which are Cr_2O_3 formers and Fe-25Cr-6Al which is an Al_2O_3 former, are the base alloys for this investigation. Conventional alloying as well as ion-implantation are the techniques for incorporating the reactive elements into the base alloys.

Keywords: Corrosion, Oxides, Scales

483. Investigation of the Effects of Microalloy Constituents, Surface Treatment, and Oxidation Conditions on Development and Breakdown of Protective Oxide Scales

FY 1987
$215,000

DOE Contact: E. E. Hoffman, (615) 576-0735; FTS 626-0735
Universal Energy Systems, Inc. (Contact No. DE-AC05-84OR21400, Martin Marietta Energy Systems Subcontract No. 86X-95901C) Contact: V. Sinivasan, (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 500-700°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

484. Mechanical Properties of Oxide Films and Correlation with Metal/Oxide Interface FY 1987 $50,000

DOE Contact: E. E. Hoffman, (615), 576-0735; FTS 626-0735
Oak Ridge National Laboratory (Contract No. DE-AC05-84OR21400) Contact J. H. DeVan: (615) 574-4451; FTS 624-4451

In May 1986 J. H. DeVan began a one-year assignment at Harwell Laboratory to conduct joint high temperature gas-metal reaction studies with researchers to Harwell's Materials Development and Metallurgy and Materials Physics Division. Concurrently, he followed research programs at the Central Electricity Research Laboratory and British Coal's Coal Research Establishment (Stoke Orchard) involving corrosion studies of FBC heat exchanger and turbine materials and of advanced steam generator materials for conventional fossil-fired boilers.

Keywords: Corrosion, Oxides, Interfaces

485. A Study of Erosive Particle Rebound Parameters FY 1987 $80,000

DOE Contact: E. E. Hoffman, (615) 576-0735; FTS 626-0735
University of Notre Dame (Contract No. DE-AC-05-84OR21400, Martin Marietta Energy Systems 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, Particles

486. In Situ Scanning Electron Microscopy Studies of Erosion-Corrosion FY 1987 $200,000

DOE Contact: E. E. Hoffman, (615) 576-0735, FTS 626-0735
Oak Ridge National Laboratory (Contact No. DE-AC05-84OR21400) 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

487. Study of Particle Rebound Characteristics and Material Erosion at High Temperature

FY 1987
$ 0[2]

DOE Contact: 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, with sizes from 5 to 200um. The target materials will be selected according to present and anticipated materials needs of coal combustion systems. Candidate materials will include stainless steel, INCO 718, Ti 6-4, and 2024 Al.

Keywords: Erosion and Wear, Corrosion, Metals, Alloys

488. Development of Nondestructive Evaluation Techniques for Structural Ceramics

FY 1987
$190,000

DOE Contact: E. E. Hoffman, (615) 576-0735, FTS 626-0735
Argonne National Laboratory (Contract No. W-31-109-eng-38) Contact: W. A. Ellingson, (312) 972-5068, FTS 972-5068

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, inclusins, 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.

Keywords: Nondestructive Evaluation, Ceramics

[2]Prefunded in FY 1986.

489. Effect of Flaws on the Fracture Behavior of Structural Ceramics FY 1987 $125,000

DOE Contact: E. E. Hoffman, (615) 576-0735, FTS 626-0735
Argonne National Laboratory (Contract No. W-31-109-eng-38) Contact: J. P. Singh, (312) 972-5123, FTS 972-5123

The purpose of this work is to (a) establish correlations between the composition, microstructure, and mechanical properties of structural ceramics (Si_3N_4 and SiC) with well-defined flaws, and (b) provide information which will be used to relate mechanical properties to nondestructive 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). Subsequently, 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

490. Joining of Silicon Carbide Reinforced Ceramics FY 1987 $75,000

DOE Contact: E. E. Hoffman, (615) 576-0735, FTS 626-0735
Idaho National Engineering Laboratory (Contract No. DE-AC07-76IDO1570) Contact: D. N. Coon, FTS 583-9738

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 composities. 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 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, Ceramics, Composites

491. Nondestructive Evaluation of Advanced Ceramic Composite Materials FY 1987 $75,000

DOE Contact: E. E. Hoffman, (615) 576-0735, FTS 626-0735
Idaho National Engineering Laboratory (Contract No. DE-AC07-76IDO570) Contact: J. B. Walter, FTS 583-0033

The purpose of this project is to develop an effective capability for nondestructive evaluation of ceramic fiber reinforced ceramic composites. The response of selected samples of sintered composite materials consisting of SiC fibers in SiC and Si_3N_4 matrices to both ultrasonic and radiographic techniques will be investigated. Experimental techniques and signal processing algorithms will be developed for (1) characterizing acoustic properties and sample morphology, including fiber size and distribution and the degree of bonding of the fibers to the matrix, (2) detecting flaws including cracks, porosity, fiber clusters, and bonding anomalies, and (3) detecting flaws in joints. The NDE techniques developed in this project will result in more effective and extensive use of advanced ceramic composite materials in fossill energy applications.

Keywords: Ceramics, Composites, Nondestructive Evaluation

492. Investigation of the Mechanisms of Failure of Ceramic Materials for Hot Gas Filtration FY 1987 $ 0[3]

DOE Contact: E. E. Hoffman, (615) 576-0735, FTS 626-0735
United Kingdom Coal Research Establishment/Oak Ridge National Laboratory (Contract No. DE-AC05-84OR21400) Contact: R. R. Judkins, (615) 574-4572, FTS 624-4572

High temperature ceramic candle filters used for removing particulates from gas streams have been under evaluation at the United Kingdom Coal Research Establishment (UKCRE). These filters have been tested at 950°C in gasification atmospheres. Cracks at the point of attachment to the manifold have been a drawback not only to the application of this specific ceramic design, but represent a phenomenon generic to most ridig ceramic filters. No detailed phenomenological explanation of the failure has been determined. This task is a cooperative project of the DOE Fossil Energy AR&TD Fossil Energy Materials Program and the UKCRE to develop an understanding of the mechanisms of failure of ceramic hot gas filtration materials and, thereby, provide a basis for material and system improvements.

Keywords: Ceramics, Filters, Failure

[3]Prefunded in FY 1985.

493. High-Temperature Creep Behavior of Refractory Bricks — FY 1987 $ 0[4]

DOE Contact: E. E. Hoffman, (615) 576-0735, FTS 626-0735
Iowa State University, Engineering Research Institute, Department of Materials Science and Engineering (Contract No. DE-AC05-84OR21400, Martin Marietta Energy Systems, Inc., Subcontract No. 19X-07940C) Contact: T. D. McGee, (515) 294-9619, FTS 865-9619

This research effort is a continuation of the study of creep of refractories used to line fossil fuel process vessels. The work will concentrate on those refractories intended for use at higher temperatures and under more severe conditions than can be tolerated by refractory concretes. Specifically, the research will focus on the creep behavior of high-chromia refractories suitable for lining the hot section of slagging gasifiers. Uniaxial creep experiments will be conducted in compression in air and mixed gases with very low oxygen partial pressures. The creep behavior of high-chromia refractories in uniaxial compression will be measured as a function of stress, oxygen partial pressure, and temperature. Oxygen partial pressures ranging from 21 kPa to 0.1 pPa will be used. Stress will be varied from 0.7 to 2 MPa. In addition, biaxial creep measurements will be made for selected refractories for which uniaxial creep measurements have been determined.

The creep data will be evaluated in cooperation with related work at the Massachusetts Institute of Technology to correlate the creep behavior of these refractories with a mathematical model.

Keywords: Ceramics, Glasses, Materials Characterization

494. Weldability Studies of Advanced Austenitic Alloys — FY 1987 $100,000

DOE Contact: E. E. Hoffman, (615) 576-0735, FTS 626-0735
Oak Ridge National Laboratory (Contact No. DE-AC05-84OR21400) Contact: R. W. Swindeman, (615) 574-5108, FTS 624-5108

Evaluation of the weldability of alloys will include a specialized technique on a device called a Sigmajig, which evaluates the hot cracking tendency of the weldments. Ranking of alloys is by the extent of cracking as a function of applied load and plate thickness. Weldments in the alloys produced as tubing will be evaluated against requirements of the ASME BPV Code Sections I and IX, which involve bend testing, tensile testing, and metallography. Additional evaluation will be based on varestraint and circular groove tests. Other tests not required by the Code may be identified during the course of this work, and those tests will be included as appropriate. The development of a suitable filler metal is an important part of this work. Oak Ridge National Laboratory will work with university and industrial subcontractors in this development.

Keywords: Steam Cycle, Materials, Mechanical Properties

495. Investigation of Corrosion-Resistant Oxide Scales on Iron-Based Alloys in Mixed Gas Environments FY 1987 $225,000

DOE Contact: E. E. Hoffman, (615) 576-0735, FTS 626-0735
Oak Ridge National Laboratory (Contact No. DE-AC05-84OR21400) 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 600-800°C. Specific objectives include (1) the development of protective oxide scales by modifying oxide chemistry and microstructure to reduce the transport of sulfur through the scale; (2) the formation of a sulfur-diffusion barrier (i.e., SiO_2 layer) under or above the protective oxide scale to minimize the sulfur attack; (3) the study of the effects of alloy chemistry, oxide morphology, and temperature on the breakdown of protective oxide scales; and (4) the examination of methods to limit internal sulfidation. The mechanical performance and adherence of oxide scales in mixed oxidant gases will be studied by impinging tungsten carbide particles on the oxide within a scanning electron microscope under controlled temperature and environmental conditions.

Keywords: Corrosion, Iron-Based, Mixed Gas, Scales

496. Solid Particle Erosion in Turbulent Flows Past Tube Banks FY 1987 $60,000

DOE Contact: 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: R. Greif, (415) 642-6462

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, Particle, Gas Streams

497. Modeling of Fibrous Preforms for CVD Infiltration — FY 1987 $45,000

DOE Contact: 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-559001C) 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.

498. Structural Reliability and Damage Tolerance of Ceramic Composites — FY 1987 $200,000

DOE Contact: E. E. Hoffman, (615) 576-0735, FTS 626-0735
National Bureau of Standards, Center for Materials Science (Contract No. DE-A105-800RS0679) Contacts: E. R. Fuller and S. J. Schneider, (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

499. Improved Ceramic Composites Through Controlled Fiber-Matrix Interaction

FY 1987
$150,000

DOE Contact: E. E. Hoffman, (615) 576-0735, FTS 626-0735
Pacific Northwest Laboratory (Contract No. DE-AC06-76RL0830) 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

500. Ceramic Catalyst Materials

FY 1987
$150,000

DOE Contact: E. E. Hoffman, (615) 576-0735, FTS 626-0735
Sandia National Laboratory (Contract No. DE-AC04-76DP00789) Contact: B. Granoff, FTS 844-8145

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

501. Evaluation of Mechanical Properties of Advanced Austenitic Alloys

FY 1987
$130,000

DOE Contact: E. E. Hoffman, (615) 576-0735, FTS 626-0735
Oak Ridge National Laboratory (Contract No. DE-AC05-84OR21400) Contact: R. W. Swindeman, (615) 574-5108, FTS 624-5108

Creep-rupture data on alloys developed in the above task (Item 17) will be gathered in the temperature range 600-760°C for times from 10 to 10,000 h. The effects of mechanical and thermal cycles will be examined, and results from testing will be used to establish cumulative damage models. Multiaxial stress testing, notched-bar stress-rupture testing, and creep crack-growth testing will be undertaken for constant and variable load conditions to verify cumulative damage models.

Keywords: Steam Cycle, Materials, Mechanical Properties

Device or Component Fabrication, Behavior or Testing

502. "Materials and Components in Fossil Energy Applications" (Newsletter) FY 1987 $100,000

DOE Contact: 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) Contact: 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

503. Studies of Materials Erosion in Coal Conversion and Utilization Systems FY 1987 $250,000

DOE Contact: E. E. Hoffman, (615) 576-0735, FTS 626-0735
Lawrence Berkeley Laboratory (Contract No. DE-AC03-76SF00098) Contact: A. V. Levy, (415) 486-4822, 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

504. Mechanisms of Galling and Abrasive Wear FY 1987 $75,000

DOE Contact: E. E. Hoffman, (615) 576-0735, FTS 626-0735
National Bureau of Standards, Center for Materials Science (Contract No. DE-AI05-83OR21322) Contact: L. K. Ives, (301) 921-2943

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

505. Thermomechanical Modeling of Refractory Brick Linings for Slagging Gasifiers

FY 1987
$65,000

DOE Contact: 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 Buyukozturg, (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 heat-up and cool-down cycles. Through simulation and parameter studies, design recommendations will be made for vessel configuration, material property combinations, and optimum heating schedules.

Keywords: Refractory Liners

506. Alkali Attack of Coal Gasifier Refractory Linings

FY 1987
$ 0[4]

DOE Contact: E. E. Hoffman, (615) 576-0735, FTS 626-0735
Virginia Polytechnic Institute and State University, Department of Materials Engineering (Contract No. DE-AC05-84OR21400, Martin Marietta Energy Systems, Inc., Subcontract No. 19X-43397C) Contact: J. J. Brown, Jr., (703) 961-6777

This task will investigate the physical and chemical characteristics of alkalai attack of coal gasifier linings under nonslagging conditions. Various refractories will be exposed to simulated coal gasification atmospheres containing alkalai metals. Phase changes and compound formations that occur in the refractories will be evaluated and compared with theoretical calculations.

Keywords: Corrosion, Ceramics, Glasses

[4]Prefunded in FY 1985.

507. Thermodynamic Properties and Phase Relations for Refractory-Slag Reactions in Slagging Coal Gasifiers — FY 1987 $ 0[5]

DOE Contact: E. E. Hoffman, (615) 576-0735, FTS 626-0735
Pennsylvania State University (Contract No. DE-AC05-84OR21400, Martin Marietta Energy Systems, Inc., Subcontract No. 19X-09006C) Contact: Arnulf Muan, (814) 865-7659

The purpose of this program is to determine the chemical constraints affecting the performance of refractory materials under experimental conditions corresponding to those prevailing in slagging gasifiers.

Keywords: Thermodynamics, Refractory, Slag, Phase

508. Evaluation of Candidate Materials for Solid Oxide Fuel Cells — FY 1987 $150,000

DOE Contact: 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 SOFCs. Specifically, the work involves determining the effects of rare earth (RE) and indium oxide additions on the electrical transport properties of $HfO_2)ZrO_2)$-RE_xO_y-In_2O_3. In addition, the study will develop an understanding of the crystallographic, microstructural, and phase equilibrium factors that influence the above properties. The compositions of the $HfO_2)ZrO_2)$-RE_xO_y-In_2O_3 are varied, and the electrical properties are measured relative to the phase equilibrium and crystallographic structures to determine the RE and In_2O_3 combinations that provide the highest electronic conductivity. 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.

Keywords: Fuel Cells

[5]Prefunded in FY 1986.

509. 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 1987 $ 0[6]

DOE Contact: 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 is 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. As part of this project, the current practice for design and engineering of ceramic filters will be researched, and the current use for such filters in industrial and utility applications similar to those in the fossil energy systems listed above will be described. Materials failure experience will be examined, and causes of failure of ceramic filters will be 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, will be identified.

Keywords: Gas Cleanup, Filters, Ceramic, Assessment

510. Development of a Design Methodology for High-Temperature Cyclic Application of Materials Which Experience Cyclic Softening FY 1987 $100,000

DOE Contact: 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-27488C) Contact: D. L. Mariott, (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

[6]Prefunded in FY 1986.

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 remmant life assessment.

Keywords: Materials, Cyclic Softening

Instrumentation and Facilities

511. Management of the AR&TD Fossil Energy Materials Program — FY 1987 $350,000

DOE Contact: E. E. Hoffman, (615) 576-0735, FTS 626-0735
Oak Ridge National Laboratory (Contract No. DE-AC05-84OR21400) Contacts: R. A. Bradley, (615) 574-6094, FTS 624-6094; R. R. Judkins, P. T. Carlson, (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

512. Coal Conversion and Utilization Plant Support Services — FY 1987 $20,000

DOE Contact: E. E. Hoffman, (615) 576-0735, FTS 626-0735
Oak Ridge National Laboratory (Contact No. DE-AC05-84OR21400) 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 Surface Coal Gasification

Surface Gasification Materials Program

Materials Preparation, Synthesis, Deposition, Growth or Forming

513. Development of Iron Aluminides for Coal Gasification Systems — FY 1987 $215,000

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Oak Ridge National Laboratory (Contact No. DE-AC05-84OR21400) Contact: C. T. Liu, (615) 574-5120, FTS 624-5120

The purpose 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 and utilization systems. Initial emphasis is on the development of iron aluminides for heat recovery applications in coal gasification systems.

Keywords: Ferrous Metals, Intermetallics, Heat Recovery

514. Ceramic Fiber-Ceramic Matrix Hot-Gas Filters — FY 1987 $90,000

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The purpose of this project is to develop a ceramic fiber-ceramic matrix composite that will be suitable as a high-temperature particulate filter for use in hot-gas cleanup systems. The goal is to produce a composite that has the requisite strength and toughness and which also has sufficient porosity to be permeaable to the gas stream, but with the proper size and distribution of porosity to be an effective filter. A practical process for fabricating porous ceramic fiber-ceramic matrix filter materials will be developed.

Keywords: Composites, Ceramics, Gas Cleanup

515. Protective Coatings and Claddings: Application/Evaluation — FY 1987 $230,000

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Argonne National Laboratory (Contract No. W-31-109-eng-38) Contact: D. J. Baxter, (312) 972-5117, FTS 972-5117

The coating/cladding development activity provides experimental evaluation and thermodynamic analysis of metallic protective coatings for coal gasifer waste heat steam

generators and superheaters as well as the development of coating inspection methods. The evaluation of procedures for the field restoration of protective coatings at welds and damaged areas is included, as is the development of NDE techniques for verifying coating integrity and quality. These protective coatings will enable conventional ferritic steel boiler and superheater alloys to operate in contact with raw product gas at metal temperatures (about 480-540°C) required for good plant efficiency.

Keywords: Coatings and Films, Nondestructive Evaluation, Corrosion, Alternative Fuels

516. Materials Development for Solid Oxide Oxygen Production Unit FY 1987 $150,000

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The development and implementation of solid oxide ceramic oxygen-generating devices in coal gasification systems is believed to have the potential for significantly reducing the total cost of synthetic coal-derived pipeline fuel gas when compared to other oxygen production systems such as cryogenic pumping. However, the economic success of the solid oxide oxygen pump is dependent on the reduction of internal power losses caused by high internal resistances in the individual ceramic oxide components. For a given component, the power loss is directly proportional to the electrical resistance which, in turn, is proportional to the resistivity of the material multiplied by the thickness of the component.

Keywords: Corrosion, Oxides, Interfaces

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KEYWORD INDEX

Alloys - 189, 191, 192, 196, 251, 260, 283, 284, 331, 342, 373, 382, 383, 396, 400, 401
Absorbents - 248
Absorption - 248, 258
Acoustic Emission - 385
Acoustic Sensors - 275
Acrylics - 376
Actinides - 289, 290, 296, 343, 352, 355, 358, 361, 363, 365, 381
Active Thermal Insulation - 205
Adherence - 191, 222, 233
Adhesion - 321
Adhesives - 378
Adiabatic Diesels - 223
Advanced Heat Engines - 231
Aerosols - 278
Aerospace - 195
AGT - 228, 231
Alloy Development - 237, 238, 380
Alternate Materials - 237, 238
Alternative Fuels - 414
Alumina - 214, 219-221, 225, 228
Aluminides - 390, 396
Aluminum - 210, 211, 375
Aluminum Chloride - 210
Aluminum Phosphate - 221
Amorphous - 385
Amorphous Alloys - 377
Amorphous Films - 344
Amorphous Materials - 254, 341
Amorphous Metals - 310
Anode - 209
Assessment - 201, 231, 411
Atomic Vapor Laser Isotope Separation (AVLIS) - 288
Auger Electron Microscopy - 313

Autoclaving - 208
Automatic Welding - 269
Automation - 326
Automobiles - 190
Barrier - 287
Batteries - 237, 238, 318
Beryllium - 375
Biomass - 194
Boiling - 267
Bonding Agents - 257, 259
Boron Doping - 324
Borosilicate Glass - 308
Brazing - 221
Breeder Reactor - 289
Building Insulation - 204, 205, 207, 208
Bulk Characterization - 257, 259
Bulk Modulus - 323
Calibration - 205
Capacitance - 370
Carbon-Based Materials - 344
Carbon Fibers - 252
Carbon Foam - 318, 322
Cast Iron - 221
Casting - 259
Catalysis - 343, 361
Catalyst - 240, 407
Cathode - 209
Cells - 256
Cements and Concrete - 208, 257, 259, 387
Ceramic Coatings - 380
Ceramic Insulators/Dielectrics - 329
Ceramic Powder - 385
Ceramics - 183, 185, 189, 198, 199, 201, 209-211, 230, 251, 281-283, 316, 331, 339, 340, 352, 373, 374, 379-382, 384, 385, 387, 391-393, 401-404, 406, 407, 409, 411, 413
Chemical Analysis - 325, 327
Chemical Sensors - 315

Chemical Synthesis - 350
Chemical Vapor Deposition - 183, 188, 218, 233, 243, 254, 255, 281, 330, 331, 377
Chemistry - 339, 355
Chromia - 220
Chromium - 342
Cladding Rupture - 301
Cleaning - 347
Coatings - 183, 184, 188, 209, 234, 235, 237, 260, 281, 282, 321, 346, 375, 377, 380, 390
Coatings and Films - 183, 186, 210, 222, 223, 233, 234, 243-246, 249-251, 254, 255, 309, 318, 329-331, 336-338, 356, 376, 377, 385, 414
Cold Pressing - 380
Combustion - 228
Combustion Synthesis - 352
Compatibility - 347
Component Design - 235
Component Test - 235
Components - 408
Composite Ceramics - 212
Composite Materials - 252
Composites - 188, 189, 209, 216-220, 228, 238, 239, 258, 277, 346, 351, 364, 365, 373, 374, 378-380, 392, 393, 402, 403, 407, 413
Computed Tomagraphy - 230
Computer Modeling - 303
Computer Program - 206
Computerized Tomography - 370
Conducting Polymers - 375
Consolidation - 390
Consolidation of Powder - 186, 187, 296
Contact Stress - 233
Containment - 373
Contour Measurement - 370
Control - 269, 270
Control Rods - 294, 295
Conventional Solidification - 208, 333-335
Coordination - 231

Corrosion - 197, 210, 227, 228, 237, 251, 258-260, 283, 284, 339-341, 346, 347, 377, 397-401, 405, 408, 409, 412, 414
Corrosion-Gaseous - 211
Corrosion Tribology - 374
Cost-Effective Analysis - 206
Crack Growth - 364
Creep - 217, 226, 229, 276, 292, 293, 323, 333, 361
Creep Rupture - 397
Crosslinks - 194
Crud - 301
Cryolite - 210, 211
Crystal Defects/Grain Boundaries - 345
Crystalline - 385
Curing - 190
Cyclic Fatigue - 226
Cyclic Softening - 412
Damage - 273
Database - 225, 305
Decomposition - 192
Defects - 310, 369
Defects/Grain Boundaries - 347
Deformation - 331, 369
Deformation Predictive Behavior Modeling - 364
Desiccants - 247-249, 344
Design Codes - 223
Design Methodology - 221
Diagnostics - 387
Diamond - 344
Dielectric Properties - 384
Diesel - 231
Diesel Combustion - 228
Diesel Engines - 224, 234, 235
Diffusion - 207, 260, 282
Direct Absorption Receiver - 253
Disassemble - 301
Disordered Media - 263, 272

Dispersion Toughened - 217
Dissolution - 258
Drilling - 257, 259
Ductility - 372
Dye Laser - 387
Dynamic Interfaces - 223
Economic Analysis - 207
Economics - 185
Eddy Currents - 293
Elasticity - 275
Electrical Insulators - 340
Electrical Resistivity - 372
Electrodeposition - 255, 342, 377
Electroforming - 342
Electrolytes - 236
Electron Beam - 387
Electron Beam Methods - 332, 350
Electron Optics - 326
Electronic Structure - 192
Electrophoretic Deposition - 329
Electroplating - 375
Electrorefining - 289
Elemental Composition - 348
Enamels - 380
Encapsulants - 322, 344, 364
Energetic Materials - 358, 359
Energies - 196
Energy Conservation - 197
Energy Savings Calculation - 205
Energy Storage - 240
Engines - 198, 199, 202, 216, 221, 225, 226, 228, 231-234
Enrichment - 288
Environmental Effects - 228
Environmental Testing - 294
Epitaxial Growth) - 255
Equation of State - 384

Erosion - 228, 400, 405
Erosion and Wear - 198, 234, 400, 401, 408
Erosion/Wear/Tribology - 332, 336, 338
Exhibits - 231
Explosives - 350
Extrusion - 211, 258, 297
Fabrication - 188, 235, 314, 384
Facilities - 371
Failure - 403
Failure Analysis - 412
Failure Testing - 292
False Color Imaging - 327
Fast Ion Conductors and Solid Electrolytes - 237, 238
Fasteners - 206
Fatigue - 227, 228, 260, 276, 292, 293, 333, 342, 355, 362
Ferrous and Non-Ferrous Metals - 277, 332, 333, 334, 342
Ferrous Metals - 294, 331, 333, 337, 345, 347, 349, 413
Ferrous Metals including Steels - 275, 276, 330
Fiber Architecture - 212
Fiber-Reinforced - 392, 393, 407
Fibers - 184, 189, 298, 323, 346, 353
Field Ion Microscopy - 313
Field Testing - 304
Filament Winding Composites - 386
Films - 311, 321, 348
Filters - 379, 403, 411
Flaws - 402
Flexure Test - 225
Fluidized Bed Combustion - 397
Fluids - 354
Fluorocarbons - 351
Foam Generation - 208
Foams - 322, 356, 368, 376
Fourier Transform Infrared Spectrometer - 327
Fracture - 217, 223, 225, 228, 229, 266, 271, 273, 275-277, 323, 331, 334, 339, 342, 345, 402

Fracture Strength - 227
Fracture Toughness - 305
Friction - 183-185, 198, 199, 310
FTIR - 347
Fuel - 281, 282
Fuel Cells - 238, 410
Fuel Cycle - 290
Fuel Degradation - 300
Fuel Rod Removal - 301
Fuel Rods - 295, 296
Fusion - 360
Gas Chromatograph - 327
Gas Cleanup - 411, 413
Gas Streams - 405
Gas-Turbine Engine - 227, 235
Gaseous Diffusion - 287, 288
Gasification - 397
Gears - 199
Glass - 322, 339, 340, 354, 404, 406, 409
Glass Ceramics - 227, 316, 364
Glass Ceramics and/or Non-Metallic Glasses - 353
Glass Encapsulated - 218
Glassy Alloys - 341
Goechemical Modeling - 303
Grain Boundary - 191, 196
Granular Explosives - 313
Graphite - 283
Green State - 200, 230
Grinding - 353
Hafnia - 220
Heat Exchangers - 212
Heat Flux Transducers - 205
Heat Recovery - 413
Heat Transfer - 204, 205, 207, 208
Heliostat - 252
High-Level Waste - 308

High Pressures - 355
High Strain Rate - 383
High Temperature - 227, 228, 317, 360, 361
High Temperature Service - 189, 196, 225, 226, 282-284, 297, 298, 379, 380
Hot Cracks - 387
Hot Isostatic Pressing - 216, 218, 379
Hot Pressing - 217, 379
Hydraulics - 291, 292
Hydrides - 355, 378, 381
Hydrogen - 352
Hydrogen Attack - 349
Hydrogen Complexes - 324
Hydrogen Effects - 381, 395
Hydrogen Getters - 344
Hydrogen Isotopes - 357
Hydrogen Storage - 240
IEA - 230
In-Place Stabilization - 308
Inconel - 387
Industrial Insulation - 208
Industrial Waste Heat Recovery - 211, 212, 238, 258
Inertial Fusion - 309, 361, 368, 386
Infiltration - 206
Infrared Detectors - 314
Infrared Reflectometer - 328
Inorganic - 194
Inorganic Solids - 313
Instrument or Technique Development - 223, 231, 279, 280, 304, 325, 326, 327, 348, 328, 358, 359, 362, 365-379
Insulation - 189
Insulation Sheathing - 207
Insulators/Dielectrics-Polymeric - 319
Insulators/Thermal - 298
Integrated Circuit Fabrication - 312
Interfaces - 392, 400, 414
Interim Dry Storage - 300

Intermetallics - 190-192, 380, 396, 413
Ion Beam - 222
Ion Implantation - 183, 187, 280, 310, 332, 336, 349, 374
Ion Plating - 377
Iron-Based - 405
Irradiation - 283, 294
Isotope - 385
Joining - 190, 199, 237, 259, 283, 284, 337, 388, 395, 396, 402
Joining/Welding - 191, 200, 221, 231, 232, 332, 334, 335, 346, 355
Laser Annealing - 186
Laser Etching - 312
Laser Fusion - 357
Laser-Induced Chemistry - 367
Laser-Induced Fluorescence - 278
Laser Isotope Separation - 288
Lasers - 335, 387
Layers - 187
Li(D,T) - 378
Life Prediction - 223
Lightweight Materials - 190, 193, 194
Liquefaction - 412
Liquid Crystal Polymers - 375
Liquid Crystals - 192, 193
Loss Tangent Measurements - 384
Low Density - 374
Low Pressure Plasma - 380
Low Temperature Service (below 77°C) - 241, 243-250
Lubrication - 183
Machining - 183, 184, 188, 197, 354, 378
Magnesium - 190
Magnesium Chloride - 210
Magnetic Field Sensors - 315
Magnetic Fusion - 331, 337, 357, 361
Management - 231, 412
Material Degradation - 257, 259
Materials - 390, 393, 404, 405, 407, 408, 412

Materials Characteristics - 239, 394, 395, 404, 406
Materials Degradation - 302
Materials Processing - 394
Materials Program - 412
Materials Science - 210, 211, 274, 371
Mathematical Modeling - 205
Matrix - 225
Mechanical - 367
Mechanical Properties - 225, 293, 294, 342, 362, 363, 365, 393, 394, 404, 407
Mechanical Testing - 349
Meetings - 231
Metal Building - 206
Metal-Ceramic - 231
Metal Powder - 385
Metal Tritides - 378
Metallic Glass - 210, 243, 329, 336, 377
Metals - 183, 184, 189, 191, 192, 195, 196, 198, 199, 221, 231, 232, 234, 240, 260, 331, 337, 341, 342, 346, 354, 362, 363, 365, 373, 375, 377, 379, 380, 383, 400, 401
Metals: Ferrous - 355, 365, 366
Metals: Ferrous and Non-Ferrous - 356, 364
Metals: Non-Ferrous - 190, 196, 295, 297, 311, 312, 334, 335, 345, 347, 349-351, 361
Metastable State - 385
Microcircuitry - 311
Microelectronics - 310
Microsensors - 311
Microstructure - 240, 282-284, 305, 331, 343, 346, 368, 379, 382-384, 394
Microstructure and Solar Cells - 255
Microwave Properties - 384
Microwaves - 381
Mildew - 206
Mixed Gas - 405
Modeling - 185, 191, 192, 346, 241
Models - 199
Moisture - 206
Molding - 217, 220, 343
Molecular Beam Epitaxy - 187

Molecular Structure - 313
Molten Metal - 190, 195
Molten Salts - 210, 253
Monolithics - 216, 223
Mullite - 219-221
National Needs for Research - 206
NBS - 230
NDE - 200, 212, 216, 229, 230, 277, 346, 369, 370
Near Field Environment - 302, 303
Near-Net-Shape - 381
Near-Net-Shape Forming - 342
Near-Net-Shape Processing - 342, 378
Nodular Cast Iron - 305, 306
Nondestructive Evaluation - 204, 208, 255, 266, 273, 275, 306, 377, 385, 401-403, 414
Nondestructive Testing - 293, 298
Nuclear Absorbers - 295
Nuclear Fuel Isotopic Separations - 287
Nuclear Reactor Materials - 293
Nuclear Reactors - 333, 379
Oils - 198, 199
Onducting Polymers - 375
Optical Components - 369
Optical Diagnostics - 330
Optical Sensing - 265
Ordered - 192
Ordered Intermetallics - 196
Organic - 241, 247, 257, 259, 321, 323, 344
Organic Foams - 344
Organic Gases - 352
Organic Solids - 313
Oxidation Predictive Behavior Modeling - 352
Oxide Ceramics - 234, 235
Oxide Powder - 220
Oxides - 398-400, 414
Parachutes - 323
Particle/Plasma Interaction - 264, 265

Particle Size - 385
Particles - 400, 405
Particulates - 195
Phase - 410
Phase Diagrams - 363, 372, 373
Photoresistant - 319
Photothermal - 243, 246
Physical Properties - 360
Physical Vapor Deposition - 255, 376, 377, 385
Plasma - 186, 312, 361
Plasma Deposition - 320
Plasma Diagnostics - 271
Plasma Etching - 320
Plasma-Flame Spraying - 380
Plasma/Particle Interaction - 268
Plasma Polymerization - 237
Plasma Processing - 264, 265, 268, 271, 344
Plasma Synthesis - 311, 329, 331, 337
Plasma Systems - 269
Plastic Deformation - 263
Plastics - 185
Plutonium - 372, 373
Plutonium Alloys - 372, 384
Polyacetylene - 375
Polyesters - 376
Polymer Membrane - 252
Polymeric Encapsulants - 323
Polymeric Insulators/Dielectrics - 329
Polymeric Precursor Route - 322
Polymers - 184, 185, 187, 190, 192-194, 236, 238, 246-249, 251, 257, 258, 267, 317-323, 343, 357, 360, 376
Polyolefins - 376
Polyphenylguinoxaline - 375
Polypyrrones - 375
Polyurethanes - 376
Powder Characterization - 230

Powder Fabrication - 374
Powder Synthesis - 195, 214, 215, 220, 343
Powders - 219, 390
Prediction Behavior Modeling - 241, 360, 222, 223, 316, 320, 354-358, 360, 361, 363-365, 333
Process Modeling - 335
Processing - 190, 216
Productivitiy Boron Modeling - 316
Purification - 190
QNDE - 273
Radiation Damage - 384, 385
Radiation Effects - 251, 279, 280, 282, 319, 357, 362, 380
Radiation Hardened Semiconductors - 314
Radiation Hardness - 310, 324
Radiative Degradation - 252
Radiative Properties - 253
Radio Frequency Synthesis - 329
Radioactive Materials - 372, 378, 381-384
Radioactive Waste Casks - 306
Radioactive Waste Host - 284-286, 302, 360
Radioactive Waste Package Development - 304
Radioactive Waste Packaging Tests - 304
Radiochemical Detectors - 385
Radiography - 385
Raman Microprobe - 327
Rapid Solidification - 342, 380
Rapid Thermal Oxidation - 324
Reaction Vessel - 361
Reactions - 358, 359
Reactive Processing - 193
Reactor Components - 292
Reactor Design - 290, 291
Reactor Safety - 290
Recommended R-Values - 206
Recycle - 185
Reference Material - 230

Reflectance Emittance - 328
Reflectors - 251
Refractory - 410
Refractory Ceramics - 189, 360
Refractory Liners - 387, 409
Refractory Metals - 311
Refractory Oxides - 343
Removal - 195
Research - 231
Research Agenda - 206
Resins - 194
RF Heating - 381
Rock-Water-Waste Interaction - 303
Roof Tester Panels - 205
Roofs - 207
Scales - 398, 399, 405
Scanning Auger Microprobe - 327
Scanning Electron Microscopy - 349
Seals and Bearings - 257
Secondary Ion Mass Spectroscopy - 327
Seismology - 291
Semiconductor Device Fabrication - 314
Semiconductor Devices - 314, 315
Semiconductors - 237, 240, 254-256, 279, 280, 296, 299, 316, 330
Separations - 188
Settled Density - 204
Shock - 313
Shock Wave - 313
Shock Wave Compaction - 342
SiAlON - 218, 219
Silica - 221
Silicon - 310, 324
Silicon Carbide - 214, 216, 218-220, 227, 228, 230, 233
Silicon Dioxide - 310
Silicon Nitride - 214-218, 227, 229, 230, 233, 310
Silicones - 376

Sintering - 186, 214-220, 281, 380, 381, 384, 387
Sintering Refractory Liners - 379
Slag - 410
Smokes - 374
Sol-Gel - 188, 220
Sol Gel Process - 316
Solar Cells (Liquid Phase Epitaxial Growth, Molecular Beam Epitaxial Growth) Solid Oxide Electrolytes - 255
Solid State Bonding - 388
Solidification - 189, 258, 346
Solidification-Conventional - 334
Solidification-Rapid - 195, 296
Specific Heat - 206
Spectrometer - 349
Spectroscopy - 348
Spent Nuclear Fuel - 300, 301
Sputtering - 210, 352, 377, 388
Sputtering and Solar Cells - 254, 255
Stability - 372
Stainless Steel - 387
Static Behavior - 227
Statistical Mechanics - 263
Statistics - 223
Steam Cycle - 393, 394, 404, 407
Strain Sensors - 315
Strain-Tolerance - 189
Strained Layer Superlattices - 314
Strained Quantum Well - 314
Strength - 258, 259, 283, 284, 339, 379, 382-384, 396
Strengthening Mechanisms - 325
Stress - 257
Stress Analysis - 274
Stretched Membrane - 252
Structural Ceramics - 186-189, 191, 196, 197, 199, 200, 202, 211, 212, 214-217, 221-235, 379
Structure - 191, 212, 227, 241, 296, 336, 338, 355-358, 360-362, 368

Structure Solidification - 355
Subcontractors - 231
Superconductivity - 316
Superconductors - 201, 353, 392
Superplastic Forming - 381
Surface - 196, 197, 228, 258, 316, 321, 336-338, 349, 350, 353, 354, 361, 365, 368
Surface Alloying - 252
Surface Characterization and Treatment - 240, 251, 255, 378, 380, 381, 382
Surface Microstructure - 185
Surface Modification - 183, 252, 374
Surface Phenomena - 247, 248
Surface Physics - 313
Surface Preparation - 188
Surface Properties - 376
Surface Topology - 185
Surface Treatment - 339
Surfaces - 347
Switchable Emittance - 205
Synthesis - 312
Target Fabrication - 309, 386
Technology Transfer - 231
Tensile Testing - 226, 229, 292
Tests - 200, 323
Thermal Conductivity - 206, 224
Thermal Expansion - 372, 384
Thermal Fluids - 251
Thermal Insulations - 195
Thermal Plasma Synthesis - 373
Thermal Shock - 379
Thermodynamics - 372, 410
Thermoelectric - 296, 298, 299
Thermomechanical Processing - 325
Thermosets - 194
Thin Films - 316
Thoria - 379
Time-Dependent Behavior - 227, 228

Titanium - 381
Toughened Ceramics - 225-227
Toughness - 292
Toxic Metal Removal - 258
Transformation - 217, 240, 243, 245, 247, 259, 332, 346, 358, 382, 383
Transformation Toughened - 219, 220, 228
Transformation Toughened Ceramics - 379
Transformation Toughened Zirconia Oxide - 225
Transition Metal - 323
Transmission Electron Microscopy - 326
Transport Properties - 269
Tribology - 183, 234
Tritiated Materials - 378
Tritium - 347, 371, 378
Tritium Charging - 349
Tt-ZrO2 - 219
Turbomilling - 214
U-Alloys - 325
U-Values - 206
Ultra-low Expansion - 221
Ultrasonic - 229, 293, 370
Ultrasonic Sensing - 265
Uncertainty Analysis - 303
UO2 Oxidation - 300
Uranium - 287, 288, 306
Uranium Alloys - 381
UV Degradation - 251
UV Photoemission Spectroscopy - 313
Vacuum Arc Remelting - 330
Vapor Deposition - 353
Varistor - 323
Varistraint - 387
Video - 387
Volume Reduction - 308
Walls - 207
Waste - 308

Waste Acceptance Specifications (OGR/B-8) - 308
Waste Form - 308
Waste Management - 257
Waste Package Performance - 303
Waste Treatment - 289
Weapons - 319, 322, 332, 333, 350, 352, 358-360, 378
Wear - 183-185, 198, 199, 223, 234, 310
Weibull - 216, 223
Welding - 265, 270, 292, 330, 337, 387
Whiskers - 189, 214, 216-220, 225, 373, 374, 379
Wood - 206
Wood Products - 206
X-Rays - 327
Yttria - 220
Zeta Potential - 385
Zircaloy Cladding - 301
Zirconia - 219-221, 225, 228
ZnO - 323

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